TESIS DE LA UNIVERSIDAD DE ZARAGOZA

2017

77

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Sistemas cuánticos abiertos: descripción geométrica, dinámica y control

Departamento
Física Teórica

Director/es
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ISSN 2254-7606

Prensas de la Universidad
Universidad Zaragoza

ISSN 2254-7606

Universidad Zaragoza
1542

Tesis Doctoral

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UNIVERSIDAD DE ZARAGOZA

Física Teórica

2017

Sistemas cuánticos abiertos: Descripción geométrica, dinámica y control

"Open quantum systems: geometric description, dynamics and control"

Memoria de Tesis Doctoral
presentada por
Jorge Alberto Jover Galtier
para acceder al grado de Doctor en Física

Trabajo dirigido por los profesores de la Universidad de Zaragoza
Dr. José Fernando Cariñena Marzo y
Dr. Jesús Jerónimo Clemente Gallardo

DEPARTAMENTO DE FÍSICA TEÓRICA - FACULTAD DE CIENCIAS
UNIVERSIDAD DE ZARAGOZA
2017

Universidad Zaragoza
1542

Zaragoza, a 21 de abril de 2017

D. José Fernando Cariñena Marzo y D. Jesús Jerónimo Clemente Gallardo,

como directores de la tesis doctoral

“Sistemas cuánticos abiertos: descripción geométrica, dinámica y control”

presentada por

D. Jorge Alberto Jover Galtier

hacemos constar que su contenido se corresponde con lo presentado en mayo de 2014 en su Plan de Investigación ante la Escuela de Doctorado de la Universidad de Zaragoza, aprobado por la comisión académica del Programa de Doctorado en Física.

Por todo ello, nuestro informe es favorable para la admisión a trámite de la tesis doctoral.

LOS DIRECTORES DE TESIS

Fdo.: D. José Fernando Cariñena Marzo

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Abstract

The main topic of this dissertation is the analysis of open quantum systems. These systems are characterised by being subjeted to the influence of the environment, which causes thier evolution to be no longer unitary. It is thus necessary to consider models different to the Schrödinger equation. Open quantum systems appear in a great variety of fields, such as Solid State Physics and Molecular Dynamics. For this reason a careful analysis of their properties and dynamics is a relevant topic, with a broad range of applications.

The approach followed along this dissertation is the development of a geometric formalism that properly describes the characteristics of open quantum systems. Differential geometry has proved to be a powerful tool in the analysis of physical systems. Since the mid years of the 20th century, a geometric description of Classical Mechanics, mainly concerning Lagrangian and Hamiltonian mechanics, has been developed with huge success. For this reason, it seems natural to also describe quantum systems in geometric terms. The adventages of such a geometric formalism are clear. When both classical and quantum systems are described in the same terms, it is simple to describe situations in which classical-quantum interactions exist. Such is the case, for example, of many models in Molecular Dynamics, when nuclei and electrons are considered respectively classical and quantum. Also, a geometrical formalism of Quantum Mechanics makes possible to understand the intrinsic differences between classical and quantum theories.

Due to its relevance in this dissertation, Chapter 1 is devoted to the review and analysis of the geometric description of the Schrödinger picture of Quantum Mechanics. In its standard (algebraic) formulation, this picture is based in the representation of states of quantum systems by means of vectors in a complex Hilbert space. The transition to a formulation based on differential geometry is straightforward for finite-dimensional systems, as finite-dimensional linear spaces are trivial cases of differentiable manifolds. The additional structures, namely the Hermitian product in Hilbert spaces and the presence of imaginary scalars, are described by tensor fields on such differentiable manifolds, forming what is called a Kähler structure. All the necessary ingredients for the analysis of quantum systems can be described on Kähler manifolds. Observables are represented by smooth functions, while dynamics is described by means of integral curves of Hamiltonian vector fields with respect to the symplectic form in the Kähler structure. This characterisation can be carried out on the Hilbert space associated to any finite-dimensional quantum system. It is also possible to analyse the geometric properties of the projective Hilbert space, which is the set of pure states of the system. Its Kähler structure can be deduced via a reduction procedure from the existing structure on the Hilbert space. As a novelty, the dissertation presents in detail this reduction procedure, with an appropriate mathematical description.

All the aspects of the Schrödinger picture can be presented in geometric terms, which allows for the use of new tools in the analysis of quantum systems. This is the topic of Chapter 2, in which Lie-Kähler systems are employed in order to solve the time-dependent Schrödinger equation. In differential geometry, a Lie system is a non-homogeneous system of differential equation that admits a superposition rule. The determination of this superposition rule is in general a difficult task, which can be lightened by the presence of additional structures preserved by the action of the Lie system. Thus, depending on the preserved structure, it is possible to consider Lie-Hamilton systems, Lie-Dirac systems, etc. In the case of Quantum Mechanics, a time-dependent Schrödinger equation is a Lie system that preserves the existing Kähler structure. It is therefore a new type of Lie system, which is natural to call a Lie-Kähler system. Chapter 2 presents the properties of these new systems and describes a rigurous method in order

to obtain their superposition rules.

It is possible to extend the geometric formalism beyond the Schrödinger picture. This is necessary in the context of open quantum systems, as both pure and mixed states are needed for their description. For this reason, Chapter 3 presents the Heisenberg picture and its representation of pure and mixed states as linear functionals on the real Lie-Jordan algebra of observables. It is also presented how the the algebraic structures of observables can be represented geometrically on the dual space of linear functionals on the algebra. This is the starting point of one of the main contributions of the dissertation. A reduction procedure, similar to the one perfomed in the analysis of the Schrödinger picture, allows to describe the geometric properties of the manifold of pure and mixed states of quantum systems. Thus, two tensor fields are obtained on the manifold of states, which correctly reproduces the algebraic structures of the observables. It can thus be concluded that the geometrical formalism presented in the dissertation is completely equivalent to the usual algebraic description, as it is possible to properly describe all the properties of quantum systems. Furthermore, the geometric formalism offer a clearer description of the intrinsic properties of Quantum Mechanics, which allows for a better understanding of the theory. On the other side, a geometric characterisation of the manifold of states allows to study its stratification and its properties. The dissertation shows how this is a manifold with boundary, whose extremal points are precisely the pure states of the system. The stratification of this manifold is important when considering the dynamics induced by gradient and Hamiltonian vector fields. With the aim of illustrating all these properties, some simple but physically relevant examples are analysed.

Different applications of the geometric formalism to the analysis of open quantum systems are offered along the dissertation. Chapter 4 presents the description of the Markovian evolution of open quantum systems. An evolution is said to be Markovian if it depends only on the present state of the system and not on the states at previous instante, i.e. if the system 'has no memory'. In Quantum Mechanics, Markovian evolution is governed by the Kossakowski-Lindblad equation, a first order differential equation on the manifold of pure and mixed states of an open quantum system. The geometric formalism describes this equation as a vector field on the manifold, and the properties of its integral curves are analysed. Thus, it is possible to consider different aspects of Markovian evolution from a geometric perspective. Any non-unitary evolution determines a change in the algebraic properties of quantum observables, which can lead to a contraction of the algebra. In geometric terms, this contraction can be understood as the limit of a family of tensor fields determined by the flow of the Kossakowski-Lindblad vector field. Another important feature of this evolution is the existence of limit manifolds. Their properties can be determined thanks to the existing affine structure, and its connection with the contraction of algebras is investigated. Lastly, control problems of open quantum systems are described in geometric terms. A geometric description of Quantum Mechanicas allows to applut to these problems the results of the theory of control of Lie groups. As a consequence, it is posible to obtain a classification of quantum systems according to their controlability properties.

Another example of open quantum systems appears in the context of Molecular Dynamics. In the study of molecular systems, the large number of particles implies that the Schrödinger equation cannot be solved even by numerical methods. It is thus useful to consider approximations to the Schrödinger equation. In particular, many models are developed considering a classical behaviour for some of the particles, usually the nuclei. In these hybrid classical-quantum system, the quantum particles conform an open quantum system that interacts with the classical nuclei. Chapter 5 reviews these molecular models, particularising to the Ehrenfest model. A geometric description of the model is possible, based on the separate descriptions of the classical and quantum subsystems. As a result, the equations of the model are characterised as Hamiltonian equations on a Poisson manifold. Starting from these properties, the dissertation presents a generalisation of the Ehrenfest model to statistical ensembles. This is an important step, as the dissertation proves that decoherence-like effect, which are not present in its initial form, appear in this statistical setting. Also, the thermodynamic limit of the model is characterised. Numerical simulations have been performed, and the computed results support the description of molecular systems by means of the Ehrenfest statistical model. Lastly, in this context it is possible to consider statistical ensembles with temperature. The dissertation analyses these ensembles and their thermodynamic limit.

The following publications are result of the investigations presented in this dissertation:

- J. L. Alonso, P. Bruscolini, A. Castro, J. Clemente-Gallardo, J. C. Cuchí, and J. A. Jover-Galtier. Ehrenfest statistical dynamics in chemistry without potential energy surfaces: Decoherence-like effects. Submitted for publication.
- J. L. Alonso, J. Clemente-Gallardo, J. C. Cuchí, D. García-Álvarez, and J. A. Jover-Galtier. Extensivity of the Hybrid Canonical Ensemble (HCE) in the thermodynamic limit. Submitted for publication.
- J. L. Alonso, J. Clemente-Gallardo, P. Echenique-Robba, and J. A. Jover-Galtier. Comment on "Correlated electron-nuclear dynamics: Exact factorization of the molecular wavefunction" [J. Chem. Phys. 137, 22A530 (2012)]. *J. Chem. Phys.*, 139(8):087101, 2013.
- J. F. Cariñena, J. Clemente-Gallardo, J. A. Jover-Galtier, and J. de Lucas. Lie systems and Schrödinger equations. *Pre-print*, arXiv:1611.05630, 2016
- J. F. Cariñena, J. Clemente-Gallardo, J. A. Jover-Galtier, and G. Marmo. Tangent bundle geometry from dynamics: application to the Kepler problem. *Int. J. Geom. Methods Mod. Phys.*, 14:1750047, 2017.
- J. F. Cariñena, J. Clemente-Gallardo, J. A. Jover-Galtier, and G. Marmo. Tensorial dynamics on the space of quantum states. Submitted for publication.
- J. A. Jover-Galtier, M. Kuś, and J. de Lucas. Characterisation of limit manifolds for Markovian evolution of open quantum system. In preparation.
- J. A. Jover-Galtier, M. Kuś, and J. de Lucas. Inner derivations of Jordan algebras and their connection with Lie structures. In preparation.

The research has been financially supported by the grant B100/13 of the 'Diputación General de Aragón' and by the grant FPU13/01587 of the 'Ministerio de Educación, Ciencia y Deporte'.

Resumen

El tema central de la tesis doctoral es el análisis de los sistemas cuánticos abiertos. Estos sistemas se caracterizan por estar sometidos a la interacción con el entorno, lo que provoca que su evolución deje de ser unitaria. Es por tanto necesario considerar modelos más allá de la ecuación de Schrödinger. Los sistemas cuánticos abiertos aparecen en numerosos campos, como la Física del Estado Sólido y la Dinámica Molecular. Por este motivo, un análisis detallado de sus propiedades y su dinámica es un tema digno de estudio con un gran abanico de aplicaciones.

El enfoque elegido en esta tesis es el desarollo de un formalismo geométrico que describa de forma adecuada las características de los sistemas cuánticos abiertos. La geometría diferencial ha demostrado ser una herramienta muy útil en el análisis de sistemas físicos. Desde mediados del siglo XX, se ha desarrollado con gran éxito una descripción geométrica de la Mecánica Clásica, principalemnte en torno a las mecánicas lagrangiana y hamiltoniana. Por este motivo, resulta natural describir también los sistemas cuánticos en términos geométricos. Las ventajas de un formalismo geométrico resultan claras. Cuando tanto los sistemas clásicos como los cuánticos se describen en los mismos términos, es sencillo describir situaciones en las que existan interacciones clásico-cuánticas. Éste es el caso, por ejemplo, de muchos modelos de Dinámica Molecular, en los que los núcleos y los electrones son considerados respectivamente como partículas clásicas y cuánticas. Por otra parte, un formalismo geométrico de la Mecánica Cuántica posibilita un mejor entendimiento de las diferencias intrínsecas entre las teorías clásicas y las cuánticas.

Dada su relevancia a lo largo de la tesis, el Capítulo 1 está enfocado al resumen y el análisis de la descripción geométrica de la imagen de Schrödinger de la Mecánica Cuántica. En formulación usual (algebraica), esta imagen se basa en la representación de los estados de los sistemas cuánticos mediante vectores en un espacio de Hilbert complejo. La transición a una formulación basada en geometría diferencial es inmediata para sistemas finito-dimensionales, dado que los espacios lineales de dimensión finita son casos triviales de variedades diferenciables. Las estructuras adicionales, en concreto el producto hermítico propio de los espacios de Hilbert y los escalares complejos, se describen mediante campos tensoriales en dichas variedades diferenciables, formando lo que se conoce como una estructura Kähler. Todos los ingredientes necesarios para el análisis de sistemas cuánticos pueden describirse en estas variedades de Kähler. Los observables se representan mediante funciones diferenciables, mientras que la dinámica se describe mediante curvas integrales de campos vectoriales hamiltonianos respecto a la forma simpléctica de la estructura Kähler. Esta caracterización puede llevarse a cabo en el espacio de Hilbert asociado a cualquier sistema cuántico finito-dimensional. Además, es posible analizar las propiedades geométricas del espacio proyectivo de Hilbert, el cual constituye el conjunto de estados puros del sistema. Su estructura Kähler puede ser deducida mediante un proceso de reducción de la estructura previamente obtenida en el espacio de Hilbert. Como aspecto novedoso, la tesis presenta en detalle este proceso de reducción, dotándolo de una descripción matemática adecuada.

Todas las características de la imagen de Schrödinger pueden describirse de forma geométrica, lo que permite utilizar nuevas herramientas en el análisis de los sistemas cuánticos. Éste es precisamente el tema principal del Capítulo 2, en el cual se utilizan los sistemas de Lie-Kähler para resolver la ecuación de Schrödinger dependiente del tiempo. En geometría diferencial, un sistema de Lie es un sistema no homogéneo de ecuaciones diferenciales que admite una regla de superposición. En general, la obtención de esta regla de superposición es una ardua tarea, la cual puede aligerarse en presencia de estructuras adicionales que sean preservadas por la acción del sistema de Lie. De esta forma, según la estructura

preservada, es posible hablar de sistemas de Lie-Hamilton, Lie-Dirac, etc. En el caso de la Mecánica Cuántica, una ecuación de Schrödinger dependiente del tiempo es un sistema de Lie que preserva la estructura de Kähler previamente descrita. Es por tanto un nuevo tipo de sistema de Lie, al que resulta natural denominar de Lie-Kähler. El Capítulo 2 presenta las propiedades de estos nuevos sistemas y describe un método riguroso para la obtención de sus reglas de superposición.

El formalismo geométrico puede extenderse más allá de la imagen de Schrödinger, lo que resulta necesario en el contexto de los sistemas cuánticos abiertos, dado que tanto estados puros como estados mezcla son necesarios para su descripción. Por este motivo, el Capítulo 3 resume la imagen de Heisenberg de la Mecánica Cuántica y su representación de los estados puros y mezcla como funcionales lineales en el álgebra de Lie-Jordan de observables. Se explica también como las estructuras algebraicas de los observables pueden representarse geométricamente en el espacio dual de funcionales lineales en el álgebra. Este es el punto de partida de una de las principales contribuciones de la tesis. Un proceso de reducción, similar al realizado en el análisis de la imagen de Schrödinger, permite describir las propiedades geométricas de la variedad de estados puros y mezcla del sistema. De esta forma, se obtienen dos campos tensoriales en la variedad de estados, los cuales representan correctamente las estructuras algebraicas de los observables. Puede por tanto concluirse que el formalismo geométrico presentado en la tesis es completamente equivalente a la descripción algebraica tradicional, ya que se logra describir adecuadamente todas las propiedades de los sistemas cuánticos. Además, el formalismo geométrico ofrece una visión más clara de las propiedades intrínsecas de la Mecánica Cuántica, lo que facilita una mejor comprensión de la teoría. Por otra parte, un análisis geométrico de la variedad de estados permite estudiar su estratificación y sus propiedades. La tesis demuestra que se trata de una variedad con borde, cuyos puntos extremales son precisamente los estados puros del sistema. La estratificación de esta variedad resulta importante a la hora de considerar la dinámica inducida por campos gradiente y hamiltonianos. Con el objetivo de ilustrar todas estas propiedades, se analizan unos casos sencillos pero con relevancia física.

A lo largo de la tesis, se muestran diversas aplicaciones del formalismo geométrico al análisis de sistemas cuánticos abiertos. El Capítulo 4 presenta la descripción de la evolución markoviana de sistemas cuánticos abiertos. Se dice que una evolución es markoviana si depende únicamente en el estado actual del sistema y no de los estados en instantes anteriores, es decir, si el sistema "no tiene memoria". En Mecánica Cuántica, la evolución markoviana se obtiene a partir de la ecuación de Kossakowski-Lindblad, una ecuación diferencial de primer orden en la variedad de estados puros y mezcla de un sistema cuántico abierto. El formalismo geométrico describe esta ecuación como un campo tensorial en esta variedad, lo que permite analizar las propiedades de sus curvas integrales. De esta manera, es posible considerar diversos aspectos de la evolución markoviana desde un punto de vista geométrico. Cualquier evolucion no-unitaria determina un cambio en las propiedades algebaicas de los observables cuánticos, lo que puede resultar en una contracción del álgebra. En términos geométricos, esta contracción puede entenderse mediante el límite de una familia de campos tensoriales definida por el flujo del campo tensorial de Kossakowski-Lindblad. Otra característica importante de esta evolución es la existencia de variedades límite. Sus propiedades pueden determinarse gracias a la estructura afín existente, lo que a su vez permite investigar su relación con las contracciones de álgebras de observables. Por último, se ofrece una descripción geométrica de los problemas de control de sistemas cuánticos abiertos. Un análisis geométrico de la Mecánica Cuántica permite aplicar a estos problemas los resultados de la teoría de control de grupos de Lie. Como consecuencia, es posible realizar una clasificación de los sistemas cuánticos abiertos según sus propiedades de controlabilidad.

Otro ejemplo de sistemas cuánticos abiertos aparece en el contexto de la Dinámica Molecular. En el estudio de sistemas moleculares, debido al gran número de partículas presentes, la ecuación de Schrödinger no puede ser resuelta ni siquiera por métodos numéricos. Por tanto, resulta útil considerar aproximaciones a la ecuación de Schrödinger. En particular, existen muchos modelos que consideran un comportamiento clásico de algunas de las partículas, normalmente los núcleos. El Capítulo 5 resume las propiedades estos modelos moleculares, y en particular del conocido como modelo de Ehrenfest. Es posible llevar a cabo una descripción geométrica de este modelo, basándose en las descripciones de los subsistemas clásico y cuántico. Como resultado, las ecuaciones del modelo pueden escribirse como ecuaciones hamiltonianas en una variedad de Poisson. A partir de estas propiedades, la tesis presenta una generalización del

modelo de Ehrenfest a distribuciones estadísticas. Este es un paso importante, ya que se demuestra que esta descripción estadística predice la aparición de efectos relacionados con el fenómeno de decoherencia, algo que no ocurre en el modelo de Ehrenfest estándar. Se han realizado simulaciones numéricas, cuyos resultados respaldan la descripción de sistemas moleculares mediante el modelo estadístico de Ehrenfest. Por último, en este contexto resulta posible considerar distribuciones estadísticas con temperatura. La tesis presenta estas distribuciones y analiza su límite termodinámico.

Las siguientes publicaciones son el resultado de investigaciones presentadas en esta tesis:

- J. L. Alonso, P. Bruscolini, A. Castro, J. Clemente-Gallardo, J. C. Cuchí, and J. A. Jover-Galtier. Ehrenfest statistical dynamics in chemistry without potential energy surfaces: Decoherence-like effects. Pendiente de publicación.

- J. L. Alonso, J. Clemente-Gallardo, J. C. Cuchí, D. García-Álvarez, and J. A. Jover-Galtier. Extensivity of the Hybrid Canonical Ensemble (HCE) in the thermodynamic limit. Pendiente de publicación.

- J. L. Alonso, J. Clemente-Gallardo, P. Echenique-Robba, and J. A. Jover-Galtier. Comment on "Correlated electron-nuclear dynamics: Exact factorization of the molecular wavefunction" [J. Chem. Phys. 137, 22A530 (2012)]. *J. Chem. Phys.*, 139(8):087101, 2013.

- J. F. Cariñena, J. Clemente-Gallardo, J. A. Jover-Galtier, and J. de Lucas. Lie systems and Schrödinger equations. *Preimpresión*, arXiv:1611.05630, 2016

- J. F. Cariñena, J. Clemente-Gallardo, J. A. Jover-Galtier, and G. Marmo. Tangent bundle geometry from dynamics: application to the Kepler problem. *Int. J. Geom. Methods Mod. Phys.*, 14:1750047, 2017.

- J. F. Cariñena, J. Clemente-Gallardo, J. A. Jover-Galtier, and G. Marmo. Tensorial dynamics on the space of quantum states. Pendiente de publicación.

- J. A. Jover-Galtier, M. Kuś, and J. de Lucas. Characterisation of limit manifolds for Markovian evolution of open quantum system. En preparación.

- J. A. Jover-Galtier, M. Kuś, and J. de Lucas. Inner derivations of Jordan algebras and their connection with Lie structures. En preparación.

La investigación ha sido financiada por la beca B100/13 de la Diputación General de Aragón y por la beca FPU13/01587 del Ministerio de Educación, Ciencia y Deporte.

To José Miguel, Susana and Laura

Acknowledgements

This dissertation marks the end of a long journey that started four years ago. But I have not travelled alone, as many people have walked with me over all these years. Without their help and support in the many tough times, it would have been impossible for me to finish this task. I therefore wish to thank all my mentors and advisers, my colleagues and my family for playing such an important part in this chapter of my professional life that now closes.

More specifically, I would like to acknowledge the lead and tutoring of my thesis advisers Jesús Clemente and José F. Cariñena. I am really thankful for their help, their kindness and their patience for all these years. To them I owe the successful results of my doctorate.

Special thanks go to professor Giuseppe Marmo. Fruitful conversations with professor Marmo were the seed for the development of a huge part of my work. I am also very thankful for the possibility to collaborate with him in Naples. I take this opportunity to thank the support by Juan Manuel Pérez Pardo, Franco Ventriglia, Patrizia Vitale and all the people from the University of Naples and the INFN.

Likewise, I thank professor Marek Kuś the invitation to work under his supervision in Warsaw. His hospitality and good advices have been very important to me, and he is responsible for many results presented in this dissertations. I also wish to express my gratitude to professor Janusz Grabowski and the other collaborators in Warsaw the possibility to attend and participate in their seminars and workshops.

I wish to thank particularly professor Javier de Lucas for his support and friendship since even before the beginning of my doctorate. Since the beginning of my doctorate, collaborations with Javier have been essential to the development of my thesis. Furthermore, and in a more personal ground, I am extremely thankful to him for his kindness and warm hospitality during my stay in Warsaw.

José Luis Alonso deserves a special mention in this lines. I really thank him his support, help and friendship for all these years. Similarly, I thank Juan Carlos Cuchí, Pierpaolo Bruscolini, Alberto Castro and Pablo Echenique for their collaborations and illuminating discussions on the topics of my thesis. I also thank Edith Padrón, Silvia Vilariño and all the people from the Spanish network of Geometry, Mechanics and Control for all the useful schools and lectures that have contributed to the development of this dissertation.

Except for my stays in distant lands, I have conducted my research in the Department of Theoretical Physics in the University of Zaragoza. I thank the Heads of Department José Vicente García Esteve and Fernando Falceto, the secretaries Pedro and Esther, my teaching supervisors José Gracia Bondía and Manuel Fernández-Rañada and the other members of the staff for the wonderful working environment. I also thank the BIFI institute for the access to computational resources and the support in the practical aspects of the research.

In a more technical matter, I thank the 'Diputación General de Aragón' (DGA) and the 'Ministerio de Educación, Ciencia y Deporte' (MECD) for the financial support to my research. I was granted by the Aragonese government for years 2014 and 2015 (DGA grant 24/1), whereupon, and until year 2017, I received an FPU grant from the MECD (FPU13/01587), which also funded my stays in Naples and Warsaw, in years 2015 and 2016, respectively.

Moving to personal matters, I wish to thank the huge support that I have recieved from all my frieds. The elaboration of a doctoral thesis is an arduous task, which is somehow ligthened with the company of beloved people. For this reason, I am really thankful to Eduardo, Alberto, Elisa, Adrián, Pablo, Carlos, Andrés, Silvia and many others for ther support and friendship along these years.

And I leave for the end the most important acknowlegments. I wish to thank my family, specially my parents and my sister, for their warm and wholehearted support. This long journey would have not been possible without them. To them I dedicate this work.

Preface

Quantum Mechanics has been one of the most relevant physical theories for more than a century. It is a theory that describes the behaviour of the constituent particles of matter: atoms, electrons, photons, etc. It has applications in a huge variety of fields: Solid State Physics, Electronics, Optics... Because of this, Quantum Mechanics plays a centre role in modern Physics.

Development of Quantum Mechanics started in the year 1900 by Max Planck. In his seminal works [220, 221], Planck offered an original solution to the problem of the black body radiation. He suggested that energy was not emitted in a continuous way, but in small discrete quantities. In the following years, many physicists extended this new theory to a large number of situations. Among them was Albert Einstein, who gave a satisfactory explanation for the photoelectric effect [119] by proposing that energy was also absorbed and transmitted in discrete quantities. Quantum theory allowed for the development of atomic models, such as Niels Bohr's model. Many other physicists contributed to the establishment of the new theory as a fundamental description of the behaviour of matter.

A rigorous description of the theory as a whole, however, was yet to be achieved. In the 1920's, Werner Heisenberg [152], in close work with Max Born and Pascual Jordan [51, 53], derived a formulation of the quantum theory known as 'matrix mechanics'. This description dealt directly with observables as the fundamental elements of the theory. A similar formulation was independently achieved by Paul Dirac [109]. At the same time, Erwin Schrödinger proposed a description of quantum systems in terms of wave functions [102, 237], mathematical objects reproducing the probabilistic nature of Quantum Mechanics that had been observed in experiments. It was proved a few years later that both approaches are equivalent [267].

Schrödinger and Heisenberg's ideas were further developed by them and other physicists, such as Paul Dirac [111], John von Neumann [267], Paul Ehrenfest [118], Louis de Broglie, Wolfgang Pauli and many others. Quantum Mechanics has since evolved and expanded. Nowadays, Quantum Mechanics is probably the most relevant and prolific theory in the development of Physics.

A full characterisation of a mechanical system requires the description of its dynamics. In the realm of Classical Mechanics, Newton's laws marked a milestone in the development of Physics, as they offered the first rigorous description of the nature of dynamics of classical systems. In the early years of the 20th century, a similar description of quantum systems was pursued. In terms of wave functions, the evolution of isolated systems is governed by the Schrödinger equation:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\psi = H\psi.$$

This differential equation determines the dynamics of an isolated quantum system, where H, the Hamiltonian operator, represents the energy observable of the system. A system is called isolated, or closed, if it does not interchange information or energy with its environment. This definition is obviously an idealisation. No physical system is truly isolated, except for the whole Universe (or so we assume). In practice, many systems are 'isolated enough' so that the Schrödinger equation describes accurately their evolution. When the action of the environment on the system cannot be neglected, however, new models are needed.

A system is called open if it is not closed, i.e. if it interacts with its environment. This environment may take any form, from a single electron to a set of molecular nuclei or a large measurement equipment.

The interaction may also appear in different ways. For example, the decay of quantum systems can be modelled by considering the interchange of energy between the system and its surroundings. Open quantum systems also appear in the study of composite systems. The subsystems of a composite, ideally isolated quantum system are not in general themselves isolated, as they typically interact with each other. A particular example of this case occurs in relation with the measurement process in Quantum Mechanics. The coupling of a quantum system with a much larger system, the measurement equipment, is expected to have a huge influence in its evolution. The Schrödiner picture reflects this interaction as an instantaneous, non-deterministic change in the state of the quantum system. The implications of this probabilistic behaviour of the Quantum Mechanics and the difficulties for its correct description are commonly known as the 'measurement problem'. An analysis of this situation in terms of open quantum systems is possible, and it sheds some light on the behaviour and properties of Quantum Mechanics, as proposed by authors such as Zeh [278] and Zurek [280, 281].

The approaches taken to study the dynamics of open quantum systems vary widely. Chemical physics [199, 215], quantum optics [87, 88, 103, 223] or condensed matter physics [47, 188, 272] are some of the many relevant fields on which open quantum systems have a great relevance. It is also possible to consider a more mathematical framework [214, 226], usually from the point of view of statistical physics. In this setting, it deserves specific mention the works by Lindblad [191] and Gorini, Kossakowski and Sudarshan [139], concerning the characterisation of Markovian evolution of open quantum systems. In a broad sense, a system is said to follow a Markovian evolution if 'it has no memory'. In other words, the dynamics at any time is determined only by the state of the system (and maybe of the environment) at such time, and it does not depend in any way on previous states. In the aforementioned works, the particular first order differential equation governing such an equation was found. For a finite-dimensional quantum system of dimension n, the generic expression of the Kossakowski-Lindblad equation is

$$\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\rho} = -\mathrm{i}\hbar^{-1}[H,\widehat{\rho}] + \sum_{j=1}^{n^2-1}\left(V_j\widehat{\rho}V_j^\dagger - \frac{1}{2}(V_j^\dagger V_j\widehat{\rho} + \widehat{\rho}V_j^\dagger V_j)\right), \tag{1}$$

where $\widehat{\rho}$ is the density matrix of the system, and with $H, V_1, \ldots, V_{n^2-1}$ traceless complex $n \times n$ matrices. The determination of these matrices for particular problems is thus enough in order to determine the dynamics of the system.

As in the case of the Kossakowski-Lindblad equation, open quantum systems are generally described in terms of density matrices. Such an approach follows from the usual algebraic description of Quantum Mechanics, in particular of the Schrödinger picture [102]. Thus, pure states of a quantum system are represented by elements in a complex Hilbert space, and observables and density matrices are self-adjoint operators acting on it. This algebraic setting fits in well with the properties of Quantum Mechanics; for example, the superposition principle of quantum systems can be easily understood by the properties Hilbert spaces. However, a geometric approach to Quantum Mechanics is more useful in many situations, such as the cases in which an open quantum system interacts with a classical environment.

In order to understand the limitations of the algebraic approach, consider a situation in which an open quantum system is interacting with a much larger environment. This situation is very common. For example, molecular dynamics typically studies the evolution of electrons as an open quantum system interacting with the nuclei. A similar approach is also taken in the analysis of the measurement problem presented above. In all these cases, tue description of the dynamics of the open quantum system strongly depends on the characterisation of this environment. It is common in these situation to describe the evolution of the environment by Classical Mechanics. Formal and practical problems arise here, as two entities, with dynamics expressed in different languages, have to be merged. This is one of the main motivations for the development of a different formalism for Quantum Mechanics, a new one that can easily be combined with the description of classical dynamics.

As taught in Physics courses, many different descriptions of Classical Mechanics exist. Among them, the geometric formalism enjoys many features that can be adapted to the quantum realm, and even shed new light on the properties of quantum systems. The second half of the 20th century was the starting point in the development of physical models based on the notions of differentiable geometry. The works

and textbooks by Abraham and Marsden [3], Arnold [28], Smale [244,245], Souriau [246] and many others authors contributed to its development. The main features of this formalism are the following. The phase space of a classical system is identified with a differentiable manifold, whose symplectic structure has a direct relation with dynamics. Typically, this manifold is either the tangent bundle (in the Lagrangian formalism) or the cotangent bundle (in the Hamiltonian one) of the configuration space. Both approaches are related by a fibre-wise Legendre transform. The cotangent bundle is naturally equipped with a symplectic form; integral curves of Hamiltonian vector fields with respect to this form are precisely the trajectories that classical systems obey. Thus, the geometric formalism offers a rich setting with many objects and features that can be easily extended and adapted to different situations. See any of the aforementioned references, especially the textbook by Abraham and Marsden [3], and the one by Cariñena, Ibort, Marmo and Morandi [81].

A geometric description of Quantum Mechanics was first proposed by Strocchi [251] and Kibble [176], aiming to obtain a similar description of quantum systems to that obtained for Classical Mechanics. It was developed by authors such as Cantoni [65–69], Cirelli and co-workers [94,95], and others [22,23,30,42,45,63,154,247]. Recent works on the topic can be found in the works by Aniello, Asorey, Cariñena, Clemente-Gallardo, Marmo and co-workers, the author among them [8,26,27,31,57,70,72–74,81,97–101,122]. Most of these works focused on a geometric description of the Schrödinger picture. Any linear space can be replaced by an appropriate differentiable manifold. In the case of complex Hilbert spaces, the additional structures are represented in terms of tensor fields on the manifold with precise characteristics. As a result, it is possible to describe a quantum system by means of a Kähler manifold, whose structure encodes all the required features. Observables on the Hilbert space are represented by real functions on this manifold. The corresponding algebraic structures, such as the commutator or the anticommutator can be implemented on the set of these functions by means of the symplectic and symmetric structures of the Kähler structure.

Similarities between geometric formalisms of Classical and Quantum Mechanics are already visible. Kähler manifolds are just symplectic manifolds with additional structures. Thus, from the perspective of open quantum systems, composition of a classical system and a quantum one is not harder to describe that that of two classical systems. Many other features of both theories can be related in the same way. Unitary evolution of quantum systems, which was described by the Schrödinger equation in the algebraic setting, is now governed by a Hamiltonian vector fields with respect to the natural symplectic form on the Kähler manifold, as in the classical case. Differences can also appreciated at this level. The additional structures present in the case of quantum systems are in direct relation with features such as the non-commutativity of quantum observables. Summing up, geometric tools prove to be very useful in the characterisation of quantum dynamics and its comparison with classical systems.

This geometric description of Quantum Mechanics can be extended to the analysis of open quantum systems. This is the main topic of this dissertation. Open quantum systems require a more general setting than the one offered by the Schrödinger picture. In fact, the approach of the Heisenberg picture offers a better description in this case. According to this picture, pure and mixed states of quantum systems are represented by real positive normalised linear functionals on the C*-algebra of quantum observables of the system. The linear space of functionals on a C*-algebra also enjoys some nice geometric characteristics [141,142]. With an appropriate description, it is possible to reduce the geometric structures to the set of quantum states of the system [72]. As a result, a new description of pure and mixed states is obtained. Geometric tools can thus be applied to the description of open quantum systems. Among the many applications of this formalisms is the analysis of Markovian evolution of open quantum systems. The 'no memory' property of this evolution makes possible to describe it in terms of a first-order differential equation, namely the Kossakowski-Lindblad equation. As a consequence, Markovian evolution can easily be implemented in the geometric formalism. Many examples can be analysed, such as decaying of quantum systems and decoherence models in molecular dynamics.

This dissertation is organised as follows. Chapter 1 is intended to be a review of the the geometric description of the Schrödinger picture of Quantum Mechanics. Most of the results presented here are derived from the aforementioned works. Some new approches are also presented, in particular in relation with the precise description of the projection onto the manifold of pure states of the system and

the reduction of the algebraic structures. Along the dissertation, knowledge of differential geometry is assumed. Unless otherwise stated, the terminology and conventions here used are those in the book by Crampin and Pirani [104]. Other interesting works on the topic are the books by Boothby [50], Kobayashi and Nozumi [177], and Nakahara [212]. Regarding the geometric approach, the main reference for this chapter is the book by Cariñena, Ibort, Marmo and Morandi [81], which presents the fundamentals of the geometric description of physical systems. Such a description makes possible to characterise quantum dynamics by means of geometric tools. This is the case of Lie systems, a powerful technique for the resolution of differential equations. Thus, Chapter 2 presents the analysis of the Schrödinger equation in terms of Lie systems, as developed in a recent paper by Cariñena, Clemente-Gallardo, de Lucas and the author [70].

Following chapters extend the geometric formalism to the description of open quantum systems. In Chapter 3 starts with a review of the algebraic properties of the Heisenberg picture and its geometric representation on the linear space of functionals on a C*-algebra [141, 142]. This motivates the presentation of two of the main contributions of the dissertation. Firstly, a characterisation of Lie-Jordan algebras is offered, based in the research carried out in joint work with Kuś and de Lucas [169]. And secondly, a detailed geometric formulation of the properties of the set of pure and mixed states of a quantum system is offered, extending the work presented in a paper by Cariñena, Clemente-Gallardo, Marmo and the author [72]. The characteristics of open quantum systems are thus described in geometrical terms, and the implications of the results thus obtained are discussed. The remaining chapters of the dissertation present the application of the developed formaism to different situations. Chapter 4 offers a geometric characterisation of Markovian evolution and the Kossakowski-Lindblad dynamics [72, 169]. Its application to several physical situations is presented. Also in this context, the relevance of geometric control theory is discussed. Finally, Chapter 5 deals with the description of hybrid classical-quantum models in the context of molecular dynamics [8]. In particular, the Ehrenfest model is studied in detail, and numerical results are offered in order to illustrate the formalism.

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Chapter 1

Geometric formulation of the Schrödinger picture

Quantum Mechanics has been one of the most relevant physical theories for more than a century. It is a theory concerned with the behaviour of the constituent particles of matter: atoms, electrons, photons, etc. Nowadays, Quantum Mechanics is probably the most relevant and prolific theory in the development of Physics.

Standard descriptions of Quantum Mechanics are based on an algebraic characterisation of the properties of systems. The Schrödinger picture, for example, represents pure states of the system by element in a complex and separable Hilbert space. By contrast, the Heisenberg picture focuses on the characterisation of observables as elements in a C*-algebra. Other descriptions of Quantum Mechanics exists, which different properties and applications. And in particular, a geometric characterisation of the theory is possible. The present chapter stablish the ground for the rest of the dissertation by presenting the geometric description of the Schrödinger picture of Quantum Mechanics.

The geometric description of physical theories has been studied for the last 50 years. It has his roots in the works by Arnold [28], Smale [244, 245] and Souriau [246]. As a result, a geometric description of Classical Mechanics was developed with very satisfactory results. See the textbook by Abraham and Marsden [3] to grasp the importance of geometric calculus in mechanical problems, and also more recent works [71, 81].

Following this spirit, a description of Quantum Mechanics based on differential geometry was proposed by Strocchi [251] and Kibble [176]. The properties of the Schrödinger picture were described in terms of geometric objects on a differentiable manifold. This first geometric approach to pure quantum systems is the topic of this first chapter, which will be addressed after a brief summary of the standard Schrödinger picture of Quantum Mechanics and its relation to the probabilistic nature of the theory.

The chapter is organised as follows. Section 1.1 offers a short summary of the Schrödinger picture of Quantum Mechanics and its properties. All its elements can be reproduced in geometric terms, as done in Section 1.2. A geometric approach allows to describe in similar terms the set of pure states of a quantum system, which has the structure of a projective Hilbert space. Section 1.3 describes a characterisation of this set. Finally, in Section 1.4, all the concepts are exemplified by their application to the study of a simple system.

1.1 The Schrödinger picture of Quantum Mechanics

This section presents a short summary of the main properties of Schrödinger picture. In its standard formulation, Schrödinger picture associates a Hilbert space $\mathcal{H}$ to each physical system. Each vector on $\mathcal{H}$, excluding the zero vector, represents a state of the system. The relation between vectors and states is not however unique (see Section 1.1.6). Observables of the quantum system are identified with essentially self-

adjoint operators acting on $\mathcal{H}$. The possible results of the measurement of an observable are the values of the spectrum of its associated operator. This leads, in the case of operators with only discrete spectrum, to the expected quantisation of the measurements. The probability of obtaining each possible value is determined by the decomposition of vectors in the basis of eigenvalues of the operator. For a complete description of Quantum Mechanics, see any of many remarkable works on the topic [81,102,143,230,243].

1.1.1 Hilbert spaces and the Dirac notation

As a starting point, some mathematical structures are defined. These are the main tools describing the Schrödinger picture. Regarding dimensionality, Schrödinger picture is valid for systems of finite and infinite dimension. In the later case, however, many properties have to be more carefully proved. The definitions and properties are presented in a language valid for both cases. More information on the properties and theorems of Linear Algebra can be found in specialised works [148,149,174,186].

Definition 1.1. *An inner product on a vector space V over a field $\mathcal{K}$ (either $\mathbb{R}$ or $\mathbb{C}$) is a function $\langle\cdot|\cdot\rangle : V \times V \to \mathcal{K}$ satisfying the following three axioms:*

1. *It is symmetric (for $\mathcal{K} = \mathbb{R}$) or conjugate symmetric (for $\mathcal{K} = \mathbb{C}$),*

$$\langle x|y\rangle = \langle y|x\rangle \text{ if } \mathcal{K} = \mathbb{R} \quad \text{or} \quad \langle x|y\rangle = \langle y|x\rangle^* \text{ if } \mathcal{K} = \mathbb{C}, \quad \forall x, y \in V. \tag{1.1}$$

2. *It is linear on its second argument,*

$$\langle x|ay + bz\rangle = a\langle x|y\rangle + b\langle x|z\rangle, \quad \forall x, y, z \in V, \quad \forall a, b \in \mathcal{K}. \tag{1.2}$$

3. *It is non-degenerate and positive-definite*

$$\langle x|x\rangle \geq 0, \forall x \in V \quad \text{and} \quad \langle x|x\rangle = 0 \Rightarrow x = 0. \tag{1.3}$$

Inner products on complex vector spaces are known as Hermitian products. The pair $(V, \langle\cdot|\cdot\rangle)$ is called an inner product space over $\mathcal{K}$.

Observe that, due to the definition, the inner product over a real vector space is linear also on its first argument, i.e. it is bilinear. This is not true, however, for Hermitian products, as scalar factors have to be conjugated: $\langle ax|y\rangle = a^*\langle x|y\rangle$. Such products are sometimes called sesquilinear.

Proposition 1.2. *Any inner product space is a normed space with respect to the norm defined as*

$$\|x\| := \sqrt{\langle x|x\rangle}, \quad x \in V. \tag{1.4}$$

The norm in V naturally defines a distance function $d(x, y) = \|x - y\|$, with $x, y \in V$.

Proposition 1.3 (Schwarz inequality)**.** *Consider an inner product space $(V, \langle\cdot|\cdot\rangle)$ over the field $\mathcal{K}$. Then,*

$$|\langle x|y\rangle| \leq \|x\|\|y\|, \quad \forall x, y \in V. \tag{1.5}$$

The equality holds if and only if $x = \lambda y$ for some $\lambda \in \mathcal{K} - \{0\}$, or if either $x = 0$ or $y = 0$.

Proof. For $x = 0$ and $y = 0$, Schwarz inequality is trivially satisfied. Consider the case $x \neq 0, y \neq 0$. Then, for any $\lambda \in \mathcal{K}$,

$$\|x - \lambda y\|^2 = \langle x - \lambda y|x - \lambda y\rangle = \|x\|^2 - \lambda\langle x|y\rangle - \lambda^*\langle y|x\rangle + |\lambda|^2\|y\|^2.$$

Because of axiom (1.3), this norm is non-negative for any $\lambda \in \mathcal{K}$. In particular, taking $\lambda = \langle y|x\rangle\|y\|^{-2}$, Schwarz inequality is obtained:

$$\|x - \lambda y\|^2 \geq 0 \Rightarrow \|x\|^2 - \frac{|\langle x|y\rangle|^2}{\|y\|^2} \geq 0 \Rightarrow \|x\|^2\|y\|^2 \geq |\langle x|y\rangle|^2. \tag{1.6}$$

Equality holds only if $\|x - \lambda y\|^2 = 0$, which by (1.3) implies that $x - \lambda y = 0$, thus completing the proof. □

Definition 1.4. *A Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle)$ over a field $\mathcal{K}$ (either $\mathbb{R}$ or $\mathbb{C}$) is an inner product space over $\mathcal{K}$ which is complete with respect to the topology defined by the norm on $\mathcal{H}$ induced by the inner product.*

In the following, if the inner product of a Hilbert space is understood, the Hilbert space is simply denoted $\mathcal{H}$.

Definition 1.5. *Consider a linear space V over a field $\mathcal{K}$. The algebraic dual space of V is defined as the linear space V^* of $\mathcal{K}$-linear functions $\alpha : V \to \mathcal{K}$. If V is a topological linear space, then the topological dual space of V is the linear space V' of continuous $\mathcal{K}$-linear functions $\alpha' : V \to \mathcal{K}$.*

The difference between algebraic and topological dual spaces is relevant for infinite-dimensional linear spaces. Continuous functionals on a topological linear space V are necessarily bounded [148]. Thus, the topological dual space V' is the subspace of bounded elements in V^*. If V is finite-dimensional, any $\mathcal{K}$-linear function on V is bounded, thus $V^* = V'$. For this reason, in the following no difference is made between topological and algebraic dual spaces of finite-dimensional linear spaces; they will be denoted by V^* and simply called dual spaces.

Theorem 1.6 (Riesz representation theorem [148])**.** *Let $\mathcal{H}$ be a Hilbert space over $\mathcal{K}$. For any $x \in \mathcal{H}$, let $\alpha_x \in \mathcal{H}^*$ be the linear functional defined as $\alpha_x(y) = \langle x|y\rangle$, with $y \in \mathcal{H}$. Then, α_x is bounded with norm $\|\alpha_x\| = \|x\|$, and therefore continuous. The application $\alpha : x \in \mathcal{H} \mapsto \alpha_x \in \mathcal{H}^*$ is a bijection between $\mathcal{H}$ and the topological dual space $\mathcal{H}'$.*

Observe that, as a result of the last assertion, if $\mathcal{H}$ is finite dimensional, the dual space is unique and α is a bijection between $\mathcal{H}$ and $\mathcal{H}^*$. The Riesz representation theorem fully characterises all the bounded linear functionals on Hilbert spaces.

The case of infinite-dimensional Hilbert spaces requires a careful description of operators. Several mathematical difficulties have to be faced, as many physically relevant operators are not bounded, which leads to continuity and domain problems. However, the geometric approach that is considered along the dissertation is only useful in its present form in the case of finite dimensional systems. For this reason, the description of operators on infinite-dimensional Hilbert spaces is skipped. The mathematical tools needed for the description of infinite-dimensional quantum systems can be found, for example, in the course by Moretti [207] or in the book by Hunter and Nachtergeale [157].

Definition 1.7. *Consider a $\mathcal{K}$-linear operator $A : \mathcal{H} \to \mathcal{H}$, with $\mathcal{H}$ a finite-dimensional Hilbert space over the field $\mathcal{K}$. The adjoint operator of A is the linear operator $A^\dagger : \mathcal{H} \to \mathcal{H}$ satisfying*

$$\langle x|Ay\rangle = \langle A^\dagger x|y\rangle, \quad \forall x, y \in \mathcal{H}. \tag{1.7}$$

A linear operator $A : \mathcal{H} \to \mathcal{H}$ is said to be self-adjoint if $A = A^\dagger$.

The infinite-dimensional case requires a formally identical definition, with the necessary consideration of the definition domain of operators. In the case of bounded operators, the domain can be considered as the whole Hilbert space, and the definition of adjoint operators is identical to the finite-dimensional case.

Regarding spectra of operators, the infinite-dimensional case also presents the need for a careful description. It is necessary to distinguish between discrete, continuous and residual spectra [157]. Thus, once again only the finite dimensional case is presented. The following theorem gives information on the properties of the eigenvalues and eigenvectors of operators.

Theorem 1.8 (Finite-dimensional spectral theorem [150])**.** *Let $\mathcal{H}$ be a finite-dimensional complex Hilbert space. Any self-adjoint operator $A : \mathcal{H} \to \mathcal{H}$ is diagonalizable, with every eigenvalue being a real number. Any two eigenvectors of A with different eigenvalue are orthogonal. Thus, it is possible to obtain an orthogonal basis of $\mathcal{H}$ composed by eigenvectors of A.*

The formulation of the Schrödinger picture of Quantum Mechanics is based on the concepts presented here. Pure states of quantum system are represented by vectors in complex Hilbert spaces. Thus, this

will be the focus of the present section. In the following, if not otherwise specified, $\mathcal{H}$ denotes a complex Hilbert space and $\langle\cdot|\cdot\rangle : \mathcal{H}\times\mathcal{H}\to\mathbb{C}$ the inner product in $\mathcal{H}$. The algebraic dual space of $\mathcal{H}$ is denoted as $\mathcal{H}^*$; following the above comments, if $\mathcal{H}$ is finite-dimensional, then $\mathcal{H}^*$ is simply called the dual space of $\mathcal{H}$.

It is common in Quantum Mechanics to use the so-called 'Dirac notation' or 'bra-ket notation' for elements in $\mathcal{H}$ and in the topological dual space $\mathcal{H}'$. This notation is based on the Riesz representation theorem 1.6, as it relates both spaces in terms of the Hermitian product. It can be, however, formally misleading, hence the next paragraphs present the necessary definitions.

Elements in the Hilbert space are denoted by 'kets' as $|\psi\rangle\in\mathcal{H}$. The notation of the inner product of any two elements $|\psi\rangle, |\phi\rangle\in\mathcal{H}$ is simplified as

$$\langle\phi|\psi\rangle := \Big\langle |\phi\rangle \Big| |\psi\rangle \Big\rangle. \tag{1.8}$$

This notation allows to simplify the concept presented by Riesz representation theorem. Given a vector $|\phi\rangle\in\mathcal{H}$, it is possible to write the linear functional $\alpha_{|\phi\rangle}$ associated to it as a 'bra' $\langle\phi|\in\mathcal{H}'$. By making use of the notation for the Hermitian product, the action of $\langle\phi|$ on $\mathcal{H}$ is denoted by juxtaposition:

$$\langle\phi| := \alpha_{|\phi\rangle} \;\Rightarrow\; \langle\phi|\Big(|\psi\rangle\Big) = \alpha_{|\phi\rangle}\Big(|\psi\rangle\Big) = \langle\phi|\psi\rangle, \quad |\psi\rangle, |\phi\rangle\in\mathcal{H}. \tag{1.9}$$

The action of a linear operator $A:\mathcal{H}\to\mathcal{H}$ is usually written as

$$A|\psi\rangle := A(|\psi\rangle), \quad |\psi\rangle\in\mathcal{H}. \tag{1.10}$$

This notation resembles multiplication of matrices and vectors. If $\mathcal{H}$ is finite-dimensional, with complex dimension n, then by choosing a basis it is possible to associate to $|\psi\rangle$ a column vector in $\mathbb{C}^n$. In a similar way, the linear operator A is represented by an $n\times n$ matrix with complex entries, and $A|\psi\rangle$ can be computed by usual matrix multiplication. Following with this analogy, the 'bra' $\langle\phi|$ is represented by a row vector, and $\langle\phi|\psi\rangle$ is obtained as the matrix product of a row vector and a column vector.

Other simplifications are introduced in the notation. For example, sums of vectors and multiplications by scalars on $\mathcal{H}$ can sometimes be written as follows:

$$|\psi+\phi\rangle := |\psi\rangle + |\phi\rangle, \quad |\lambda\psi\rangle := \lambda|\psi\rangle, \quad |\psi\rangle, |\phi\rangle\in\mathcal{H}, \quad \lambda\in\mathbb{C}. \tag{1.11}$$

The norm in $\mathcal{H}$ is simply written as $\|\psi\| := \big\||\psi\rangle\big\|$, for any $|\psi\rangle\in\mathcal{H}$. Observe that the norm of elements in $\mathcal{H}'$ is the same as their corresponding element in $\mathcal{H}$ by Theorem 1.6, thus it is consistent to write $\|\psi\| = \big\|\langle\psi|\,\big\|$ for any 'bra' $\langle\psi|\in\mathcal{H}'$.

The mathematical tools sketched here are the basic ingredients for a formal description of Quantum Mechanics. They are the necessary ingredient for an appropriate identification of the properties of quantum systems, presented in the following sections.

1.1.2 The postulates of Quantum Mechanics

The Schrödinger picture of Quantum Mechanics describes the properties of quantum systems in terms of complex Hilbert spaces and their characteristics. The prominent textbook by Cohen-Tannoudji *et al.* [102] presents in a clear and systematic way the postulates of Quantum Mechanic that formally describe this relation between Hilbert spaces and quantum systems. Such postulates are reproduced here; refer to pages 215 and following of Cohen-Tannoudji's first volume for a more detailed presentation.

POSTULATE 1. *The state of a quantum system at a fixed time is defined by specifying a vector in a complex separable Hilbert space $\mathcal{H}$.*

A quantum system is said to be finite-dimensional if its associated Hilbert space is of finite dimension. Evidently, a quantum system is said to be infinite-dimensional if its associated Hilbert space is separable and infinite-dimensional.

POSTULATE 2. *An observable, i.e. a measurable quantity on the system, is represented by an essentially self-adjoint operator on $\mathcal{H}$.*

This postulate is also valid for infinite-dimensional systems [207]. Operators associated to physical quantities in infinite-dimensional systems are not, however, necessarily bounded. Such is the case, for example, of the energy of a quantum oscillator or of the hydrogen atom. Non-boundedness of physical observables leads to many mathematical difficulties.

In the following, the name 'observable' denotes both measurable quantities and self-adjoint operators associated to them. Recall that, due to the spectral theorem 1.8, the spectrum $\mathrm{spec}(A)$ of an essentially self-adjoint operator A is always a set of real numbers. This feature is fundamental in the following statement.

POSTULATE 3. *The possible results of the measurement of an observable of a quantum system are the elements in its spectrum.*

POSTULATE 4 (Finite-dimensional systems)**.** *Consider a finite-dimensional quantum system. If an observable A with spectrum, $\mathrm{spec}(A) = \{a_1, a_2, \ldots\}$ is measured when the system is in a state represented by $|\psi\rangle \in \mathcal{H}$, the result of the measurement is $a \in \mathrm{spec}(A)$ with probability.*

$$p_\psi(a) = \sum_{k=1}^{d_a} \frac{|\langle e_k^a|\psi\rangle|^2}{\langle\psi|\psi\rangle}, \tag{1.12}$$

where d_a is the degeneracy of the eigenvalue a and $\{|e_1^a\rangle, |e_2^a\rangle, \ldots, |e_{d_a}^a\rangle\}$ is an orthonormal basis of the corresponding eigenspace.

The postulate for infinite-dimensional systems is formally similar. It is necessary to distinguish between discrete and continuum spectra of self-adjoint operators. See references [102,207] for a description of the measurement process in the infinite-dimensional case.

It is an empirical fact that, when a measure is carried on a quantum system, its state changes. This is a non-deterministic change that depends on the outcome of the measurement process. This behaviour of quantum states is described by the following postulate.

POSTULATE 5. *Let $a \in \mathrm{spec}(A)$ be the result of the measurement of an observable A when the system is in a state represented by $|\psi\rangle \in \mathcal{H}$. Immediately after the measurement process, the state of the system collapses onto the state represented by the vector*

$$|\psi_a\rangle = P_a|\psi\rangle, \tag{1.13}$$

where P_a is the orthogonal projector onto the eigenspace of a. If the system is finite-dimensional, then

$$P_a = \sum_{k=1}^{d_a} |e_k^a\rangle\langle e_k^a|. \tag{1.14}$$

POSTULATE 6. *The evolution of a quantum system between two measurements is governed by the Schrödinger equation:*

$$\mathrm{i}\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle, \tag{1.15}$$

where $H(t)$ is called the Hamiltonian operator and is the observable representing the energy of the quantum system.

These postulates are the canonical starting point of the description of Quantum Mechanics. It should be noticed that they provide a suitable mathematical description for the main elements of a theory. Namely, postulates determine which objects represent the state of the system and the quantities that can be measured, how the measurement process is implemented and how the system evolves. The

interpretation of the physical meaning of the postulates has been object of deep studies and debates among physicists since the conception of Quantum Mechanics.

Observe that, as a consequence of Postulate 1, there exists a superposition principle on $\mathcal{H}$ and it is possible to consider linear superpositions of states. This is a purely quantum phenomenon that reflects the wave-particle duality found in experiments [102]. Its interpretation is in deep connection with statement of Postulate 4. This postulate determines in a mathematical way the probabilistic nature that is intrinsic to quantum systems. According to it, it is impossible to know in advance the result of any measurement in any state, even if the state is completely determined. The probabilistic nature of Quantum Mechanics is one of the most important aspects of the theory, and represents a qualitative difference with Classical Mechanics, a fully deterministic theory.

Postulate 5 describes the change in the state of a quantum system after the measure of an observable. This change is immediate and is also an important element in the description of quantum probability. The correct interpretation of this behaviour, usually known as the 'measurement problem', is an open debate in Quantum Mechanics [163, 234, 274, 278]. Several interpretations to this phenomenon have been proposed, from the existence of hidden variables [48, 49, 116] to the many-world interpretation [125, 126]. One of the most successful proposals is based in the concept of quantum decoherence [164, 218, 235, 236, 278, 280, 281]. The measurement problem will be discussed again when dealing with the geometric description of decoherence of quantum systems.

1.1.3 The observables of quantum systems

As stated by Postulate 2, observable quantities are represented by essentially self-adjoint operators on Hilbert spaces. It is important to properly describe the properties of the set $\mathcal{O}$ of observables. In finite-dimensional systems, the concepts of self-adjoint and Hermitian operators are equivalent. Thus, for these systems, the set of observables is $\mathcal{O} = \mathrm{Herm}(\mathcal{H})$.

Observables of quantum systems are the main object of the Heisenberg picture of Quantum Mechanics. Thus, it is natural that the algebraic properties of observables were first studied by their main contributors. Pascal Jordan indeed proposed a new type of algebraic structure [165, 166] in order to understand the properties of observables in a formal and abstract way. In the following deacdes, many works have dealt with the study of Jordan algebras [160–162, 192, 200–202, 248]. Jordan algebras will be presented in detail in Chapter 3 when discussing Heisenberg picture. For now, let us simply present the needed definitions to understand the algebraic structure of the set of quantum observables.

Definition 1.9. *An algebra $(A, *)$ over a field $\mathcal{K}$ is a pair where V is a linear space over $\mathcal{K}$ equipped with a bilinear product $*$, i.e. with an inner composition rule satisfying the following relations:*

$$(\lambda x+\mu y)*z = \lambda(x*z)+\mu(y*z), \quad x*(\lambda y+\mu z) = \lambda(x*y)+\mu(x*z), \quad \forall x,y,z \in A, \quad \forall \lambda,\mu \in \mathcal{K}. \tag{1.16}$$

The algebra is called associative or commutative if the product $*$ is associative or commutative, respectively.

Several examples of associative algebras appear along this dissertation. Smooth functions on a manifold M form an associative and commutative algebra $C^\infty(M)$ with respect to the point-wise product fg of functions, defined as $(fg)(x) = f(x)g(x)$. C*-algebras, and in particular linear operators on finite-dimensional linear spaces, are also associative algebra. Other types of algebras can be obtained by assuming different axioms on the bilinear product. Lie and Jordan algebras, which play a key role in the description of Quantum Mechanics, are defined next.

Definition 1.10. *A Lie algebra $(A, [\![\cdot,\cdot]\!])$ over the field $\mathcal{K}$ (either $\mathbb{R}$ or $\mathbb{C}$) is an algebra over $\mathcal{K}$ whose bilinear product $[\![\cdot,\cdot]\!]$, called the Lie bracket of the algebra, is skew-symmetric and satisfies Jacobi identity:*

$$[\![x,y]\!] = -[\![y,x]\!], \quad [\![x,[\![y,z]\!]]\!] + [\![y,[\![z,x]\!]]\!] + [\![z,[\![x,y]\!]]\!] = 0, \quad \forall x,y,z \in A. \tag{1.17}$$

Definition 1.11. *A linear Jordan algebra $(A, odot)$ over the field $\mathcal{K}$ (either $\mathbb{R}$ or $\mathbb{C}$) is an algebra over $\mathcal{K}$ whose associative product, called the Jordan product of the algebra, is symmetric and satisfies Jordan identity:*

$$x \odot y = y \odot x, \quad (x \odot y) \odot (x \odot x) = x \odot (y \odot (x \odot x)), \quad \forall a, b \in A. \tag{1.18}$$

A linear Jordan algebra is called unital if there exists an element $1 \in A$, called the unit element, such that $x \odot 1 = x$ for any $x \in A$.

Different algebraic structures can be defined on a same linear space. If they satisfy some compatibility conditions, then a new structure is obtained. This is the case of Lie-Jordan algebras, in which compatible Lie bracket and Jordan product exist on the same linear space.

Definition 1.12. *A triple $(A, [\![\cdot,\cdot]\!], \odot)$ is called a Lie-Jordan algebra over the field $\mathcal{K}$ (either $\mathbb{R}$ or $\mathbb{C}$) if $(A, [\![\cdot,\cdot,]\!])$ is a Lie algebra over $\mathcal{K}$, $(A, \odot)$ is a linear Jordan algebra over $\mathcal{K}$ and the following compatibility relations between the Lie bracket and the Jordan product are satisfied:*

$$[\![x, y \odot z]\!] = [\![x, y]\!] \odot z + y \odot [\![x, z]\!], \quad (x \odot y) \odot z - x \odot (y \odot z) = \lambda [\![[\![x, z]\!], y]\!], \quad \forall x, y, z \in A, \tag{1.19}$$

with λ a positive real number. A Lie-Jordan algebra is called unital if there exists a unit element for the Jordan product

If $(A, [\![\cdot,\cdot]\!], \odot)$ is a unital Lie-Jordan algebra, then the unit element commutes with any other element, i.e. $[\![x, 1]\!] = 0$ for any $x \in A$. This can be proved by taking $y = z = 1$ in the first compatibility relation in (1.19).

Proposition 1.13. *The triple $(\mathcal{O}, [\![\cdot,\cdot]\!], \odot)$, with $\mathcal{O} = \mathrm{Herm}(\mathcal{H})$ being the set of Hermitian operators on a finite-dimensional complex Hilbert space $\mathcal{H}$, is a unital Lie-Jordan algebra over $\mathbb{R}$ with respect to the products*

$$[\![A, B]\!] = -\mathrm{i}(AB - BA) = -\mathrm{i}[A, B], \quad A \odot B = AB + BA, \quad A, B \in \mathcal{O}, \tag{1.20}$$

with $[\cdot,\cdot]$ the usual commutator, $[A, B] = AB - BA$, and with $\frac{1}{2}I$ as the unit element.

Proof. Products $[\![A, B]\!]$ and $A \odot B$ are by definition inner composition laws of $\mathrm{Herm}(\mathcal{H})$. Notice the factor needed for the first product to be an inner operation. They are respectively skew-symmetric and symmetric. The required identities are proved to be satisfied by direct computation. For example,

$$\begin{aligned}(A \odot B) \odot (A \odot A) &= (AB + BA) \odot (2A^2) = 2ABA^2 + 2A^3B + 2BA^3 + 2A^2BA,\\ A \odot (B \odot (A \odot A)) &= A \odot (2BA^2 + 2A^2B) = 2ABA^2 + 2BA^3 + 2A^3B + 2A^2BA,\end{aligned}$$

which proves that Jordan identity is satisfied. Notice that the second identity in (1.19) is satisfied for $\lambda = 1$. □

Consider the complexification $\mathcal{O}_{\mathbb{C}}$ of the linear space $\mathcal{O}$, obtained by extending the field of scalars from $\mathbb{R}$ to $\mathbb{C}$. By extending also the Lie bracket and the Jordan product, it is possible to recover the associative product of operators as

$$AB = \frac{1}{2} A \odot B + \frac{\mathrm{i}}{2} [\![A, B]\!], \quad A, B \in \mathcal{O}_{\mathbb{C}}. \tag{1.21}$$

The connection between Lie-Jordan algebras and associative algebras will be described in detail in Chapter 3.

1.1.4 The probabilistic nature of Quantum Mechanics

The probabilistic nature of the measurement can be described mathematically in the concept of expectation values of observables. Even if it is not possible to predict the exact result of a measurement, the probability of each possible result is known. It is thus possible to define the expectation value of the measurement, which represents the average value that would be obtained on a large ensemble of identically prepared systems.

Definition 1.14. *The expectation value of an observable A on a state of a quantum system described by $|\psi\rangle \in \mathcal{H}$ is the sum of the possible results of its measurement, weighted by their corresponding probabilities:*

$$\langle A\rangle_\psi = \sum_{a\in \mathrm{spec}(A)} p_\psi(a)a = \frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle} \tag{1.22}$$

Consider an ensemble consisting of a large number of identical quantum systems, all of them in the same state $|\psi\rangle$. The expectation value $\langle A\rangle_\psi$ represents the average value of the measurements of A on this ensemble [102]. Within a statistical perspective, it is natural to consider also the standard derivation of A, defined as

$$\Delta_\psi A := \sqrt{\langle A^2\rangle_\psi - \langle A\rangle_\psi^2}. \tag{1.23}$$

Theorem 1.15 (Schrödinger uncertainty relation)**.** *The standard derivations of two observables $A, B \in \mathcal{O}$ satisfy the following relation:*

$$(\Delta_\psi A)(\Delta_\psi B) \geq \left(\frac{1}{2}\langle A\odot B\rangle_\psi - \langle A\rangle_\psi\langle B\rangle_\psi\right)^2 + \left(\frac{1}{2}\langle[\![A,B]\!]\rangle_\psi\right)^2, \quad \forall|\psi\rangle\in\mathcal{H}. \tag{1.24}$$

Proof. Given a vector $|\psi\rangle \in \mathcal{H} - \{0\}$, consider the observables $C = A - \langle A\rangle_\psi I$, $D = B - \langle B\rangle_\psi I$. It is immediate to compute that the expectation values of these observables are

$$\langle C^2\rangle_\psi = (\Delta_\psi A)^2, \quad \langle D^2\rangle_\psi = (\Delta_\psi B)^2.$$

Define two new vectors in $\mathcal{H}$ as $|\phi_C\rangle = C|\psi\rangle$, $|\phi_D\rangle = D|\psi\rangle$. Schwarz inequality (1.5) can be applied to these vectors:

$$\|\phi_C\|\|\phi_D\| \geq |\langle\phi_C|\phi_D\rangle| = |\langle\psi|CD|\phi_D\rangle| = \left|\frac{1}{2}\langle\psi|C\odot D|\psi\rangle + \frac{\mathrm{i}}{2}\langle\psi|[\![C,D]\!]|\psi\rangle\right|,$$

where relation (1.21) has been used. Taking the square of this equation and dividing by $\|\psi\|^4$ yields the following relation:

$$\langle C^2\rangle_\psi\langle D^2\rangle_\psi \geq \left(\frac{1}{2}\langle C\odot D\rangle_\psi\right)^2 + \left(\frac{1}{2}\langle[\![C,D]\!]\rangle_\psi\right)^2. \tag{1.25}$$

The Lie bracket and Jordan product of C and D are obtained by direct computation:

$$[\![C,D]\!] = [\![A,B]\!], \qquad C\odot B = A\odot B - 2\langle A\rangle_\psi B - 2\langle B\rangle_\psi A + 2\langle A\rangle_\psi\langle B\rangle_\psi I.$$

By substituting these relations on (1.25), Schrödinger inequality is obtained. □

Corollary 1.16 (Robertson uncertainty relation)**.** *Any two observables $A, B \in \mathcal{O}$ of a quantum system satisfy the following relation:*

$$(\Delta_\psi A)(\Delta_\psi B) \geq \frac{1}{2}\langle[\![A,B]\!]\rangle_\psi, \quad \forall|\psi\rangle\in\mathcal{H}. \tag{1.26}$$

The implications of these results are some of the main characteristics of quantum systems. There exists an inherent limitation to the amount of information that can be extracted from quantum systems. Even if the state of a system is fully determined, arbitrary pairs of observables cannot have both zero standard deviation at the same state of the system. From an empirical perspective, this property means that these observables cannot be measured simultaneously with perfect accuracy.

A well-known case corresponds to position and momentum observables of a free quantum particle. Notice that this is an infinite-dimensional system, with the already mentioned limitation to the algebraic treatment of observables. Consider a particle moving in a one-dimensional space, and let X and P be respectively the position and momentum P observables of the particles. The commutator of these operators is known to be $[X, P] = \mathrm{i}\hbar I$ [102]. Thus, the application of the Robertson inequality yields the following result:

$$(\Delta_\psi X)(\Delta_\psi P) \geq \frac{\hbar}{2}. \tag{1.27}$$

This famous inequality is known as the Heisenberg uncertainty principle [153]. The fact that positions and momenta of quantum particles cannot be determined simultaneously is one of the most important differences with classical systems.

Expectation values are in fact very important tools in Quantum Mechanics. They are, after all, the only possible way in which information can be obtained about the state of a quantum system. It is indeed possible to reformulate Quantum Mechanics in terms of these expectation values, instead of operators. This formulation is known as the Ehrenfest picture, in honour to Paul Ehrenfest, who first introduced the idea in his seminal work [118]. The geometric characterisation of Quantum Mechanics, which is the topic of this dissertation, expands the idea of the Ehrenfest picture [101]. Expectation values are seen as functions on a differentiable manifold whose points correspond to the vectors of the Hilbert space. The second part of this chapter deals deeply with this geometric description.

Observe that Quantum Mechanics is an intrinsically probabilistic theory, unlike Classical Mechanics. Expectation values of observables are required for a correct description of quantum phenomenons even if the state of the system is completely determined, in other words, if the state is pure. This 'quantum probability' is fundamental in the understanding of this theory. Nevertheless, it is also possible to introduce statistical ensembles as in Classical Mechanics. In other words, it is possible to consider probability distributions on the space of pure states. In this case, it is said that the state of the system is mixed, as it is not completely determined. The study of Statistical Quantum Mechanics is a fascinating issue, as it mixes classical statistical properties with the intrinsic quantum probability of the theory. Many relevant works have been devoted to the topic, such as the seminal work by Gleason [136], the more recent contributions by Moretti and Pastorello [206, 208, 209], and others [15, 61, 62, 64, 117]. It is not possible, however, to dwell on the details of the topic. A brief review of the topic will be presented in Section 3.1.5, and its connections with the geometric formalism and hybrid quantum-classical models wil be discussed in Section 5.3.

1.1.5 The Schrödinger equation

Postulate 6 determines the differential equation that governs the free evolution of autonomous quantum systems between two measurements. It is however possible to describe quantum evolution in a more fundamental way, by means of families unitary transformations acting on the Hilbert space [81, 230], as presented in this section.

Consider a quantum system whose state at an initial time t_0 is described by a vector $|\psi_0\rangle \in \mathcal{H}$. The states of the system at every time $t \geq t_0$ define a trajectory $|\psi(t)\rangle$ on $\mathcal{H}$, with $|\psi(t_0)\rangle = |\psi_0\rangle$. It is thus possible to define the map $U(t, t_0) : \mathcal{H} \to \mathcal{H}$, by

$$U(t, t_0)|\psi_0\rangle := |\psi(t)\rangle, \quad t \geq t_0. \tag{1.28}$$

Physically, evolution of closed quantum systems preserves both linear superpositions and quantum probabilities [102]. Therefore, if no measurement has been taken on the system in the interval $[t_0, t]$, the maps $U(t, t_0)$ are necessarily symmetries of the system, i.e they preserve the linearity and the Hermitian

product in $\mathcal{H}$. They are unitary operators on $\mathcal{H}$, and thus the evolution (1.28) is called unitary evolution of quantum systems.

Continuity of the evolution requires two further conditions for these operators:

$$U(t_1,t_1)=I, \quad U(t_2,t_1)U(t_1,t_0)=U(t_2,t_0), \quad t_2\geq t_1\geq t_0. \tag{1.29}$$

Theorem 1.17. *Consider a family of unitary operators $\{U(t,t_0), t\geq t_0\}$ on $\mathcal{H}$ such that conditions in (1.29) hold. They satisfy the following differential equation:*

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0)=H(t)U(t,t_0), \tag{1.30}$$

with $H(t)\in\mathcal{O}$ and $t\geq t_0$.

Proof. For a fixed value of t_0, the set $\{U(t,t_0), t\geq t_0\}$ is a one-parameter family on the Lie group $U(\mathcal{H})$ of unitary operators on $\mathcal{H}$. The differential equation generating the family can be obtained from (1.29) by taking $t_2=t$:

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0)=\left(\frac{\mathrm{d}}{\mathrm{d}t}U(t,t_1)\right)U(t_1,t_0), \quad t\geq t_1\geq t_0.$$

As $U(t_1,t_0)=U(t,t_1)^{-1}U(t,t_0)$, the following relation holds for all possible values of t_1 and t_0:

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0)\right)U(t,t_0)^{-1}=\left(\frac{\mathrm{d}}{\mathrm{d}t}U(t,t_1)\right)U(t,t_1)^{-1}$$

Thus, both sides of the equation depend only on t. As $U(\mathcal{H})$ is a Lie group, this is precisely the expression of an element in the tangent space to $U(t_0,t_0)=I$, therefore in the Lie algebra of the unitary group. This is the algebra of skew-Hermitian operators on $\mathcal{H}$. Hence, it is possible to rewrite this expression as

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}U(t,t_0)\right)U(t,t_0)^{-1}=-\mathrm{i}\hbar^{-1}H(t), \quad t\geq t_0, \tag{1.31}$$

with $H(t)$ an Hermitian operator on $\mathcal{H}$. □

Proposition 1.18. *Take a trajectory $|\psi(t)\rangle$ on $\mathcal{H}$ starting at a vector $|\psi_0\rangle=|\psi(t)\rangle$. If the trajectory is determined by a family of time-evolution operators as in (1.28) such that conditions (1.29) hold, then the differential equation of the trajectory is the time-dependent Schrödinger equation*

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle=H(t)|\psi(t)\rangle. \tag{1.32}$$

Proof. Derivation of (1.28), together with (1.30), yields as a result the proposed equation. □

Observe that the resulting equation is more general than the time-independent Schrödinger equation proposed in Postulate 6. By considering the unitary operators defining the evolution, it is possible to describe also non-autonomous quantum systems. Therefore, the approach presented here is more general and with a broader range of applications. Chapter 2, in particular, deals with the analysis of time-dependent Schrödinger equations from the point of view of Lie systems.

1.1.6 The projective Hilbert spaces

Up to this point, Quantum Mechanics has been described in terms of linear algebra, yielding important results. However, from an empirical point of view, there exists some ambiguity in the description of states in terms of vectors in $\mathcal{H}$. The measurable aspects of Quantum Mechanics, namely the probabilities of measurements presented in (1.12) and the expectation values of observables (1.22), suffer from this ambiguity. Therefore, if the theory is assumed to characterise mathematically the empirical properties of quantum systems, this aspect has to been taken into account.

Proposition 1.19. *Consider two non-zero vectors $|\psi\rangle, |\psi'\rangle \in \mathcal{H}$. Expectation values at both states are equal for any observable if and only if the vectors are proportional:*

$$\langle A\rangle_\psi = \langle A\rangle_{\psi'},\ \forall A \in \mathcal{O} \ \Leftrightarrow\ |\psi\rangle = c|\psi'\rangle,\ c \in \mathbb{C} - \{0\}. \tag{1.33}$$

Proof. If the vectors are proportional, then (1.22) shows that expectation values of observables are always equal. Assume now that $\langle A\rangle_\psi = \langle A\rangle_{\psi'}$ is satisfied for any $A \in \mathcal{O}$. In particular, consider the equality for the projector onto the subspace generated by $|\psi\rangle$:

$$A = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} \Rightarrow 1 = \frac{\langle\psi'|\psi\rangle\langle\psi|\psi'\rangle}{\langle\psi|\psi\rangle\langle\psi'|\psi'\rangle} \Rightarrow \|\psi\|^2\|\psi'\|^2 = |\langle\psi|\psi'\rangle|^2. \tag{1.34}$$

By Schwarz inequality (1.5), both vectors are proportional. □

A proper description of this feature requires the definition of an equivalence relation between vectors in $\mathcal{H} - \{0\}$. From a purely empirical perspective, states are described not by vectors in $\mathcal{H}$, but rather by equivalence classes in $\mathcal{H} - \{0\}$. In other words, the set of states is the quotient space defined by this equivalence relation. In the case of Hilbert spaces, this particular equivalence relation define the corresponding projective spaces. Refer to the books by Halmos [150], Nakahara [212] and other similar works for descriptions of equivalence classes, quotient spaces and projective spaces.

Definition 1.20. *Two vectors $|\psi\rangle, |\psi'\rangle \in \mathcal{H} - \{0\}$ are said to be related, $|\psi\rangle \sim |\psi'\rangle$, if there exists a non-zero complex number c such that $|\psi\rangle = c|\psi'\rangle$.*

Proposition 1.21. *The relation $\sim$ is an equivalence relation in $\mathcal{H} - \{0\}$.*

Proof. This assertion is immediately proved, as the relation is reflexive, symmetric and transitive. □

Definition 1.22. *The projective Hilbert space $\mathcal{P}$ is the quotient space defined by the equivalence relation in Definition 1.20, $\mathcal{P} = \mathcal{H}_0/\sim$.*

Hence the states of a quantum system are in a one-to-one correspondence with points in $\mathcal{P}$. It is important to notice that $\mathcal{P}$ is not a linear space. The usual way to deal with the projective Hilbert space in Quantum Mechanics is to embed in a natural way $\mathcal{P}$ into the whole Hilbert space by choosing a representative of each equivalence class, i.e. by 'fixing the norm and the global phase' of the vectors. In this setting, it is always compulsory to prove that dynamics does not modify the constraints imposed on the norm and the phase of vectors.

A geometric approach to Quantum Mechanics presents advantages in this respect. The projective Hilbert space $\mathcal{P}$ can be described as a differentiable manifold. Hence a geometric formalism can describe Quantum Mechanics directly on $\mathcal{P}$ without constraints.

1.1.7 A first approach to the 2-level system

As an application of the concepts presented in the dissertation, it is useful to consider particular cases of practical examples. The 2-level system results appealing due to its simplicity, while at the same time illustrates correctly almost all of the characteristics of generic systems. For these reasons, the 2-level system is analysed in detail along the dissertation.

In Quantum Mechanics, an n-level system is any quantum system with n different states and their combinations. When a basis is chosen, the Hilbert space of the system is isomorphic to $\mathbb{C}^n$. Some examples of n-level systems are spin particles, transitions of atoms between its ground and excited states, etc. In particular, the 2-level system is the simplest relevant case that can be studied (as the dynamics of a one-level system is trivial). Physically, 2-level systems appear mainly in the study of $\frac{1}{2}$-spin particles. They play a key role in quantum computing, where 2-level systems, also known as qubits, are the basic unit of information.

Pure states of the 2-level system are represented by elements in a complex 2-dimensional Hilbert space. By choosing an orthonormal basis in $\mathcal{H}$, states are represented by vectors in $\mathbb{C}^2$:

$$|\psi\rangle = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \in \mathbb{C}^2, \quad z_1, z_2 \in \mathbb{C}. \tag{1.35}$$

The Hermitian product takes the following coordinate expression in the chosen orthonormal basis of $\mathcal{H}$:

$$|\psi\rangle = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}, \quad |\psi'\rangle = \begin{pmatrix} z_1' \\ z_2' \end{pmatrix} \Rightarrow \langle\psi|\psi'\rangle = z_1^* z_1' + z_2^* z_2', \quad z_1, z_2, z_1', z_2' \in \mathbb{C}. \tag{1.36}$$

Thus, in matrix notation, the covector $\langle\psi|$ associated to a vector $|\psi\rangle$ is represented by the following row matrix:

$$|\psi\rangle = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \in \mathbb{C}^2 \Rightarrow \langle\psi| = (z_1^*, z_2^*), \quad z_1, z_2 \in \mathbb{C}. \tag{1.37}$$

Observables of the system are Hermitian operators on the Hilbert space of the system. Once that the basis is fixed, observables are represented by 2×2 complex self-adjoint matrices. The set of such matrices is denoted as Herm(2). A basis of such matrices is given by

$$\sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.38}$$

Matrices $\sigma_1, \sigma_2, \sigma_3$ are known as Pauli matrices. This particular basis of Herm(2) is appropriate for the description of its Lie-Jordan algebraic structure, with Lie bracket and Jordan product defined by (1.20). The products of the elements in the basis are

$$\begin{aligned} &[\![\sigma_1, \sigma_2]\!] = 2\sigma_3, \quad [\![\sigma_2, \sigma_3]\!] = 2\sigma_1, \quad [\![\sigma_3, \sigma_1]\!] = 2\sigma_2, \quad [\![\sigma_0, A]\!] = 0, \quad \forall A \in \mathrm{Herm}(2), \\ &\sigma_1 \odot \sigma_1 = \sigma_2 \odot \sigma_2 = \sigma_3 \odot \sigma_3 = 2\sigma_0, \quad \sigma_0 \odot A = 2A, \quad \forall A \in \mathrm{Herm}(2). \end{aligned} \tag{1.39}$$

Consider now a simple case. Let H be a diagonal matrix in the given representation, with the following expression:

$$H = \begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix}, \quad E_0, E_1 \in \mathbb{R}. \tag{1.40}$$

If $E_0 < E_1$, then E_0 is the energy of the ground state of the system $|0\rangle$, while the excited state $|1\rangle$ of the system has energy E_1. In the given basis,

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{1.41}$$

The Schrödinger equation for this system takes the following form

$$\mathrm{i}\hbar \frac{d}{dt} \begin{pmatrix} z_1(t) \\ z_2(t) \end{pmatrix} = H \begin{pmatrix} z_1(t) \\ z_2(t) \end{pmatrix} = \begin{pmatrix} E_0 z_1(t) \\ E_1 z_2(t) \end{pmatrix}. \tag{1.42}$$

Let us denote the initial conditions by $z_1(0) = z_{10}$, $z_2(0) = z_{20}$. The evolution in $\mathcal{H}$ is obtained by integrating the above differential equation:

$$|\psi(t)\rangle = \begin{pmatrix} e^{-\mathrm{i}\hbar^{-1} E_0 t} z_{10} \\ e^{-\mathrm{i}\hbar^{-1} E_1 t} z_{20} \end{pmatrix}. \tag{1.43}$$

The norm of the states is constant along the evolution:

$$\|\psi(t)\|^2 = \langle\psi(t)|\psi(t)\rangle = \left(e^{i\hbar^{-1} E_0 t} z_{10}^*, e^{i\hbar^{-1} E_1 t} z_{20}^*\right) \begin{pmatrix} e^{-\mathrm{i}\hbar^{-1} E_0 t} z_{10} \\ e^{-\mathrm{i}\hbar^{-1} E_1 t} z_{20} \end{pmatrix} = |z_{10}|^2 + |z_{20}|^2 = \|\psi(0)\|^2, \quad t \in \mathbb{R}. \tag{1.44}$$

If a similar treatment is tried to be carried on $\mathcal{P}$, mathematical problems arise. The set of equivalence classes on $\mathcal{H}$ is not a linear space, and thus a matrix treatment cannot fully describe its properties. As seen at the end of the present chapter, differential geometry is much more useful in this task, as $\mathcal{P}$ is a differentiable manifold.

1.2 The geometric formulation of Quantum Mechanics

The standard formulation of Schrödinger picture in terms of vector spaces presents problems when the probabilistic nature of Quantum Mechanics is taken into account. As it has been seen, an accurate description of the states of a quantum system is done in terms of a projective Hilbert space. This is not a linear space, but a manifold that cannot be described with a global chart. Therefore, any algebraic approach to Quantum Mechanics is unable to adequately describe this space. That is the reason why most physicists ignore, at least partially, the consequences of the probabilistic interpretation. It is common to simply describe quantum systems in terms of vectors of a subset of the Hilbert space, usually normalised vectors with a common global phase. Although useful for computational purposes, this description fails to properly represent the quantum properties of systems.

It is however possible to describe Quantum Mechanics with a formalism that intrinsically incorporates the probabilistic interpretation. Differential geometry, developed along the 20th century, comprehends the needed tools to appropriately describe the properties of manifolds. A geometric description of Quantum Mechanics was first proposed by Strocchi [251] and Kibble [176], and developed by authors such as Cantoni [65–69], Cirelli and co-workers [94, 95], and others [22, 23, 30, 42, 45, 63, 154, 247]. Recent works on the topic can be found in the works by Aniello, Asorey, Cariñena, Clemente-Gallardo, Marmo and co-workers, the author among them [8, 26, 27, 31, 57, 70, 72–74, 81, 97–101, 122].

The geometric description of Quantum Mechanics presents advantages from multiple perspectives. Many analogies exist between the Hamiltonian description of Classical Mechanics and the geometric formulation of Quantum Mechanics. For example, the Schrödinger equation is geometrically described by a Hamilton-like equation on a differentiable manifold [251]. The geometric tools developed for the study of classical systems can be easily adapted for the description of quantum systems. The theory of Lie systems, for example, has been found to be useful in order to solve the Schrödinger equation, as it will be seen in Chapter 2. Geometric control theory, which was first developed in the context of classical mechanical systems, has also interesting applications in the study of quantum systems; this topic is analysed in Chapter 4. Finally, mixed quantum-classical systems, appearing commonly in models of molecular dynamics, have been recently studied from a geometric perspective [8, 10, 14]. As shown in Chapter 5, a geometric characterisation of both the classical and quantum parts of these systems allows for a consistent description of the composite system. Many other interesting topics, such as the analysis of the classical limit of quantum systems, can be easily approached within this formalism.

This section presents the geometric description of the Schrödinger picture. In this way, the properties of the Hilbert spaces associated to any physical system are described in terms of geometric objects on a differentiable manifold.

Notice that only finite-dimensional quantum systems, i.e. systems whose associated Hilbert space is finite-dimensional, are considered here. Differential geometry presents problems when dealing with infinite-dimensional manifolds. Some advance on the topic is being carried out by Michor and co-workers in terms of Convenient Calculus [38, 204]. However, a geometric description for infinite-dimensional system is an open problem that lays beyond the scope of this dissertation. Nevertheless, the study of finite-dimensional problems is enough to deal with most physical problems.

1.2.1 Notation in differential geometry

Before describing the geometric formalism of Quantum Mechanics, some comments on the notation are useful. The following conventions are considered along this dissertation. The notation is similar to that used by Crampin and Pirani [104]; refer to this work for more details.

Consider a differentiable manifold M. The set of smooth functions on the manifold is denoted as $C^\infty(M)$. The tangent and cotangent spaces at a point $p \in M$ are denoted respectively as T_pM and T_p^*M. The corresponding tangent and cotangent bundles of the manifold are $\tau : TM \to M$ and $\tau^* : T^*M \to M$, with $TM := \cup_p T_pM$ and $T^*M := \cup_p T_p^*M$. In the same way, there exist bundles r times contravariant

and s times covariant $\tau^{r,s} : T^{r,s}M \to M$, or simply (r,s)-bundles, on the manifold M, where

$$T^{r,s}M := \bigcup_{p\in M} T^{r,s}_p M, \quad T^{r,s}_p M := \underbrace{T_pM \otimes \cdots \otimes T_pM}_{r} \otimes \underbrace{T^*_pM \otimes \cdots \otimes T^*_pM}_{s}, \quad r,s \geq 0 \tag{1.45}$$

As a consequence of this definition, $T^{1,0}M = TM$, $T^{0,1}M = T^*M$ and $T^{0,0}M = M$.

The set of vector fields on M is denoted as $\mathfrak{X}(M)$. As sections of the tangent bundle, a vector field $X \in \mathfrak{X}(M)$ defines at each point $p \in M$ a tangent vector to the manifold, denoted as $X_p \in T_pM$. Identical notation is used for 1-forms, i.e. sections of the cotangent bundle. The set of 1-forms is denoted as $\bigwedge^1(M)$. In general, a section χ of the (r,s)-bundle is an (r,s)-tensor field. At each point $p \in M$, it defines a tensor $\chi_p \in T^{r,s}_p M$. The set of (r,s)-tensor fields on the manifold is denoted as $\mathcal{T}^{r,s}(M)$

Recall that an (r,s)-tensor on a linear space V is a multilinear map on r copies of V^* and s copies of V. New tensors can be obtained simply by fixing its arguments. This can be extrapolated to tensor fields. An (r,s)-tensor field $\chi \in \mathcal{T}^{r,s}(M)$ is a map

$$\chi : \underbrace{\textstyle\bigwedge^1(M) \times \cdots \times \bigwedge^1(M)}_{r} \times \underbrace{\mathfrak{X}(M) \times \cdots \times \mathfrak{X}(M)}_{s} \to C^\infty(M). \tag{1.46}$$

If $s > 0$, the contraction of χ by a vector field $X \in \mathfrak{X}(M)$, written as $\iota_X\chi$, is the $(r, s-1)$-tensor field obtained by fixing as X the first argument on vector fields. The contraction by 1-forms, say $\iota_\alpha\chi$ with $\alpha \in \bigwedge^1(M)$ and $r > 0$, is similarly defined.

Another important operation on tensor fields is the exterior product. This product is usually defined on forms, i.e. skew-symmetric covariant tensor fields, although it can be easily extended to any type of tensor fields. Thus, the exterior product of two tensor fields ξ, ϕ is defined as $\xi \wedge \phi = \xi \otimes \phi - \phi \otimes \xi$.

1.2.2 Geometric description of Hilbert spaces

General knowledge of differential geometry is assumed along the dissertation. For further analysis on the properties of differentiable manifolds, see for example the textbooks by Boothby [50], Crampin and Pirani [104], Kobayashi and Nomizu [177], or Nakahara [212].

Proposition 1.23. *Any n-dimensional linear space V over a field $\mathcal{K}$ (either $\mathbb{R}$ or $\mathbb{C}$) is a real differentiable manifold of dimension $m = n \dim \mathcal{K}$, with $\dim \mathbb{R} = 1$ and $\dim \mathbb{C} = 2$.*

Proof. Let $E = \{e_1, e_2, \ldots, e_n\}$ be a basis on the linear space V. For every $v \in V$, there exists a unique n-tuple $(v_1, \ldots, v_n) \in \mathcal{K}^n$ such that

$$v = v_1 e_1 + \ldots + v_n e_n. \tag{1.47}$$

If the field is $\mathcal{K} = \mathbb{R}$, then $m = n$ and there exists a global chart (V, ϕ_E), with $\phi_E : V \to \mathbb{R}^m$ being the map defined by the coordinates of the vectors. In the case $\mathcal{K} = \mathbb{C}$, then (1.47) can be rewritten as

$$\begin{aligned} v &= (\operatorname{Re} v_1 + \mathrm{i} \operatorname{Im} v_1)e_1 + \ldots + (\operatorname{Re} v_n + \mathrm{i} \operatorname{Im} v_n)e_n \\ &= (\operatorname{Re} v_1)e_1 + (\operatorname{Im} v_1)\mathrm{i}\, e_1 + \ldots + (\operatorname{Re} v_n)e_n + (\operatorname{Im} v_n)\mathrm{i}\, e_n. \end{aligned}$$

Thus, any vector v can be written as a linear combination with real coefficients of elements in the set $E_{\mathbb{R}} = \{e_1, \mathrm{i}\, e_1, e_2, \mathrm{i}\, e_2, \ldots, e_n, \mathrm{i}\, e_n\}$. It is possible to define a map $\phi_E : V \to \mathbb{R}^m$, with $m = 2n$, by $\phi_E(v) = (\operatorname{Re} v_1, \operatorname{Im} v_1, \ldots, \operatorname{Re} v_n, \operatorname{Im} v_n)$.

Let E' be a different basis on V. The change of coordinates is obtained as the composed function $\phi_{E'} \circ \phi_E^{-1}$, which is linear by the properties of linear spaces, and therefore differentiable. The set of all such global charts on V define an atlas, hence a differentiable structure on V. □

In the particular case of Quantum Mechanics, let $\mathcal{H}$ be an n-dimensional complex Hilbert space with $n \geq 2$ (hence isomorphic to $\mathbb{C}^n$). As a result of Proposition 1.23, the Hilbert space $\mathcal{H}$ is a $2n$-dimensional real differentiable manifold. In the following, the notation M_Q is used when the differentiable structure is

considered on $\mathcal{H}$. As graphically represented by Figure 1.1, there exists a bijection $\nu : M_Q \to \mathcal{H}$ between the differentiable manifold and the Hilbert space. In a sense, the differentiable manifold carries also, by definition, a linear structure, that is naturally described in terms of the Hilbert space. For this reason, the following convention is used in order to simplify the notation. For any $\psi \in M_Q$, its image by ν is written in Dirac notation as

$$|\psi\rangle := \nu(\psi), \quad \psi \in M_Q. \tag{1.48}$$

Global coordinates on M_Q are related with bases on $\mathcal{H}$. Let $E = \{|e_1\rangle, |e_2\rangle, \ldots, |e_n\rangle\}$ be an orthonormal basis of $\mathcal{H}$. Any vector $|\psi\rangle \in \mathcal{H}$ can be uniquely written as

$$|\psi\rangle = \sum_{j=1}^{n} z_j |e_j\rangle, \quad z_j = \langle e_j|\psi\rangle \in \mathbb{C}, \quad j = 1, 2, \ldots, n.$$

The associated global chart (M_Q, ϕ_E) is defined by taking the real and imaginary parts of the complex coordinates. They are denoted respectively as q_j and p_j, following the notation of positions and momenta of the Hamiltonian formalism of Classical Mechanics; thus,

$$\phi_E(\psi) = (q_1, p_1, \ldots, q_n, p_n), \quad z_j = \frac{1}{\sqrt{2}}(q_j + \mathrm{i}p_j),\ j = 1, 2, \ldots, n. \tag{1.49}$$

It should be noticed that, although this notation allows to relate the properties of Classical and Quantum Mechanics, the coordinates q_j and p_j have no physical meaning in the sense of positions and momenta.

The analysis

Proposition 1.24. *The tangent bundle to M_Q can be trivialised as a product bundle:*

$$TM_Q \cong M_Q \times M_Q. \tag{1.50}$$

Proof. This results is a simple application of the fact that, indeed, any linear space is a particular case of an affine space. The differential of the bijection $\nu : M_Q \to \mathcal{H}$ at each point $\psi \in M_Q$ is $\nu_{*\psi} : T_\psi M_Q \to T_{|\psi\rangle}\mathcal{H} \cong \mathcal{H}$, which is also a bijection. Thus, the fibre $T_\psi M_Q$ at each point of the base manifold is identified with M_Q. □

The isomorphism $\nu_{*\psi} : T_\psi M_Q \to \mathcal{H}$ identifies tangent vectors to M_Q at each point $\psi \in M_Q$ with vectors in $\mathcal{H}$. Following with the above convention, the image by $T_\psi \nu$ of any tangent vector $v \in T_\psi M_Q$ is simply denoted as follows (see also Figure 1.2):

$$|v\rangle := \nu_{*\psi}(v) \in \mathcal{H}. \tag{1.51}$$

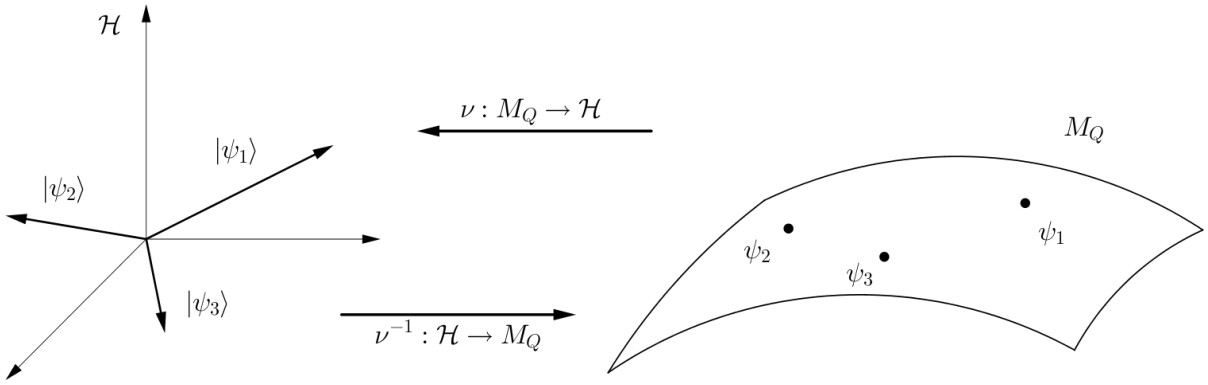


Figure 1.1: Formal relation between the Hilbert space $\mathcal{H}$ and the differentiable manifold M_Q. Vectors $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle \in \mathcal{H}$ are uniquely identified with points $\psi_1, \psi_2, \psi_3 \in M_Q$. Observe the use of Dirac notation for vectors in $\mathcal{H}$. This makes easier the relation between the geometric formalism and the properties of Hilbert spaces.

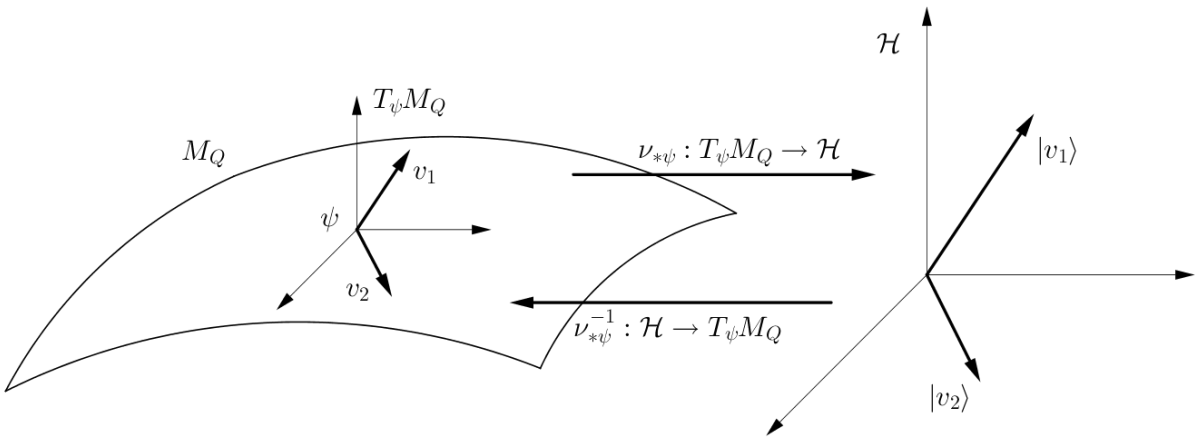


Figure 1.2: At each point $\psi \in M_Q$, there exists a tangent space $T_\psi M_Q$, which is naturally isomorphic to $\mathcal{H}$. Thus, it is possible to identify tangent vectors to M_Q with vectors in $\mathcal{H}$. Observe, that, as a consequence, there exists a natural connection in M_Q.

Consider the global coordinate chart on M_Q described by (1.49). Coordinates are given in terms of the real and imaginary parts of the coordinates of vectors in $\mathcal{H}$ for the given basis $E = \{|e_1\rangle, \ldots, |e_n\rangle\}$. Thus, applying the reasoning of Proposition 1.23, and with the notation in (1.51), the relations between the vector fields associated to the coordinate functions $q_1, p_1, \ldots, q_n, p_n$ and the elements in the basis are

$$\left| \frac{\partial}{\partial q_j}\right|_\psi \Big\rangle = \frac{1}{\sqrt{2}}|e_j\rangle, \quad \left| \frac{\partial}{\partial p_j}\right|_\psi \Big\rangle = \frac{\mathrm{i}}{\sqrt{2}}|e_j\rangle, \quad j = 1, 2, \ldots, n, \quad \forall \psi \in M_Q. \tag{1.52}$$

The trivialization of the tangent bundle alone does not describe the complex structure of $\mathcal{H}$. For any $\psi \in M_Q$, let us consider a tangent vector $\phi \in T_\psi M_Q$ and the corresponding vector $|\phi\rangle \in \mathcal{H}$. As $T_\psi M_Q$ is a real linear space, then for any $a \in \mathbb{R}$ the relation $|a\phi\rangle = a|\phi\rangle$ holds. However, a different structure is needed to describe the multiplication by complex numbers. This structure is represented by a $(1,1)$-tensor field called a complex structure [81, 212].

Definition 1.25. *An almost complex structure on a differentiable manifold M is a $(1,1)$-tensor field J satisfying that, for any $x \in M$,*

$$(J_x)^2 = -I_x, \tag{1.53}$$

with $I_x : T_x M \to T_x M$ the identity $(1,1)$-tensor at x. If it is also integrable[1]*, then J is called a complex structure.*

A complex structure on M_Q can be obtained by transporting the multiplication by the imaginary unit on $\mathcal{H}$ to the tangent bundle. At each point $\psi \in M_Q$, it is possible to define a $(1,1)$-tensor $J_\psi : T_\psi M_Q \to T_\psi M_Q$ acting on tangent vectors such that the diagram presented in Figure 1.3 commutes. In other words, the $(1,1)$-tensor J_ψ is defined by its action on tangent vectors as

$$J_\psi(w) = \nu_{*\psi}^{-1}\big(\mathrm{i}\,\nu_{*\psi}(w)\big) \;\Leftrightarrow\; |J_\psi(w)\rangle = \mathrm{i}\,|w\rangle, \quad w \in T_\psi M_Q. \tag{1.54}$$

Proposition 1.26. *The section $J : \psi \to (\psi, J_\psi)$ of the $(1,1)$-tensor bundle of M_Q is a differentiable tensor field. Furthermore, it is a complex structure on M_Q.*

[1] A tensor field on a differentiable manifold is called integrable if it is can be expressed with constant coefficients for some global chart on the manifold.

Proof. The differentiability of section J can be deduced by computing its coordinate expression. From (1.52), the action of J on the coordinate vector fields of the chosen coordinate system is the following:

$$J\left(\frac{\partial}{\partial q_j}\right) = \frac{\partial}{\partial p_j}, \quad J\left(\frac{\partial}{\partial p_j}\right) = -\frac{\partial}{\partial q_j}, \quad j = 1, 2, \ldots, n. \tag{1.55}$$

The coordinate expression of J is therefore

$$J = \sum_{j=1}^{n} \left(\mathrm{d}q_j \otimes \frac{\partial}{\partial p_j} - \mathrm{d}p_j \otimes \frac{\partial}{\partial q_j} \right), \tag{1.56}$$

so J is differentiable and integrable. Furthermore, it satisfies condition (1.53), hence it is a complex structure on M_Q. □

The definition of the complex structure in terms of its action on $\mathcal{H}$ is only the first of many examples in which the structures on $\mathcal{H}$ determine geometric objects on M_Q. This is possible because of the natural identification of the tangent space $T_\psi M_Q$ with $\mathcal{H}$ at any point $\psi \in M_Q$, as seen in Proposition 1.24. Particular attention is paid to the case of $\mathbb{C}$-linear maps on $\mathcal{H}$.

Proposition 1.27. *Any $\mathbb{C}$-linear map $A : \mathcal{H} \to \mathcal{H}$ defines a vector field $Z_A \in \mathfrak{X}(M_Q)$. It is defined as*

$$Z_A(\psi) = (\psi, \widehat{A}(\psi)), \quad \forall \psi \in M_Q, \tag{1.57}$$

with $\widehat{A} := \nu_{*\psi}^{-1} \circ A \circ \nu$.

Two of such vector fields have a particular interest in the geometric description of Quantum Mechanics. These are the dilation vector field and the phase-change vector field. As shown below, these vector fields define a regular foliation on $M_Q - \{0\}$ (i.e. with leaves of constant dimension), whose leaves are the image by $\nu^{-1} : \mathcal{H} \to M_Q$ of the equivalence classes defined on $\mathcal{H}$. Thus, the projective Hilbert space $\mathcal{P}$ is recovered as the set of leaves on $M_Q - \{0\}$ of this foliation.

Definition 1.28. *The vector field Δ associated to the identity map $I : \mathcal{H} \to \mathcal{H}$ is called the dilation vector field:*

$$\Delta(\psi) := Z_I(\psi) = (\psi, \widehat{\psi}), \quad \psi \in M_Q, \tag{1.58}$$

with $\widehat{\psi} := \left(\nu_{*\psi}^{-1} \circ \nu\right)(\psi)$. The vector field Γ associated with the multiplication by the imaginary unit, i.e. with the map $\mathrm{i}I : \mathcal{H} \to \mathcal{H}$, is called the phase-change vector field:

$$\Gamma(\psi) := Z_{\mathrm{i}I}(\psi) = (\psi, J_\psi(\widehat{\psi})), \quad \psi \in M_Q. \tag{1.59}$$

Proposition 1.29. *Both the dilation and phase-change vector fields are differentiable. They are related by the complex structure as follows:*

$$\Gamma = J(\Delta) \tag{1.60}$$

$$\begin{array}{ccc} T_\psi M_Q & \xrightarrow{\nu_{*\psi}} & \mathcal{H} \\ {\scriptstyle J_\psi}\downarrow & & \downarrow{\scriptstyle \mathrm{i}} \\ T_\psi M_Q & \xrightarrow{\nu_{*\psi}} & \mathcal{H} \end{array}$$

Figure 1.3: Commutative diagram defining for each $\psi \in M_Q$ the $(1,1)$-tensor J_ψ acting on $T_\psi M_Q$ as the transport by $\nu_{*\psi}$ of the multiplication by the imaginary unit on $\mathcal{H}$.

Proof. The coordinate expressions of both vector fields are

$$\Delta = \sum_{j=1}^{n} \left(q_j \frac{\partial}{\partial q_j} + p_j \frac{\partial}{\partial p_j} \right), \quad \Gamma = \sum_{j=1}^{n} \left(-p_j \frac{\partial}{\partial q_j} + q_j \frac{\partial}{\partial p_j} \right). \tag{1.61}$$

Hence they are differentiable vector fields The relation between Δ and Γ is obtained directly from definitions (1.58) and (1.59). In the given coordinate chart, it can be checked using also (1.56). □

In general, applications on $\mathcal{H}$, satisfying linearity properties on all of its arguments, can be interpreted as a geometric object acting on tangent vectors to the manifold M_Q. This is the case of complex functions on $\mathcal{H}$.

Proposition 1.30. *Given a complex function $f : \mathcal{H}^r \to \mathbb{C}$ which is $\mathbb{R}$-linear on each argument, there exist two differentiable $(0,r)$-tensor fields τ_f^R, τ_f^I on M_Q defined at each point $\psi \in M_Q$ by*

$$\begin{aligned} (\tau_f^R)_\psi(v_1,\dots,v_r) &= \operatorname{Re} f(|v_1\rangle,\dots,|v_n\rangle), \\ (\tau_f^I)_\psi(v_1,\dots,v_r) &= \operatorname{Im} f(|v_1\rangle,\dots,|v_n\rangle), \end{aligned} \qquad \forall v_1,\dots,v_r \in T_\psi M_Q. \tag{1.62}$$

The inner product $\langle\cdot|\cdot\rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ satisfies the axioms of Proposition 1.30. The tensor fields defined in this way are hence the geometric objects representing the Hermitian structure of Quantum Mechanics [26, 27, 72–74, 81, 97–101, 122].

Theorem 1.31. *Given a point $\psi \in M_Q$, let the maps $g_\psi, \omega_\psi : T_\psi M_Q \times T_\psi M_Q \to \mathbb{R}$ be defined as*

$$g_\psi(\phi,\chi) := \langle\phi|\chi\rangle + \langle\chi|\phi\rangle = 2\operatorname{Re}\langle\phi|\chi\rangle, \quad \omega_\psi(\phi,\chi) := -\mathrm{i}\Big(\langle\phi|\chi\rangle - \langle\chi|\phi\rangle\Big) = 2\operatorname{Im}\langle\phi|\chi\rangle, \quad \forall \phi,\chi \in T_\psi M_Q. \tag{1.63}$$

The sections $g : \psi \mapsto (\psi, g_\psi)$ and $\omega : \psi \mapsto (\psi, \omega_\psi)$ of the twice-covariant tensor bundle of M_Q are differentiable tensor fields. Furthermore, g is a metric tensor field and ω is a symplectic form.

Proof. Differentiability of the tensor fields g and ω is proved by computing their coordinate expressions. By hypothesis, the chosen basis $E = \{|e_1\rangle,\dots,|e_n\rangle\}$ for $\mathcal{H}$ is orthonormal, with elements satisfying $\langle e_j|e_k\rangle = \delta_{jk}$, for $j,k = 1,2,\dots,n$. By taking into account (1.52), the coordinate expressions g and ω are determined by the real and imaginary part of the inner products of vectors $|e_j\rangle$ and $\mathrm{i}|e_j\rangle$:

$$\operatorname{Re}\langle e_j|e_k\rangle = \operatorname{Re}\langle \mathrm{i}\, e_j|\mathrm{i}\, e_k\rangle = \delta_{jk}, \quad \operatorname{Im}\langle e_j|\mathrm{i}\, e_k\rangle = -\operatorname{Im}\langle \mathrm{i}\, e_j|e_k\rangle = \delta_{jk}, \quad j,k = 1,2,\dots,n, \tag{1.64}$$

Thus the coordinate expressions for g and ω are

$$g = \sum_{j=1}^{n} (\mathrm{d}q_j \otimes \mathrm{d}q_j + \mathrm{d}p_j \otimes \mathrm{d}p_j), \quad \omega = \sum_{j=1}^{n} \mathrm{d}q_j \wedge \mathrm{d}p_j. \tag{1.65}$$

Both tensor fields are therefore differentiable and of constant rank. Non-degeneracy of the tensor fields follows directly from the non-degeneracy of the Hermitian product in $\mathcal{H}$, stated in (1.3). The tensor g is clearly symmetric, so it is a metric tensor on M_Q. Similarly, ω is skew-symmetric, and also closed, as it has constant coefficients, hence symplectic. □

The tensor fields g and ω are related by means of the complex structure J. They reflect on the (real) differentiable manifold M_Q the complex linear structure inherited from the complex Hilbert space $\mathcal{H}$. A differentiable manifold that has such an structure is called a Kähler manifold. Further information on Kähler manifold can be found in works dealing with the topic of complex manifold [30, 37, 212].

Definition 1.32. *An almost Kähler manifold (M_Q, g, ω, J) is a 4-tuple where M is a differentiable manifold and g, ω and J are tensor fields on M such that g is a metric, ω is a symplectic form, J is an almost complex structure, and the following compatibility relation is satisfied:*

$$\omega(X,Y) = g(J(X),Y), \quad \forall X,Y \in \mathfrak{X}(M), \tag{1.66}$$

In addition, if J is integrable, hence a complex structure, then (M_Q, g, ω, J) is called a Kähler manifold.

Proposition 1.33. *The 4-tuple (M_Q, g, ω, J), with M_Q the differentiable manifold associated to a Hilbert space and tensor fields g, ω and J defined in Proposition 1.26 and Theorem 1.31, is a Kähler manifold.*

Proof. To prove that ω is indeed the Kähler form of the manifold, relation (1.66) has to be satisfied. By Proposition 1.26 and Theorem 1.31:

$$g_\psi(J_\psi(\phi), \chi) = \langle J_\psi(\phi)|\chi\rangle + \langle \chi|J_\psi(\phi)\rangle = -\mathrm{i}\langle\phi|\chi\rangle + \mathrm{i}\langle\chi|\phi\rangle = \omega_\psi(\phi, \chi),$$

for any $\phi, \chi \in T_\psi M_Q$ and any $\psi \in M_Q$. □

In the following, the Kähler manifold (M_Q, g, ω, J) will be referred to simply as M_Q. The Kähler structure reproduces the properties of $\mathcal{H}$. The next proposition relates orthogonality of vectors in $\mathcal{H}$, defined with respect to the Hermitian product, and the action of tensor fields g and ω.

Proposition 1.34. *Two tangent vectors $v, w \in T_\psi M_Q$ at $\psi \in M_Q$ satisfy $g_\psi(v, w) = \omega_\psi(v, w) = 0$ if and only if their corresponding vectors $|v\rangle, |w\rangle \in \mathcal{H}$ are orthogonal with respect to the Hermitian product, i.e. $\langle v|w\rangle = 0$.*

Proof. By definition,

$$g_\psi(v, w) = \mathrm{Re}\,\langle v|w\rangle, \quad \omega_\psi(v, w) = \mathrm{Im}\,\langle v|w\rangle \;\Leftrightarrow \langle v|w\rangle = g_\psi(v, w) + \mathrm{i}\;\omega_\psi(v, w) \tag{1.67}$$

Hence $\langle v|w\rangle = 0$ if and only if $g_\psi(v, w) = \omega_\psi(v, w) = 0$. □

1.2.3 Hamiltonian and gradient vector fields

Once that the Kähler structure of M_Q is defined, let us consider the maps $\widehat{\omega}, \widehat{g} : \mathfrak{X}(M_Q) \to \bigwedge^1(M_Q)$, defined as

$$\widehat{\omega}(X) := \iota_X(\omega), \quad \widehat{g}(X) := \iota_X(g), \quad \forall X \in \mathfrak{X}(M_Q). \tag{1.68}$$

Relation (1.66) can be given a simple form in terms of these maps.

$$\widehat{g} \circ J = \widehat{\omega} \;\Leftrightarrow \widehat{g} = -\widehat{\omega} \circ J. \tag{1.69}$$

Due to the non-degeneracy of both tensor fields ω and g, the new maps $\widehat{\omega}, \widehat{g}$ are invertible. The inverse maps $\widehat{\omega}^{-1}, \widehat{g}^{-1} : \bigwedge^1(M_Q) \to \mathfrak{X}(M_Q)$ are relevant in the description of vector fields.

Definition 1.35. *The Hamiltonian vector field and the gradient vector field of a function $f \in C^\infty(M_Q)$ are respectively the vector fields $X_f, Y_f \in \mathfrak{X}(M_Q)$ defined as*

$$X_f := \widehat{\omega}^{-1}(\mathrm{d}f), \quad Y_f := \widehat{g}^{-1}(\mathrm{d}f). \tag{1.70}$$

Proposition 1.36. *The gradient and vector fields of a given function $f \in C^\infty(M_Q)$ are related by the complex structure J in the following way:*

$$J(X_f) = Y_f. \tag{1.71}$$

Proof. By relation (1.69), the inverse maps $\widehat{\omega}^{-1}, \widehat{g}^{-1}$ satisfy the relation

$$\widehat{g}^{-1} = -J^{-1} \circ \widehat{\omega}^{-1} = J \circ \widehat{\omega}^{-1},$$

as $J^{-1} = -J$ by (1.53). This relation can be evaluated on an exact 1-form $\mathrm{d}f$ in order to obtain the result. □

Proposition 1.37. *The coordinate expressions of the Hamiltonian and gradient vector fields associated to the coordinate functions previously defined are, respectively,*

$$X_{q_j} = -\frac{\partial}{\partial p_j}, \quad X_{p_j} = \frac{\partial}{\partial q_j}, \quad Y_{q_j} = \frac{\partial}{\partial q_j}, \quad Y_{p_j} = \frac{\partial}{\partial p_j}, \quad j = 1, 2, \ldots, n. \tag{1.72}$$

Proof. These expressions are obtained by solving the equations:

$$\widehat{\omega}(X_{q_j}) = \mathrm{d}q_j, \quad \widehat{\omega}(X_{p_j}) = \mathrm{d}p_j, \quad \widehat{g}(Y_{q_j}) = \mathrm{d}q_j, \quad \widehat{g}(Y_{p_j}) = \mathrm{d}p_j. \tag{1.73}$$

Solutions are found by assuming generic expressions for the vector fields. For example, consider the following expression for the vector field X_{q_j}:

$$X_{q_j} = \sum_{k=1}^{n} \left(a_k \frac{\partial}{\partial q_k} + b_k \frac{\partial}{\partial p_k} \right), \quad a_1, \ldots, a_n, b_1, \ldots, b_n \in \mathbb{R}.$$

Due to the coordinate expression of ω give in (1.65), the action of the map $\hat{\omega}$ on this vector field yields

$$\widehat{\omega}(X_{q_j}) = \sum_{k=1}^{n} \left(a_k \mathrm{d}p_k - b_k \mathrm{d}q_k \right).$$

These expressions can be substituted in (1.73) in order to obtain the coordinate form of X_{q_j}. The remaining coordinate expressions are computed in a similar way. □

The correspondence between functions and Hamiltonian vector fields is unique up to constant functions. Following the same procedure as in symplectic geometry, it is thus possible to use these relations to define two products on the algebra of functions on the manifold, determined respectively by ω and g.

Proposition 1.38. *There exist two inner composition laws on the algebra of functions $C^\infty(M_Q)$ defined by the tensor fields g and ω:*

$$\{f, f'\} := \omega(X_f, X_{f'}), \quad (f, f') := g(Y_f, Y_{f'}), \quad \forall f, f' \in C^\infty(M_Q). \tag{1.74}$$

Both are $\mathbb{R}$-linear in their two arguments. The product $(\cdot,\cdot)$ is symmetric, while $\{\cdot,\cdot\}$ is skew-symmetric. They satisfy the relations

$$\{f, f'\} = X_{f'}(f) = -X_f(f'), \quad (f, f') = Y_{f'}(f) = Y_f(f'), \quad f, f' \in C^\infty(M_Q). \tag{1.75}$$

Proof. The properties of the composition laws are directly derived from (1.70). The definitions of the composition laws can be rewritten as

$$\omega(X_f, X_{f'}) = \mathrm{d}f(X_{f'}) = X_{f'}(f), \quad g(Y_f, Y_{f'}) = \mathrm{d}f(Y_{f'}) = Y_{f'}(f) \tag{1.76}$$

The proof is completed by considering the symmetry of g and the skew-symmetry of ω. □

Recall that ω is a symplectic form. This implies that $\{\cdot,\cdot\}$ is in fact a Poisson bracket, a very important tool in the field of symplectic geometry and Hamiltonian mechanics [3].

Definition 1.39. *A Poisson bracket $\{\cdot,\cdot\}$ on a differentiable manifold M is a composition law of differentiable functions such that $(C^\infty(M), \{\cdot,\cdot\})$ is a Lie algebra and, for any $f \in C^\infty(M)$, the map $g \mapsto \{f, g\}$ is a derivation of the associative algebra of functions.*

Proposition 1.40. *The composition law $\{\cdot,\cdot\}$ defined in (1.75) is a Poisson bracket on $C^\infty(M_Q)$.*

Proof. This is a direct consequence of ω being a symplectic form, hence closed, which implies that the composition law $\{\cdot,\cdot\}$ satisfies Jacobi identity [3]. □

Observe that coordinate functions for the global chart defined in (1.49) satisfy the following relations:

$$\{q_j, q_k\} = \{p_j, p_k\} = 0, \quad \{q_j, p_k\} = \delta_{jk}, \quad (q_j, q_k) = (p_j, p_k) = \delta_{jk}, \quad (q_j, p_k) = 0, \quad j, k = 1, 2, \ldots, n. \tag{1.77}$$

These expressions are computed directly from the definitions of the products (1.74) and from the coordinate expressions of g, ω and the Hamiltonian and gradient vector fields of the coordinate functions. It can be concluded that these are precisely the Darboux coordinates for the symplectic form defining the Kähler structure on M_Q.

The symmetric product and Poisson bracket presented here act in a differential way on functions, as seen in (1.75). They can be thus written in a tensorial way.

Proposition 1.41. *There exist two contravariant tensor fields G and Ω satisfying the relations*

$$\Omega(\mathrm{d}f, \mathrm{d}f') := \{f, f'\}, \quad G(\mathrm{d}f, \mathrm{d}f') := (f, f'), \quad f, f' \in C^\infty(M_Q). \tag{1.78}$$

These tensor fields are well-defined and differentiable. Let $\widehat{\Omega}, \widehat{G} : \bigwedge^1(M_Q) \to \mathfrak{X}(M_Q)$ be the maps defined by $\widehat{\Omega}(\alpha)(f) = \Omega(\alpha, \mathrm{d}f)$ and $\widehat{G}(\alpha)(f) = G(\alpha, \mathrm{d}f)$, with $\alpha \in \bigwedge^1(M_Q)$ and $f \in C^\infty(M_Q)$. These maps satisfy the relations

$$\widehat{\Omega} = -\widehat{\omega}^{-1}, \quad \widehat{G} = \widehat{g}^{-1} \tag{1.79}$$

In particular, $\widehat{\Omega}(\mathrm{d}f) = -X_f$ and $\widehat{G}(\mathrm{d}f) = Y_f$ for any differentiable function $f \in C^\infty(M_Q)$.

Proof. Due to $C^\infty(M_Q)$-linearity, tensor fields Ω and G are completely determined by its action on exact 1-forms. Furthermore, the products $\{\cdot,\cdot\}$ and $(\cdot,\cdot)$ act on a differential way on function. Thus, equation (1.78) is a good definition for the tensor fields. Regarding relation (1.79), let us compute the expression of $\widehat{\Omega}(\mathrm{d}f)$ for a differentiable function f:

$$\widehat{\Omega}(\mathrm{d}f)(f') = \{f, f'\} = -X_f(f'), \quad f, f' \in C^\infty(M_Q),$$

Thus, $\widehat{\Omega}(\mathrm{d}f) = -X_f$. A similar computation shows that $\widehat{G}(\mathrm{d}f) = Y_f$. As both $\widehat{\Omega}$ and $\widehat{G}$ are by definition $C^\infty(M_Q)$-linear maps, again it is enough to consider their action on exact 1-forms, which proves the result. □

Observe that, due to the non-degeneracy of g and ω, invertible maps $\widehat{\omega}, \widehat{g} : \mathfrak{X}(M_Q) \to \bigwedge^1(M_Q)$ transport not only elements, but also structures from the algebra of vector fields to the algebra of 1-forms. In particular, Ω and G are the result of transporting by $\widehat{\omega}$ and $\widehat{g}$ the tensor fields ω and g, respectively:

$$\Omega(\widehat{\omega}(X), \widehat{\omega}(Y)) = \omega(X, Y), \quad G(\widehat{g}(X), \widehat{g}(Y)) = g(X, Y), \quad \forall X, Y \in \mathfrak{X}. \tag{1.80}$$

By use of the compatibility condition (1.69) of the Kähler structure, it is immediate to compute that

$$\Omega(\widehat{g}(X), \widehat{g}(Y)) = \omega(X, Y), \quad G(\widehat{\omega}(X), \widehat{\omega}(Y)) = g(X, Y), \quad \forall X, Y \in \mathfrak{X}. \tag{1.81}$$

The coordinate expressions of contravariant tensor fields Ω and G in the global chart defined in (1.49) are derived from the products computed in (1.77):

$$\Omega = \sum_{j=1}^{n} \frac{\partial}{\partial q_j} \wedge \frac{\partial}{\partial p_j}, \quad G = \sum_{j=1}^{n} \left(\frac{\partial}{\partial q_j} \otimes \frac{\partial}{\partial q_j} + \frac{\partial}{\partial p_j} \otimes \frac{\partial}{\partial p_j} \right), \tag{1.82}$$

It is now a simple task to compute the commutators of gradient and Hamiltonian vector fields. Their values can be written in terms of the Poisson and symmetric products of functions.

Proposition 1.42. *Hamiltonian and gradient vector fields satisfy the following commutation relations:*

$$[X_f, X_h] = -X_{\{f,h\}}, \quad [X_f, Y_h] = -Y_{\{f,h\}}, \quad [Y_f, Y_h] = X_{\{f,h\}} \quad f, h \in C^\infty(M_Q). \tag{1.83}$$

The commutator of vector fields provides the set $\mathfrak{X}_H(M_Q)$ of Hamiltonian vector fields with a Lie algebra structure, isomorphic to $(C^\infty(M_Q), \{\cdot,\cdot\})$. The set spanned by Hamiltonian and gradient vector fields is also a real Lie algebra, isomorphic to the complexification of $(\mathfrak{X}_H(M_Q), [\cdot,\cdot])$.

Proof. The first relation is a standard result in symplectic geometry [3, Corollary 3.3.18]. For the second one, recall that Hamiltonian vector fields are Killing with respect to the metric g. Therefore, by using the properties of the Lie derivative, the following relation holds:

$$\begin{aligned}
&(\mathcal{L}_{X_f} g)(Z, Z') = X_f(g(Z, Z')) - g([X_f, Z], Z') - g(Z, [X_f, Z']) = 0 \Rightarrow \\
&\quad \Rightarrow X_f(g(Z, Z')) = g([X_f, Z], Z') + g(Z, [X_f, Z']), \qquad \forall Z, Z' \in \mathfrak{X}(M_Q), \quad \forall f \in C^\infty(M_Q).
\end{aligned}$$

To find the value of the commutator $[X_f, Y_h]$, compute its image by $\widehat{g}$:

$$\widehat{g}([X_f, Y_h])(Z) = g([X_f, Y_h], Z) = X_f(g(Y_h, Z)) - g(Y_h, [X_f, Z]) = X_f(Z(h)) - [X_f, Z](h) = \\ = Z(X_f, h) = Z(\{h, f\}), \quad \forall Z \in \mathfrak{X}(M_Q), \quad \forall f, h \in C^\infty(M_Q),$$

where (1.74) and (1.75) have been taken into account. Therefore, the relation

$$\widehat{g}([X_f, Y_h]) = -\mathrm{d}(\{f, h\}), \quad \forall f, h \in C^\infty(M_Q),$$

holds, which proves the result. The last relation is proved in a similar way. □

Up to this point, multiple geometric objects have been defined on the quantum manifold M_Q. There exists a symplectic structure that resembles the geometric description of Classical Mechanics [3]. The existence of a Poisson bracket and Hamiltonian vector fields have clear analogies with classical systems. The quantum case, however, is much richer. There exist additional structures, namely the metric g and the almost complex structure J, that introduce differences between classical and quantum manifolds. The deep implications of these new structures are some of the topics of study of this dissertation. After the introduction of observables and dynamics on the manifold, more analogies and differences between classical and quantum systems can be observed. It is possible to compare both theories and to analyse in detail the implications of the different geometric structures appearing in the quantum manifold.

1.2.4 Geometric representation of observables

The next step in the development of the formulation is to find a suitable characterization of the observables of the quantum system in terms of tensor fields on the manifold. The Ehrenfest picture describe the proper way to represent observables in terms of expectation values [101]. This approach was first proposed by Ehrenfest [118] and later developed by Koopman [180] and von Neumann [266], who proved that both Classical and Quantum Mechanics can be described only in terms of expectation values. The Ehrenfest picture of Quantum Mechanics offers an alternative approach to both Schrödinger and Heisenberg pictures, and it is particularly well suited for a geometric treatment.

Following the spirit of the Ehrenfest picture, observables are represented by the following functions defined on the manifold M_Q, related to their expectation values (1.22). Recall from Section 1.1.3 that the set $\mathcal{O}$ of observables on a finite-dimensional quantum system is the Lie-Jordan algebra of Hermitian operators on its associated Hilbert space $\mathcal{H}$, i.e. $\mathcal{O} = \mathrm{Herm}(\mathcal{H})$.

Definition 1.43. *Given a Hermitian operator $A \in \mathcal{O}$, let us denote by f_A the real function on the manifold M_Q defined as*

$$f_A(\psi) := \langle \psi | A | \psi \rangle, \quad \psi \in M_Q. \tag{1.84}$$

Theorem 1.44. *The map $\varphi_{\mathcal{O}} : A \in \mathcal{O} \mapsto f_A \in C^\infty(M_Q)$ that associates to each Hermitian operator on $\mathcal{H}$ a function on M_Q is injective. It is therefore invertible on the image set $\mathcal{F}_{\mathcal{O}}(M_Q) := \varphi_{\mathcal{O}}(\mathcal{O})$.*

Proof. In order to prove that the map is injective, consider two observables $A, A' \in \mathcal{O}$ such that $f_A = f_{A'}$. By linearity of the Hermitian product in $\mathcal{H}$:

$$f_A(\psi) = f_{A'}(\psi) \Rightarrow \langle \psi | A | \psi \rangle = \langle \psi | A' | \psi \rangle \Rightarrow \langle \psi | (A - A') | \psi \rangle = 0. \tag{1.85}$$

This implies that $A - A' = 0$, hence $A = A'$ and the applications is injective. □

This theorem proves that the relation between Hermitian operators and functions of the type of (1.84) is in fact one-to-one. Therefore, the description of an observable A in terms of a smooth function f_A is completely analogous to its realisation in terms of operators on a Hilbert space.

In order to simplify the notation, given an observable $A \in \mathcal{O}$, let us write X_A and Y_A instead of X_{f_A} and Y_{f_A} for the Hamiltonian and gradient vector fields, respectively, of the function f_A.

Lemma 1.45. *For any $A \in \mathcal{O}$, the associated Hamiltonian and gradient vector fields at a given point $\psi \in M_Q$ take the values*

$$|(X_A)_\psi\rangle = -\mathrm{i}A|\psi\rangle, \quad |(Y_A)_\psi\rangle = A|\psi\rangle. \tag{1.86}$$

Proof. Let $Z \in \mathfrak{X}(M_Q)$ be a vector field and denote by $\gamma_Z(\psi_0, t)$ its integral curve starting at $\psi_0 \in M_Q$. When translated to the Hilbert space $\mathcal{H}$, for small values of t the integral curve takes the form

$$|\gamma_Z(\psi_0, t)\rangle = |\psi_0\rangle + t|Z_{\psi_0}\rangle + \vartheta(t^2). \tag{1.87}$$

The action of Z on the function f_A associated to an observable $A \in \mathcal{O}$ can be computed directly:

$$Z(f_A)(\psi) = \frac{d}{dt} f_A(\gamma_Z(\psi, t))\Big|_{t=0} = 2\,\mathrm{Re}\,\langle Z_\psi|A|\psi\rangle, \quad \psi \in M_Q. \tag{1.88}$$

On the other hand, by definition of the gradient vector field Y_A, the following relation holds:

$$Z(f_A)(\psi) = g(Z, Y_A)(\psi) = 2\,\mathrm{Re}\,\langle Z_\psi|(Y_A)_\psi\rangle, \quad \psi \in M_Q. \tag{1.89}$$

These relations hold for any vector field Z. In particular, by taking different vector fields such that they span the tangent space to the point ψ, the relation $|(Y_A)_\psi\rangle = A|\psi\rangle$ is obtained. Finally, by (1.53) and (1.71), the relation $X_A = -J(Y_A)$ gives the value of the Hamiltonian vector field X_A at each point. □

The algebraic structure of the set of Hermitian operators is recovered in terms of the Poisson bracket and symmetric product of functions on the manifold already presented.

Proposition 1.46. *The Poisson bracket and symmetric product of functions associated to observables are*

$$\{f_A, f_B\} = f_{[\![A,B]\!]}, \quad (f_A, f_B) = f_{A \odot B}, \quad A, B \in \mathcal{O}. \tag{1.90}$$

Proof. By direct computation, and with expressions (1.20), (1.63) and (1.86), the following expression is obtained:

$$\{f_A, f_B\}(\psi) = \omega(X_A, X_B)(\psi) = -\mathrm{i}\Big(\langle\psi|AB|\psi\rangle - \langle\psi|BA|\psi\rangle\Big) = \langle\psi|[\![A, B]\!]|\psi\rangle = f_{[\![A,B]\!]}(\psi), \quad \forall \psi \in M_Q.$$

An analogous computation gives the value of the symmetric product of functions. □

Corollary 1.47. *Hamiltonian vector fields of functions associated to Hermitian operators close a algebra isomorphic to $\mathfrak{u}(\mathcal{H})$, the Lie algebra of skew-symmetric $\mathbb{C}$-linear operators on $\mathcal{H}$. Similarly, the Lie algebra of Hamiltonian and gradient vector fields of functions associated to Hermitian operators is isomorphic to $\mathfrak{gl}(\mathcal{H})$, the Lie algebra of $\mathbb{C}$-linear operators on $\mathcal{H}$*

Proof. By Proposition 1.42, the following commutation relations hold

$$[X_A, X_B] = -X_{[\![A,B]\!]}, \quad [X_A, Y_B] = -Y_{[\![A,B]\!]}, \quad [Y_A, Y_B] = X_{[\![A,B]\!]}, \quad \forall A, B \in \mathcal{O}. \tag{1.91}$$

Together with Lemma 1.45, this allows to identify the obtained Lie algebras. □

Some interesting results can be derived also from (1.91). Due to their definitions, the dilation vector field Δ and the phase-change vector field Γ are easily related with the gradient and Hamiltonian vector fields of the identity observable $I \in \mathcal{O}$, respectively:

$$\Delta = Y_I, \quad \Gamma = -X_I. \tag{1.92}$$

Also, it is immediate in this description to determine the vector field that describes the evolution of isolated quantum systems, governed by the Schrödinger equation. This result gives a particularly interesting relation between Quantum Mechanics and Classical Hamiltonian Mechanics.

Theorem 1.48. *Consider the Schrödinger equation, given in natural units (with $\hbar = 1$) by*

$$\mathrm{i}\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle, \quad H \in \mathcal{O}. \tag{1.93}$$

The solutions to the Schrödinger equation are the image by $\nu : M_Q \to \mathcal{H}$ of the integral curves of the Hamiltonian vector field X_H associated to the Hamiltonian operator H of the quantum system.

Proof. Consider the Hamiltonian vector field X_H associated to $H \in \mathcal{O}$, the Hamiltonian observable of the system. A curve $\psi : I \subset \mathbb{R} \to M_Q$ is an integral curve of X_H if its tangent point at each point $\psi(t_0)$ is $(X_H)_{\psi(t_0)}$. Curves and tangent vectors can be mapped onto $\mathcal{H}$. The result is a curve $|\psi(t)\rangle$ on $\mathcal{H}$ whose derivative at each point is

$$\frac{d}{dt}|\psi(t)\rangle\Big|_{t_0} = \big|(X_H)_{\psi(t_0)}\big\rangle = -\mathrm{i}H|\psi(t_0)\rangle, \tag{1.94}$$

where (1.86) has been used. Thus, $|\psi(t)\rangle$ is a solution of the Schrödinger equation (1.93). □

Therefore, unitary evolution of quantum systems is, from a geometric point of view, a Hamiltonian evolution with respect to a Hamiltonian dynamical system. All the results developed in the study of symplectic geometry can thus be applied here. For example, the evolution of coordinates in M_Q is governed by Hamilton equations:

$$\frac{\mathrm{d}q_j}{\mathrm{d}t} = \frac{\partial f_H}{\partial p_j}, \quad \frac{\mathrm{d}p_j}{\mathrm{d}t} = -\frac{\partial f_H}{\partial q_j}. \tag{1.95}$$

The additional structures in M_Q, namely the complex structure J and the metric g, are useful in order to obtain additional interesting results. This is important in the study of quantum Lie systems, as seen in Chapter 2.

1.2.5 Natural units in Quantum Mechanics

As mentioned above, the geometric formalism presented here reproduces the equations of Quantum Mechanics when expressed in natural units. This system of units is based on the values of physical constants, such as the reduced Planck constant $\hbar$, the electron charge e and mass m_e, or the vacuum permittivity ϵ_0. For simplicity, they are given the following values:

$$\hbar = 1, \quad e = 1, \quad m_e = 1, \quad \epsilon_0 = \frac{1}{4\pi}. \tag{1.96}$$

Mathematical expressions of the theory are thus given in a simple way. However, in the spirit of comparison with a classical theory, it is relevant to understand the role of this constants, in particular the reduced Planck constant $\hbar$, in the geometric description of Quantum Mechanics.

Recall that the Schrödinger equation has the expression

$$\mathrm{i}\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle, \quad H \in \mathcal{O}. \tag{1.97}$$

The factor $\hbar$ has to be included in the definitions of the structures in such a way that the solution to this equation are the integral curves of the Hamiltonian vector field associated to H. Hence, instead of (1.86) the desired expressions for Hamiltonian and gradient vector fields are

$$|(X_A^\hbar)_\psi\rangle = -\mathrm{i}\hbar^{-1}A|\psi\rangle, \quad |(Y_A^\hbar)_\psi\rangle = \hbar^{-1}A|\psi\rangle. \tag{1.98}$$

Due to the definition of Hamiltonian and gradient vector fields, (1.70), these expresions imply that the reduced Planck constant appears in the definition of contravariant tensor fields, presented in (1.63). Thus, consider the following expressions:

$$g_\psi^\hbar(\phi,\chi) = 2\hbar\,\mathrm{Re}\,\langle\phi|\chi\rangle, \quad \omega_\psi^\hbar(\phi,\chi) = 2\hbar\,\mathrm{Im}\,\langle\phi|\chi\rangle, \quad \phi,\chi \in T_\psi M_Q, \quad \psi \in M_Q. \tag{1.99}$$

All the results computed above would be modified accordingly to these new definitions. In particular, Hamiltonian and gradient vector fields with respect to $g^\hbar$ and $\omega^\hbar$ are given by (1.98). The Poisson bracket and symmetric product of two functions associated to operators are

$$\{f_A, f_B\}^\hbar := \omega^\hbar(X_A^\hbar, X_B^\hbar) = \hbar^{-1} f_{[\![A,B]\!]}, \quad (f_A, f_B)^\hbar := g^\hbar(X_A^\hbar, X_B^\hbar) = \hbar^{-1} f_{A\odot B}, \quad A, B \in \mathcal{O}. \tag{1.100}$$

As expected, the reduced Planck constant appears indeed in this geometric formalism. Therefore, the quantum properties represented by this constant are always present in the geometric formulation of Quantum Mechanics. For the purpose of this dissertation, however, it is safe to simplify the computation by making use of natural units.

1.3 The manifold of pure states

The probabilistic interpretation of Quantum Mechanics requires to deal with an equivalence relation between elements in the Hilbert space of the system, as explained in Section 1.1.6. It can also be described in a geometric setting, in terms of a Lie group action on the quantum manifold. This action is free and transitive on $M_Q - \{0\}$, with 0 the point in M_Q representing the zero vector in $\mathcal{H}$. It is thus possible to define a projection to a quotient manifold, whose points are in a one-to-one correspondence with the pure states of the quantum system.

The behaviour of geometric structures under this projection has to be carefully analysed. Particular attention will be paid to the Kähler structure on M_Q. By Proposition 1.38, tensor fields g and ω define algebraic structures on smooth functions. Thus, the projection of the Kähler structure is in direct connection with the reduction of algebras of functions. The reduction procedure has been studied by many authors, among them Marsden and Ratiu [196], Dubrovin, Giordano, Marmo and Simoni [115], and Falceto, Ferro, Ibort and Marmo [127–129].

The present section presents a first approach to the reduction of algebras by summarising some of the results in [127]. After a description of the foliation in terms of the action of the group $\mathbb{C}_0 = \mathbb{R}_* \times U(1)$, a reduction of the Kähler structure is proposed.

1.3.1 Reductions of function algebras

In his work [127], Falceto, Ferro, Ibort and Marmo presented the reduction procedure of Lie-Jordan-Banach algebras in some particular cases. The reduction procedure can be formulated in a generic language that emphasises its main features.

Let M be a differentiable manifold and $(C^\infty(M), *)$ an algebra of smooth functions on the manifold. Consider a Lie group action $\phi : G \times M \to M$, and let $\mathfrak{X}_G \subset \mathfrak{X}(M)$ be the set of fundamental vector fields of this action. If the action is smooth, free and proper, then the orbit set M/G is a differentiable manifold [187, p. 544]. Let $\pi_G : M \to M/G$ denote the projection. Then, the image of the set $C^\infty(M/G)$ of smooth functions on the orbit set by the pull-back of π_G is precisely the set $\mathfrak{G}$ of invariant functions under the Lie group action:

$$(\pi_G)^*(C^\infty(M/G)) = \mathfrak{G} := \{f \in C^\infty(M) \mid X(f) = 0,\ \forall X \in \mathfrak{X}_G\}. \tag{1.101}$$

As a consequence, an algebraic structure on $\mathfrak{G}$ immediately determines an algebra of smooth functions on the orbit set.

Theorem 1.49. [127] *Consider an algebra $(C^\infty(M), *)$ of smooth functions on the manifold M. If the set $\mathfrak{G}$ of invariant functions with respect to the Lie group action $\phi : G \times M \to M$ is a subalgebra, then the restriction of the composition law $*$ to $\mathfrak{G}$ defines an algebraic structure on the set of smooth functions on the orbit set M/G.*

The Lie group action induces transformations of smooth functions on the manifold. For any $a \in G$, let $\phi_a : M \to M$ be the smooth map defined by $\phi_a(x) = \phi(a, x)$. Then, the set of invariant functions is a

subalgebra of $(C^\infty(M), *)$ if and only if $\phi_a^* : C^\infty(M) \to C^\infty(M)$ is an algebra homomorphism for every $a \in G$.:

$$\phi_a^*(f * f') = \phi_a^*(f) * \phi_a^*(f'), \quad \forall f, f' \in C^\infty(M). \tag{1.102}$$

The property presented in Theorem 1.49 can be considered in a tensorial way. Assume that the composition law $*$ acts on a differentiable way on functions, and thus there exists a contravariant $(2,0)$-tensor field Ξ on the manifold such that

$$\Xi(\mathrm{d}f, \mathrm{d}f') = f * f', \quad \forall f, f' \in C^\infty(M). \tag{1.103}$$

Consider the action of the group G on M and the projection $\pi_G : M \to M/G$. The condition given in Theorem 1.49 is equivalent to the assumption that Ξ is π-projectable. Thus, the new composition law of smooth functions on M_G is determined by a tensor field Ξ_G on M/G which is π_G-related with Ξ.

In a dynamical system, the reduction procedure typically is considered when symmetries and constraints are considered. In this way, the new tensor field Ξ_G describes dynamics on the reduced systems. In some cases, however, technical difficulties may arise with this description. The orbit set M/G may lack many properties that were present in the ambient manifold M, such as linearity or global coordinate charts. For this reason, it may be useful to embed in an appropriate way the reduced system into the ambient manifold M. Take the tensor field Ξ_G describing the reduced dynamics on M/G, and the set of its π_g-related tensor fields on M, among them being the initial tensor field Ξ. It is possible however to find another element $\widetilde{\Xi}_G$ in this set with better properties. Namely, $\widetilde{\Xi}_G$ should be a tensor field generating a distribution on M which, at each point, is orthogonal to the fibres of the foliation by $\mathfrak{X}_G$. Let us state this with detail.

Consider a metric manifold (M, g), a free and proper action of a Lie group G and the projection $\pi_G : M \to M/G$ onto the orbits set. Any contravariant $(2,0)$-tensor field Ξ on the manifold M defines a map $\widehat{\Xi} : \bigwedge^1(M) \to \mathfrak{X}(M)$ by

$$\beta\left(\widehat{\Xi}(\alpha)\right) = \Xi(\alpha, \beta), \quad \forall \alpha, \beta \in \bigwedge^1(M). \tag{1.104}$$

In particular, consider the action of $\widehat{\Xi}$ on the differentials of invariant functions $f \in \mathfrak{G}$. At each point $\psi \in M$, the map $\widehat{\Xi}$ generates a subspace of $T_\psi M$ by

$$D_\psi^{\mathfrak{G}} = \mathrm{span}\left\{\left(\widehat{\Xi}(\mathrm{d}f)\right)_\psi, \ f \in \mathfrak{G}\right\} \subset T_\psi M. \tag{1.105}$$

In general, the image by $\widehat{\Xi}$ of arbitrary 1-forms is not in this subset of the tangent space at ψ. It is however possible to decompose in a unique way any tangent vector $v \in T_\psi M$ as

$$v = v^{\mathfrak{G}} + v^\perp, \quad v^{\mathfrak{G}} \in D_\psi^{\mathfrak{G}}, \quad v^\perp \in \left(D_\psi^{\mathfrak{G}}\right)^\perp. \tag{1.106}$$

The reduction procedure is done in terms of invariant functions with respect to the group action. Thus, if Ξ is π_G-related with a reduced tensor field Ξ_G on M/G, it is natural to choose instead a tensor field $\widetilde{\Xi}_G$ on M whose associated generalised distribution of tangent vectors is given by (1.105). As decomposition (1.106) is unique, it is immediate to obtain $\widetilde{\Xi}_G$ by subtracting the orthogonal components of the vector fields obtained by $\widehat{\Xi}$. A practical example will be offered later in the context of the analysis of quantum systems.

1.3.2 Foliation of the quantum manifold

Recall the equivalence relation presented in Definition 1.20. It can be described as an action of the multiplicative group $\mathbb{C}_0 := \mathbb{C} - \{0\}$ on $\mathcal{H}$ by $|\psi\rangle \mapsto c|\psi\rangle$, with $c \in \mathbb{C}_0$. This is a transitive and free action. The equivalence relation is defined by the group action, the orbits of the action being the equivalence classes.

Due to the bijection $\nu : \mathcal{H} \to M_Q$, it is possible to consider the group action of $\mathbb{C}_0$ on M_Q. If the group is written as a direct product $\mathbb{C}_0 = \mathbb{R}_+ \times U(1)$, then it is immediate to describe this action as

$$r : \begin{array}{ccc} (\mathbb{R}_+ \times U(1)) \times M_Q & \to & M_Q \\ ((\rho, e^{\mathrm{i}\alpha}), \psi) & \mapsto & \psi' \end{array}, \qquad |\psi'\rangle = \rho\, e^{\mathrm{i}\alpha}|\psi\rangle. \tag{1.107}$$

Theorem 1.50. *The fundamental vector fields of the action $r : (\mathbb{R}_+ \times U(1)) \times M_Q \to M_Q$ are the dilation Δ and phase-change Γ vector fields. They define a regular foliation $\mathcal{F}_{\Delta,\Gamma}$ on the open manifold $M_{Q,0} := M_Q - \{0\}$, with $0 \in M_Q$ the image by ν of the zero-vector in $\mathcal{H}$.*

Proof. By (1.92), the dilation and phase-change vector fields are respectively related with observables I and $\mathrm{i}I$. It is thus immediate to deduce that they are the generators of the multiplication by real numbers and the change in phase on $\mathcal{H}$. In fact, if $\Phi^\Delta_t, \Phi^\Gamma_t : M_Q \to M_Q$, with $t \in \mathbb{R}$, are their associated flows, then

$$|\Phi^\Delta_t(\psi)\rangle = e^t|\psi\rangle, \quad |\Phi^\Gamma_t(\psi)\rangle = e^{\mathrm{i}t}|\psi\rangle, \quad \psi \in M_Q, \quad t \in \mathbb{R}. \tag{1.108}$$

Thus, these vector fields generate the group action of $\mathbb{C}_0 = \mathbb{R}_+ \times U(1)$ on M_Q. As $\mathbb{C}_0$ is Abelian, see (1.91) and (1.92), the fundamental vector fields Δ and Γ of the group action commute. As they are non-zero everywhere except on $0 \in M_Q$, by Frobenius theorem they generate a regular foliation $\mathcal{F}_{\Delta,\Gamma}$ on $M_{Q,0}$. □

Observe that, as $M_{Q,0}$ is an open submanifold of M_Q, it is immediate to restrict any geometric object on M_Q to $M_{Q,0}$. From now onwards, this restriction is implicitly assumed, thus simplifying the notation.

Pure states of the quantum system are identified with points in the set $\mathcal{P}$ of leaves of the foliation $\mathcal{F}_{\Delta,\Gamma}$. This set $\mathcal{P}$ can be endowed with a differentiable structure, as it is the projective Hilbert space of $\mathcal{H}$. See the textbook by Nakahara for a complete treatment of projective spaces [212].

The foliation defines a projection $\pi : M_{Q,0} \to \mathcal{P}$ onto the set of leaves. The notation from equivalence relations can be kept, thus denoting by $[\psi] := \pi(\psi)$ the elements in $\mathcal{P}$. Due to the commutativity of Δ and Γ, their respective flows commute. Thus, it is possible to carry out the projection $\pi : M_{Q,0} \to \mathcal{P}$ in two steps and in any order. This motivates the following definitions.

Definition 1.51. *Let $\mathcal{F}_\Gamma$ and $\mathcal{F}_\Delta$ denote respectively the regular foliations of $M_{Q,0}$ by Γ and Δ. The set of leaves of $\mathcal{F}_\Gamma$ will be denoted by $\mathcal{R}$, being $\pi_{M\mathcal{R}} : M_{Q,0} \to \mathcal{R}$ the corresponding projection. Similarly, the set of leaves of $\mathcal{F}_\Delta$ will be denoted by $\mathcal{Q}$, being $\pi_{M\mathcal{Q}} : M_{Q,0} \to \mathcal{Q}$ the corresponding projection.*

Foliations of a manifold define equivalence relations. Two elements in $M_{Q,0}$ are said to be Γ-equivalent if the belong to the same leaf of $\mathcal{F}_\Gamma$, and Δ-equivalent if the belong to the same leaf of $\mathcal{F}_\Delta$. Thus, both $\mathcal{R}$ and $\mathcal{Q}$ are sets of equivalent classes. For these reason, the usual notation for equivalence classes will be use. For every $\psi \in M_{Q,0}$, the corresponding images by $\pi_\mathcal{R}$ and $\pi_\mathcal{Q}$ will be denoted as $[\psi]_\mathcal{R} \in \mathcal{R}$ and $[\psi]_\mathcal{Q} \in \mathcal{Q}$. Observe also that $\mathcal{R}$ and $\mathcal{Q}$ are differentiable manifolds.

Proposition 1.52. *The differentiable manifold $\mathcal{Q}$ is isomorphic to the unit sphere $S^{2n-1} \subset \mathbb{R}^{2n}$, where n denotes the complex dimension of the initial Hilbert space.*

Proof. The manifold $M_{Q,0}$ is a $2n$-dimensional differentiable manifold with a global chart $(M_{Q,0}, \phi_E)$ described in (1.49). Elements of $\mathcal{Q}$ are the orbits of Δ. Because of the expression (1.108) of the flow of Δ, it is possible to consider the inclusion $\iota_\mathcal{Q} : \mathcal{Q} \to M_Q$ that associates to each orbit the only point in it with unit norm. As seen in the previous chapter, the norm in M_Q is equivalent to the canonical norm in $\mathbb{R}^{2n}$. Thus, the set $\iota_\mathcal{Q}(\mathcal{Q})$ is mapped onto the points of $\mathbb{R}^{2n}$ with unit norm, hence $(\phi_E \circ \iota_\mathcal{Q})(\mathcal{Q}) \simeq S^{2n-1}$. □

Both $\mathcal{R}$ and $\mathcal{Q}$ are $(2n-1)$-dimensional differentiable manifold. New projections can be established in each manifold, thus completing the projection onto the manifold $\mathcal{P}$, previously defined.

Proposition 1.53. *The vector field Δ projects onto $\mathcal{R}$, defining a regular foliation. Likewise, the vector field Γ projects onto $\mathcal{Q}$, defining also a regular foliation. The diagram shown in Table 1.4 is commutative, i.e. the projections $\pi_{\mathcal{R}\mathcal{P}} : \mathcal{R} \to \mathcal{P}$ and $\pi_{\mathcal{Q}\mathcal{P}} : \mathcal{Q} \to \mathcal{P}$ satisfy that*

$$\pi_{\mathcal{R}\mathcal{P}} \circ \pi_{M\mathcal{R}} = \pi_{\mathcal{Q}\mathcal{P}} \circ \pi_{M\mathcal{Q}} = \pi. \tag{1.109}$$

Proof. The commutativity of both vector fields makes possible to project Δ on $\mathcal{R}$, and also Γ onto $\mathcal{Q}$. As Δ and Γ are non-zero at every point of $M_{Q,0}$, their respective projections to $\mathcal{R}$ and $\mathcal{Q}$ define regular foliations. The commutativity of the diagram is a straightforward consequence. □

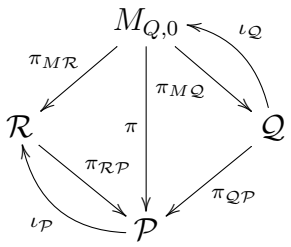


Figure 1.4: The diagram illustrates the differentiable manifolds appearing in the study of quantum systems. The projections and natural inclusions are indicated.

An additional inclusion can be defined. Namely, the projective manifold $\mathcal{P}$ can be naturally mapped into the manifold $\mathcal{R}$, as shown next.

Proposition 1.54. *There exists a differentiable embedding $\iota_{\mathcal{P}} : \mathcal{P} \to \mathcal{R}$ such that $\pi_{\mathcal{R}\mathcal{P}} \circ \iota_P = \mathrm{Id}_{\mathcal{P}}$.*

Proof. Due to the commutativity of the diagram in Table 1.4, for every element of $\mathcal{P}$ there exists an element of $\mathcal{Q}$ projecting to it under $\pi_{\mathcal{Q}\mathcal{P}}$. Let $f_{\mathcal{Q}\mathcal{R}} : \mathcal{Q} \to \mathcal{R}$ be the map defined as $f_{\mathcal{Q}\mathcal{R}} := \pi_{M\mathcal{R}} \circ \iota_{\mathcal{Q}}$. Hence, $\pi_{\mathcal{R}\mathcal{P}} \circ f_{\mathcal{Q}\mathcal{R}}(\mathcal{Q}) = \mathcal{P}$ and $\pi_{\mathcal{R}\mathcal{P}}|_{f_{\mathcal{Q}\mathcal{R}}(\mathcal{Q})} : f_{\mathcal{Q}\mathcal{R}}(\mathcal{Q}) \to \mathcal{P}$ is surjective.

It can be shown that it is also injective. Take $\psi_1, \psi_2 \in \iota_{\mathcal{Q}}(\mathcal{Q})$, which implies that $\|\psi_1\| = \|\psi_2\|$. Consider their equivalence classes $[\psi_1]_{\mathcal{R}}, [\psi_2]_{\mathcal{R}} \in \mathcal{R}$. Then, if $\pi_{\mathcal{R}\mathcal{P}}([\psi_1]_{\mathcal{R}}) = \pi_{\mathcal{R}\mathcal{P}}([\psi_2]_{\mathcal{R}})$, necessarily $|\psi_1\rangle = e^{\mathrm{i}\alpha}|\psi_2\rangle$ with $\alpha \in \mathbb{R}$. As equivalence classes in $\mathcal{R}$ are defined by the action of the $U(1)$, it is immediate that $[\psi_1]_{\mathcal{R}} = [\psi_2]_{\mathcal{R}}$. Therefore, $\pi_{\mathcal{R}\mathcal{P}}$ is a bijection when restricted to $f_{\mathcal{Q}\mathcal{R}}(\mathcal{Q})$. The inverse map, defined as $\iota_{\mathcal{P}}$, is thus a differentiable embedding. □

In Chapter 2, these manifolds will be revisited, and the properties of Lie systems determined by time-dependent Schrödinger equations will be considered on each one of the differentiable manifolds $\mathcal{R}$, $\mathcal{Q}$ and $\mathcal{P}$. For obvious reasons, they will be collectively referred to as the quantum quotient manifolds.

1.3.3 Lie derivatives of the Kähler structure

The Kähler structure on $M_{Q,0}$ cannot be projected directly onto $\mathcal{P}$. The reason is that the values of the tensor fields along the leaves of the foliation $\mathcal{F}_{\Delta,\Gamma}$ are not preserved by the Lie group action r described in (1.107). Explicit computations of the changes in the Kähler structures are presented next.

Proposition 1.55. *The Lie derivatives with respect to Δ and Γ of the tensor fields ω, g and J defining the Kähler structure are*

$$\mathcal{L}_\Delta \omega = 2\omega, \quad \mathcal{L}_\Gamma \omega = 0; \qquad \mathcal{L}_\Delta g = 2g, \quad \mathcal{L}_\Gamma g = 0; \qquad \mathcal{L}_\Delta J = \mathcal{L}_\Gamma J = 0. \tag{1.110}$$

Proof. Take an element $a = (\rho, e^{\mathrm{i}\alpha}) \in \mathbb{R} \times U(1)$ and consider the map $r_a(\psi) := r(a, \psi)$ induced by (1.107). For each $\psi \in M_{Q,0}$, the push-forward $(r_a)_{*\psi} : T_\psi M_{Q,0} \to T_{r_a(\psi)} M_{q,0}$ is defined as

$$(r_a)_{*\psi(t_0)} \left(\frac{\mathrm{d}}{\mathrm{d}t} \psi(t) \Big|_{t_0} \right) := \frac{\mathrm{d}}{\mathrm{d}t} (r_a \circ \psi)(t) \Big|_{t_0}, \tag{1.111}$$

for every smooth curve $\psi(t)$ on $M_{Q,0}$. In particular, by considering curves of the form $|\psi(t)\rangle = |\psi_0\rangle + t|v\rangle$, it is immediate to find the expression for the push forward as

$$(r_a)_{*\psi}(v) = \rho \cos\phi \, v + \rho \sin\phi \, J_{r(\psi)}(v) \;\Leftrightarrow\; |(r_a)_{*\psi}(v)\rangle = \rho e^{\mathrm{i}\phi} |v\rangle, \quad \forall \psi \in M_{Q,0} \quad \forall v \in T_\psi M_{Q,0}. \tag{1.112}$$

The pull-back by r_a of any covariant $(0,2)$-tensor τ at $r_a(\psi) \in M_{Q,0}$ is, by definition:

$$(r_a)^*_\psi(\tau)(v,v') = \tau((r_a)_{*\psi}(v),(r_a)_{*\psi}(v')), \quad \forall v,v' \in T_\psi M_{Q,0}, \quad \forall \psi \in M_{Q,0}.$$

Thus, particularising to tensor fields ω and g, (1.63) and (1.112) are enough to compute their pull-backs:

$$r_a^*(\omega) = \rho^2 \omega, \quad r_a^*(g) = \rho^2 g, \quad \forall a = (\rho, e^{\mathrm{i}\alpha}) \in \mathbb{R} \times U(1). \tag{1.113}$$

Both tensor fields are invariant under phase changes, but not under dilations. The Lie derivative with respect to Δ is computed by by considering the flow (1.108) of this vector field. Thus, replacing $\rho = e^t$ and taking the time derivative, the Lie derivatives of tensor fields ω and g are obtained.

Regarding the complex structure J, it is immediate from (1.112) to see that J commutes with r_{a*}:

$$J(r_{a*}(Z)) = \rho \cos\phi\, J(Z) - \rho \sin\phi\, Z = r_{a*}(J(Z)). \tag{1.114}$$

It is therefore equivariant under the Lie group action. □

Proposition 1.56. *The Lie derivatives with respect to Δ and Γ of the contravariant tensor fields Ω and G are*

$$\mathcal{L}_\Delta \Omega = -2\Omega, \quad \mathcal{L}_\Delta G = -2G, \quad \mathcal{L}_\Gamma \Omega = \mathcal{L}_\Gamma G = 0. \tag{1.115}$$

Proof. Let $t \in \mathcal{T}^{(0,2)}(M_Q)$ be a non-degenerate twice-covariant tensor field on M_Q. It defines a map $\widehat{t} : \mathfrak{X}(M_Q) \to \bigwedge^1(M_Q)$ by $\widehat{t}(X)(Y) = t(X,Y)$, with $X, Y \in \mathfrak{X}(M_Q)$. As t is non-degenerate, $\widehat{t}$ is an invertible map. Let $\widehat{T} : \bigwedge^1(M_Q) \to \mathfrak{X}(M_Q)$ be its inverse, $\widehat{T} = \widehat{t}^{-1}$, and $T \in \mathcal{T}^{(2,0)}(M_Q)$ be the twice-contravariant tensor field defined by $T(\alpha,\beta) = \beta(\widehat{T}(\alpha))$. Given a 1-form $\alpha \in \bigwedge^1(M_Q)$ and its image vector field $X_\alpha = \widehat{T}(\alpha)$, the following holds for any $Z \in \mathfrak{X}(M_Q)$:

$$\mathcal{L}_Z \alpha = \mathcal{L}_Z(\iota_{X_\alpha} t) = \iota_{X_\alpha}(\mathcal{L}_Z t) + \iota_{[Z,X_\alpha]} t = \iota_{X_\alpha}(\mathcal{L}_Z t) + \widehat{t}([Z,X_\alpha]) \Rightarrow \widehat{T}(\mathcal{L}_Z \alpha) = \widehat{T}(\iota_{X_\alpha}(\mathcal{L}_Z t)) + [Z,X_\alpha].$$

On the other hand,

$$[Z,X_\alpha] = \mathcal{L}_Z(X_\alpha) = \mathcal{L}_Z(\iota_\alpha T) = \iota_\alpha(\mathcal{L}_Z T) + \iota_{\mathcal{L}_Z \alpha} T = \iota_\alpha(\mathcal{L}_Z T) + \widehat{T}(\mathcal{L}_Z \alpha).$$

With both expressions, the following result is obtained:

$$\widehat{T}(\iota_{X_\alpha}(\mathcal{L}_Z t)) = -\iota_\alpha(\mathcal{L}_Z T), \quad \forall \alpha \in \textstyle\bigwedge^1(M_Q). \tag{1.116}$$

In particular, if $\mathcal{L}_Z t = \lambda\, t$, it is immediate to find that $\mathcal{L}_Z T = -\lambda T$. By taking t equal to ω and g and using (1.110), the results follow. □

As a consequence of Proposition 1.55, only the complex structure J is constant along the fibres of the foliation $\mathcal{F}_{\Delta,\Gamma}$ of $M_{Q,0}$. The Riemannian tensor g and the symplectic form ω are not, which means that they are not π-related to tensors on the set of leaves $\mathcal{P}$. It is possible, however, to define new tensor fields on $M_{Q,0}$ with better properties, by using the reduction procedure introduced in Section 1.3.1.

1.3.4 Reduction of tensor fields to the projective manifold

The group action $r : (\mathbb{R}_+ \times U(1)) \times M_Q \to M_Q$ defines a foliation of the manifold, which is regular on $M_{Q,0}$, as proved in Theorem 1.50. Consider the reduction procedure presented in Section 1.3.1, and its applications to observable functions on $M_{Q,0}$, defined in (1.84):

$$f_A(\psi) = \langle \psi | A | \psi \rangle, \quad \psi \in M_{Q,0}, \quad A \in O. \tag{1.117}$$

As proved above, these functions form a Lie-Jordan algebra $\mathcal{F}_\mathcal{O}(M_{Q,0})$ of functions. They are not, however, invariant under the group action:

$$\Delta(f_A) = 2 f_A, \quad \Gamma(f_A) = 0, \quad \forall f_A \in \mathcal{F}_\mathcal{O}(M_{Q,0}). \tag{1.118}$$

Thus, the first step in the reduction procedure is to find a suitable set of invariant functions under the action.

Proposition 1.57. *For any observable $A \in O$, let us define a function e_A on $M_{Q,0}$ is defined as*

$$e_A(\psi) := \frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle}, \quad \psi \in M_{Q,0}. \tag{1.119}$$

The function e_A is known as the expectation value function of A. The set of expectation value functions on $M_{Q,0}$ is denoted by $\mathcal{E}_{\mathcal{O}}(M_{Q,0})$. Expectation value functions are invariant under the group action of $\mathbb{R}_+ \times U(1)$ on $M_{Q,0}$.

Proof. It is immediate to check that $\Delta(e_A) = \Gamma(e_A) = 0$, for any $e_A \in \mathcal{E}_{\mathcal{O}}(M_{Q,0})$. Alternatively, if (1.119) is seen as a function on $\mathcal{H}_0$, there exists a symmetry under the change $|\psi\rangle \mapsto \lambda|\psi\rangle$, for any $\lambda \in \mathbb{C}_0$, hence the functions are invariant under the described group action. □

Proposition 1.58. *The Poisson bracket and symmetric product of expectation value functions are*

$$\{e_A, e_B\} = \frac{1}{f_I} e_{[\![A,B]\!]}, \quad (e_A, e_B) = \frac{1}{f_I}\left(e_{A\odot B} - 2e_A e_B\right), \quad \forall A, B \in \mathcal{O}. \tag{1.120}$$

Proof. Expression (1.119) can be rewritten as $e_A = f_I^{-1} f_A$. Together with relations in (1.119), the Poisson bracket of expectation value functions e_A and e_B is

$$\{e_A, e_B\} = \left\{\frac{f_A}{f_I}, \frac{f_B}{f_I}\right\} = \frac{1}{f_I^2} f_{[\![A,B]\!]} = \frac{1}{f_I} e_{[\![A,B]\!]}.$$

The symmetric product of functions is computed in a similar way:

$$(e_A, e_B) = \left(\frac{f_A}{f_I}, \frac{f_B}{f_I}\right) = \frac{1}{f_I^2} f_{A\odot B} - 4\frac{f_A f_B}{f_I^3} + 2\frac{f_A f_B}{f_I^3} = \frac{1}{f_I}\left(e_{A\odot B} - 2e_A e_B\right),$$

Observe that the last term is obtain because of $\frac{1}{2}I$ being the identity element of the Jordan product of observables; see (1.20). □

It is thus concluded that $\mathcal{E}_{\mathcal{O}}(M_{Q,0})$ is not a closed set under these composition laws. In other words, the Poisson bracket and symmetric product cannot be reduced directly onto $\mathcal{P}$. This is in accordance with Proposition 1.56, as the contravariant tensor fields describing these composition laws are not invariant under the described group action. However, relations in (1.56) offer a simple way to solve this problem. It is possible to define new composition laws of smooth functions on $M_{Q,0}$ such that they satisfy the conditions in Theorem 1.49. Consider the composition laws in $C^\infty(M_{Q,0})$ defined by

$$\{f, f'\}'(\psi) := \|\psi\|^2\{f, f'\}(\psi), \quad (f, f')'(\psi) := \|\psi\|^2(f, f')(\psi), \quad \forall f, f' \in C^\infty(M_{Q,0}), \quad \forall \psi \in M_{Q,0}, \tag{1.121}$$

with $\|\psi\|^2 = \langle\psi|\psi\rangle = f_I(\psi)$. Consider the products of functions in $\mathcal{E}_{\mathcal{O}}(M_{Q,0})$. By (1.120), the compositions of any two expectation value functions are

$$\{e_A, e_B\}' = e_{[\![A,B]\!]}, \quad (e_A, e_B)' = e_{A\odot B} - 2e_A e_B, \quad \forall A, B \in \mathcal{O}. \tag{1.122}$$

which are preserved by the described group action. Observe that the second product $(e_A, e_B)'$ is not an expectation value function, yet it is invariant by the group action. Thus, it is possible to reduce these composition laws through the projection $\pi : M_{Q,0} \to \mathcal{P}$. They can be given a tensorial description. Let Ω', G' be the contravariant $(2,0)$-tensor fields on $M_{Q,0}$ defined as

$$\Omega'_\psi := \|\psi\|^2\Omega_\psi, \quad G'_\psi := \|\psi\|^2 G_\psi, \quad \forall \psi \in M_{Q,0}. \tag{1.123}$$

By (1.121), the action of these tensor fields on exact 1-forms yields the required composition laws:

$$\Omega'(\mathrm{d}f, \mathrm{d}f') = \{f, f'\}', \quad G'(\mathrm{d}f, \mathrm{d}f') = (f, f')', \quad \forall f, f' \in C^\infty(M_{Q,0}). \tag{1.124}$$

However, the comments presented in Section 1.3.1 have to be taken into consideration. While these are, by definition, π-projectable tensor fields, they are not the best choice to represent on $M_{Q,0}$ the composition laws existing on $\mathcal{P}$. A better characterisation can be obtained by describing the generalised distributions of vector fields associated with expectation value functions.

Proposition 1.59. *Consider the maps* $\widehat{\Omega}', \widehat{G}' : \bigwedge^1(M_{Q,0}) \to \mathfrak{X}(M_{Q,0})$ *defined as* $\widehat{\Omega}'(\alpha) := \iota_\alpha \Omega$ *and* $\widehat{G}'(\alpha) := \iota_\alpha G$*, for any* $\alpha \in \bigwedge^1(M_{Q,0})$*. The image by these maps of the differentials of expectation value functions are*

$$X'_A := \widehat{\Omega}'(\mathrm{d}e_A) = X_A + e_A \Gamma, \quad Y'_A := \widehat{G}'(\mathrm{d}e_A) = Y_A - e_A \Delta, \quad \forall A \in \mathcal{O}. \tag{1.125}$$

For any $A \in \mathcal{O}$*, vector fields* X'_A *and* Y'_A *are orthogonal (with respect to the metric* g*) to* Δ *and* Γ *at each point:*

$$g(X'_A, \Delta) = g(X'_A, \Gamma) = 0, \quad g(Y'_A, \Delta) = g(Y'_A, \Gamma) = 0. \tag{1.126}$$

Proof. The expressions of X'_A and Y'_A are deduced from the $C^\infty(M_{Q,0})$-linearity of tensor fields and maps defined from them, in particular of $\widehat{\Omega}'$ and $\widehat{G}'$. By definitions given in (1.123),

$$\begin{aligned} X'_A &= \widehat{\Omega}'(\mathrm{d}e_A) = f^{-1}\widehat{\Omega}'(\mathrm{d}f_A) - f^{-2} f_A \widehat{\Omega}'(\mathrm{d}f_I) = \widehat{\Omega}(\mathrm{d}f_A) - e_A \widehat{\Omega}(\mathrm{d}f_I) = X_A + e_A \Gamma, \\ Y'_A &= \widehat{G}'(\mathrm{d}e_A) = f^{-1}\widehat{G}'(\mathrm{d}f_A) - f^{-2} f_A \widehat{G}'(\mathrm{d}f_I) = \widehat{G}(\mathrm{d}f_A) - e_A \widehat{G}(\mathrm{d}f_I) = Y_A - e_A \Delta, \end{aligned}$$

where relations $e_A = f_I^{-1} f_A$ and (1.92) have been used. Orthogonality can be proved by considering the values of these vector fields at each $\psi \in M_{Q,0}$ and their corresponding vectors on $\mathcal{H}$. Thus,

$$\big|(X'_A)_\psi\big\rangle = -\mathrm{i} A|\psi\rangle + \mathrm{i}\, \frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle}|\psi\rangle, \quad \big|(Y'_A)_\psi\big\rangle = A|\psi\rangle - \frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle}|\psi\rangle, \tag{1.127}$$

obtained from (1.58), (1.59) and (1.86). These vectors are orthogonal to $|\psi\rangle$ with respect to the Hermitian structure, hence orthogonal to both Δ and Γ with respect to tensor fields g and ω, as proved in Proposition 1.34. □

In order to characterise in an appropriate way the structure of the projective manifold $\mathcal{P}$, it is advisable to consider new tensor fields on $M_{Q,0}$ which behave in a similar way to Ω' and G' when acting on expectation value functions. In particular, vector fields associated to any function (not only to expectation value functions) should be orthogonal to both Δ and Γ, hence to the fibres of the foliation $\mathcal{F}_{\Delta,\Gamma}$.

Theorem 1.60. *Consider the tensor fields* $\widetilde{\Omega}_{\mathcal{P}}$ *and* $\widetilde{G}_{\mathcal{P}}$ *on* $M_{Q,0}$ *defined, at each point* $\psi \in M_{Q,0}$*, by*

$$(\widetilde{\Omega}_{\mathcal{P}})_\psi := \|\psi\|^2 \Omega_\psi - \frac{1}{2}\Delta_\psi \otimes \Gamma_\psi + \frac{1}{2}\Gamma_\psi \otimes \Delta_\psi, \quad (\widetilde{G}_{\mathcal{P}})_\psi := \|\psi\|^2 \Omega_\psi - \frac{1}{2}\Delta_\psi \otimes \Delta_\psi - \frac{1}{2}\Gamma_\psi \otimes \Gamma_\psi. \tag{1.128}$$

These are the only tensor fields such that, when evaluated on differentials of expectation value functions, yield the same results as Ω' *and* G'*, and such that the generalised distributions generated by their contractions with 1-forms are always orthogonal to both* Δ *and* Γ*.*

Proof. These vector fields can be directly constructed from Ω' and G', thus proving uniqueness. Consider the tangent space $T_\psi M_{Q,0}$ at any point $\psi \in M_{Q,0}$. The values of vector fields Δ and Γ generate a certain subspace $V_\psi := \mathrm{span}\{\Delta_\psi, \Gamma_\psi\} \subset T_\psi M_{Q,0}$. As a consequence of Proposition 1.34, orthogonality with respect to this subspace can be equivalently defined with respect to g and to ω. Thus, any tangent vector $v \in T_\psi M_{Q,0}$ can be decomposed in a unique way as

$$v = v^\perp + a\ \Delta_\psi + b\ \Gamma_\psi,$$

such that $v^\perp$ is orthogonal to V_ψ and real coefficients a and b take the values

$$a = \frac{g(\Delta_\psi, v)}{g(\Delta_\psi, \Delta_\psi)} = \frac{g(\Delta_\psi, v)}{2\|\psi\|^2} = -\frac{\omega(\Gamma_\psi, v)}{2\|\psi\|^2}, \quad b = \frac{g(\Gamma_\psi, v)}{g(\Gamma_\psi, \Gamma_\psi)} = \frac{g(\Gamma_\psi, v)}{2\|\psi\|^2} = \frac{\omega(\Delta_\psi, v)}{2\|\psi\|^2}, \tag{1.129}$$

where relation (1.69) between tensor fields g, ω and J has been taken into account. The orthogonal component $v^\perp$ is thus uniquely determined. Consider now, for a generic 1-form $\alpha \in \bigwedge^1(M_{Q,0})$, the vector

fields $\widehat{\Omega}'(\alpha)$ and $\widehat{G}'(\alpha)$. At each point $\psi \in M_{Q,0}$, the orthogonal components to V_ψ of the tangent vectors defined by these vector fields are

$$\begin{aligned}
\left(\widehat{\Omega}'(\alpha)\right)^\perp_\psi &= \left(\widehat{\Omega}'(\alpha)\right)_\psi + \frac{\omega\left(\Gamma, \widehat{\Omega}'(\alpha)\right)(\psi)}{2\|\psi\|^2}\,\Delta_\psi - \frac{\omega\left(\Delta, \widehat{\Omega}'(\alpha)\right)(\psi)}{2\|\psi\|^2}\,\Gamma_\psi \\
&= \|\psi\|^2\left(\widehat{\Omega}(\alpha)\right)_\psi - \frac{1}{2}\,\omega\left(\widehat{\Omega}(\alpha), \Gamma\right)(\psi)\,\Delta_\psi + \frac{1}{2}\,\omega\left(\widehat{\Omega}(\alpha), \Delta\right)(\psi)\,\Gamma_\psi \\
&= \|\psi\|^2\left(\widehat{\Omega}(\alpha)\right)_\psi + \frac{1}{2}\,\alpha_\psi(\Gamma_\psi)\,\Delta_\psi - \frac{1}{2}\,\alpha_\psi(\Delta_\psi)\,\Gamma_\psi, \\
\left(\widehat{G}'(\alpha)\right)^\perp_\psi &= \left(\widehat{G}'(\alpha)\right)_\psi - \frac{g\left(\Delta, \widehat{G}'(\alpha)\right)(\psi)}{2\|\psi\|^2}\,\Delta_\psi - \frac{g\left(\Gamma, \widehat{G}'(\alpha)\right)(\psi)}{2\|\psi\|^2}\,\Gamma_\psi \\
&= \|\psi\|^2\left(\widehat{G}(\alpha)\right)_\psi - \frac{1}{2}\,g\left(\widehat{G}(\alpha), \Delta\right)(\psi)\,\Delta_\psi + \frac{1}{2}\,g\left(\widehat{G}(\alpha), \Gamma\right)(\psi)\,\Gamma_\psi \\
&= \|\psi\|^2\left(\widehat{\Omega}(\alpha)\right)_\psi - \frac{1}{2}\,\alpha_\psi(\Delta_\psi)\,\Delta_\psi - \frac{1}{2}\,\alpha_\psi(\Gamma_\psi)\,\Gamma_\psi,
\end{aligned}$$

where C^∞-linearity of tensor fields and relations $\widehat{\Omega} = -\widehat{\omega}^{-1}$, $\widehat{G} = \widehat{g}^{-1}$, presented in (1.79), have been used. These expressions are valid for any $\alpha \in \bigwedge^1(M_{Q,0})$ and any $\psi \in M_{Q,0}$, thus they define tensor fields $\widetilde{\Omega}_\mathcal{P}$ and $\widetilde{G}_\mathcal{P}$ on the manifold $M_{Q,0}$. □

These are the appropriate tensor fields to describe the structure of the projective manifold $\mathcal{P}$ on the ambient manifold $M_{Q,0}$ [97, 99]. Their existence is relevant in relation with the habitual way in which most physicists describe Quantum Mechanics. All the analysis of group actions, equivalence relations and projective manifolds are put aside, and computations are done on Hilbert spaces. Some attention is paid to the norm of states, which is assumed to be constant along evolution. Thus, the projective manifold $\mathcal{P}$ is 'embedded' into the Hilbert space. Such embedding is, in fact, not possible. As pointed out in the diagram of Figure 1.4, the only two possible embeddings are $\iota_\mathcal{P} : \mathcal{P} \to \mathcal{R}$ and $\iota_\mathcal{Q} : \mathcal{Q} \to M_{Q,0}$. The reason is that the fibration induced by Γ is not trivial, thus a differentiable embedding of $\mathcal{P}$ into $M_{Q,0}$ does not exist. Habitual computations of Quantum Mechanics never take this fact into account, yet they produce valid results. Theorem 1.60 proves that, in fact, there exists a mathematically rigorous way to describe the properties of $\mathcal{P}$ in $M_{Q,0}$, not through an embedding, but by the definition of appropriate geometric objects. Dynamics associated with these tensor fields is naturally orthogonal to the fibres. Expectation value functions, which happen to be the appropriate representations of observables, are constant along the fibres, and these tensor fields act on them in the desired way. As a summary, the structures presented here reproduce in an appropriate way the properties of quantum system by taking into account the natural fibration induced by the group action $\mathbb{C}_0$ on the quantum manifold $M_{Q,0}$.

1.3.5 The Kähler structure of the projective manifold of pure states

The reduction procedure yields a pair of tensor fields on $\mathcal{P}$ as the push-forward by $\pi : M_{Q,0} \to \mathcal{P}$ of the tensor fields $\widetilde{\Omega}_\mathcal{P}$ and $\widetilde{G}_\mathcal{P}$:

$$\Omega_\mathcal{P} := \pi_*\left(\widetilde{\Omega}_\mathcal{P}\right), \quad G_\mathcal{P} := \pi_*\left(\widetilde{G}_\mathcal{P}\right). \tag{1.130}$$

The tensorial description makes possible to define composition laws for arbitrary smooth functions on $\mathcal{P}$, not only expectation value functions. It is convenient to consider the following definitions:

$$\{f, f'\}_\mathcal{P} = \Omega_\mathcal{P}(\mathrm{d}f, \mathrm{d}f'), \quad (f, f')_\mathcal{P} = G_\mathcal{P}(\mathrm{d}f, \mathrm{d}f') + 2ff', \quad \forall f, f' \in C^\infty(\mathcal{P}). \tag{1.131}$$

Proposition 1.61. *For any $A \in O$, there exists a unique function $\epsilon_A \in \mathcal{P}$ such that*

$$\pi^*(\epsilon_A) = e_A \in \mathcal{E}(M_{Q,0}). \tag{1.132}$$

This function ϵ_A is called the expectation value function of A on $\mathcal{P}$. Let $\mathcal{E}(\mathcal{P})$ be the set of expectation value functions on $\mathcal{P}$. Composition laws defined in (1.131) determine a Lie-Jordan structure on the set:

$$\{\epsilon_A, \epsilon_B\}_{\mathcal{P}} = \epsilon_{[\![A,B]\!]}, \quad (\epsilon_A, \epsilon_B)_{\mathcal{P}} = \epsilon_{A \odot B}, \quad \forall A, B \in \mathcal{O}. \tag{1.133}$$

Proof. Consider the fibration $\mathcal{F}_{\Delta\Gamma}$ on $M_{Q,0}$ and the projection onto $\mathcal{P}$. Any function which is constant along the fibres is the pull-back of a function on $\mathcal{P}$. This is the case of expectation value functions. Composition laws are immediately computed from (1.131) and (1.122). □

As in the case of the quantum manifold M_Q, a covariant description of the structure is also possible. In this way, a Kähler structure is obtained on the manifold $\mathcal{P}$.

Lemma 1.62. *Consider the maps $\widehat{\Omega}_{\mathcal{P}}, \widehat{G}_{\mathcal{P}} : \bigwedge^1(\mathcal{P}) \to \mathfrak{X}(M_{Q,0})$ defined by*

$$\widehat{\Omega}_{\mathcal{P}}(\alpha) := \iota_\alpha(\Omega_{\mathcal{P}}), \quad \widehat{G}_{\mathcal{P}}(\alpha) := \iota_\alpha(G_{\mathcal{P}}) \tag{1.134}$$

These maps are invertible.

Proof. Consider the definition (1.128) of the π-projectable tensor fields. Observe that the initial tensor fields Ω and G on $M_{Q,0}$ are of maximum rank, while the additional terms ensure that the reduced tensor fields are constant along the fibres. Hence, after the projection by π, which eliminates the directions along the fibres, invertibility is recovered. □

Theorem 1.63. *Let $\omega_{\mathcal{P}}$ and $g_{\mathcal{P}}$ be the covariant $(0,2)$-tensor fields on $\mathcal{P}$ defined by*

$$\omega_{\mathcal{P}}(X,Y) = \Omega_{\mathcal{P}}\left(\widehat{\Omega}_{\mathcal{P}}^{-1}(X), \widehat{\Omega}_{\mathcal{P}}^{-1}(Y)\right), \quad g_{\mathcal{P}}(X,Y) = G_{\mathcal{P}}\left(\widehat{G}_{\mathcal{P}}^{-1}(X), \widehat{G}_{\mathcal{P}}^{-1}(Y)\right), \quad \forall X, Y \in \mathfrak{X}(\mathcal{P}). \tag{1.135}$$

The projective manifold $\mathcal{P}$ is an almost Kähler manifold with respect to the tensors field $g_{\mathcal{P}}, \omega_{\mathcal{P}}$ and $J_{\mathcal{P}}$, where $J_{\mathcal{P}}$ is the tensor field on $\mathcal{P}$ π-related with the complex structure J on $M_{Q,0}$.

Proof. Compatibility between these structures can be proved by computing their counterparts on $M_{Q,0}$. Let $\tilde{g}_{\mathcal{P}} := \pi^*(g_{\mathcal{P}})$ and $\tilde{\omega}_{\mathcal{P}} := \pi^*(\omega_{\mathcal{P}})$ denote the corresponding pull-backs onto $M_{Q,0}$. Their expressions are

$$\tilde{g}_{\mathcal{P},\psi}(v,w) = \frac{g_\psi(v,w)}{\|\psi\|^2} - 2\mathrm{Re}\,\frac{\langle v|\psi\rangle\langle\psi|w\rangle}{\|\psi\|^4}, \qquad \tilde{\omega}_{\mathcal{P},\psi}(v,w) = \frac{\omega_\psi(v,w)}{\|\psi\|^2} - 2\mathrm{Im}\,\frac{\langle v|\psi\rangle\langle\psi|w\rangle}{\|\psi\|^4}, \tag{1.136}$$

for any $\psi \in M_{Q,0}$ and any $v, w \in T_\psi M_{Q,0}$. They satisfy the relation

$$\tilde{g}_{\mathcal{P}}(J(X), Y) = \tilde{\omega}_{\mathcal{P}}(X,Y), \quad \forall X, Y \in \mathfrak{X}(M_{Q,0}). \tag{1.137}$$

Therefore, the corresponding π-related tensor fields $\mathcal{P}$, say $g_{\mathcal{P}}$, $\omega_{\mathcal{P}}$ and $J_{\mathcal{P}}$, define an almost Kähler structure on the manifold $\mathcal{P}$. □

The tensor fields $g_{\mathcal{P}}$ and $\omega_{\mathcal{P}}$ obtained on $\mathcal{P}$ are known in the literature of complex manifolds as the Fubini-Study metric. It was first introduced in the first years of the 20th century by Fubini and Study [132, 254]. The Fubini-Study has been described in many works [91, 216, 217]. See in particular the geometric approach of Anandan [22], which share many similarities with the reduction procedure presented here.

Hamiltonian and gradient vector fields on the projective manifold are defined as usual. For any smooth function $f \in C^\infty(\mathcal{P})$, their Hamiltonian and gradient vector fields are, respectively,

$$X_{\mathcal{P},f} := -\widehat{\Omega}_{\mathcal{P}}(\mathrm{d}f), \quad Y_{\mathcal{P},f} := \widehat{G}_{\mathcal{P}}(\mathrm{d}f). \tag{1.138}$$

Proposition 1.64. *Hamiltonian and gradient vector fields on $\mathcal{P}$ satisfy the following commutation relations:*

$$[X_{\mathcal{P},f}, X_{\mathcal{P},h}] = -X_{\mathcal{P},\{f,h\}_{\mathcal{P}}}, \quad [X_{\mathcal{P},f}, Y_{\mathcal{P},h}] = -Y_{\mathcal{P},\{f,h\}_{\mathcal{P}}}, \quad [Y_{\mathcal{P},f}, Y_{\mathcal{P},h}] = X_{\mathcal{P},\{f,h\}_{\mathcal{P}}} \quad f, h \in C^\infty(\mathcal{P}). \tag{1.139}$$

Proof. Similar to Proposition 1.42. □

Observe the similarities and differences between this result and Proposition 1.42. In both cases, Hamiltonian vector field close a Lie algebra with respect to the commutator. The complexification of this algebra is obtained by considering also gradient vector fields. Differences arise between both proposition for the case of gradient and Hamiltonian vector fields associated to observables. As before, the notation is shortened as $X_{\mathcal{P}A} := X_{\mathcal{P}\epsilon_A}$ and $Y_{\mathcal{P}A} := Y_{\mathcal{P}\epsilon_A}$. The Lie algebra generated by these Hamiltonian and gradient vector fields is isomorphic to $\mathfrak{sl}(\mathcal{H})$, the Lie algebra of traceless linear operators on the complex Hilbert space $\mathcal{H}$. Compare these properties with Corollary 1.47. As expected, as a result of the projection from $M_{Q,0}$ to $\mathcal{P}$, smaller Lie algebras of vector fields are obtained. This is in agreement with the decomposition $\mathfrak{gl}(\mathcal{H}) = \mathfrak{sl}(\mathcal{H}) \oplus \mathbb{C}$.

Due to the commutation relations in Proposition 1.42, Hamiltonian vector fields on $M_{Q,0}$ are π-related with Hamiltonian vector fields on $\mathcal{O}$. In particular, it is possible to recover the description of unitary evolution by Hamiltonian vector fields, in this case on $\mathcal{P}$.

Theorem 1.65. *The unitary dynamics of quantum systems, generated by the Schrödinger equation in the algebraic formalism, is described on the manifold of states $\mathcal{P}$ by the Hamiltonian vector field $X_{\mathcal{P}H}$ associated to the Hamiltonian operator H of the system. This vector field is π-related with the Hamiltonian vector field X_H on $M_{Q,0}$.*

As a last result regarding expectation value functions, observe that the differential $\mathrm{d}\epsilon_A$ give information on the spectral decomposition of the observable A.

Theorem 1.66. *Consider an observable A.*

The critical points of an expectation value function $\epsilon_A \in \mathcal{E}_{\mathcal{O}}(\mathcal{P})$ are the equivalence classes $[\psi_\lambda] \in \mathcal{P}$ of the points $\psi_\lambda \in M_{Q,0}$ representing the eigenvectors of $A \in \mathcal{O}$. The values of ϵ_A at such critical points give the corresponding eigenvalues of A. In other words, if $|\psi_\lambda\rangle \in \mathcal{H}$ is an eigenvector of A with (real) eigenvalue λ, then

$$(\mathrm{d}\epsilon_A)_{[\psi_\lambda]} = 0, \quad \epsilon_A([\psi_\lambda]) = \lambda. \tag{1.140}$$

Proof. If $|\psi_\lambda\rangle \in \mathcal{H}$ is an eigenvector of A, then

$$\epsilon_A([\psi_\lambda]) = \frac{\langle\psi_\lambda|A|\psi_\lambda\rangle}{\langle\psi_\lambda|\psi_\lambda\rangle} = \lambda.$$

In order to compute the differential $\mathrm{d}\epsilon_A$, consider a trajectory $|\psi_\lambda\rangle + t|v\rangle$ in $\mathcal{H}$. By direct computation, if $A|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\langle\psi_\lambda + tv|A|\psi_\lambda + tv\rangle}{\langle\psi_\lambda + tv|\psi_\lambda + tv\rangle}\bigg|_{t=0} = 0. \tag{1.141}$$

for any $|v\rangle \in \mathcal{H}$. This proves that the function $e_A = \pi^*(\epsilon_A)$ satisfies $X(e_A)(\psi_\lambda) = \mathrm{d}e_A(X)(\psi_\lambda) = 0$ for any vector field $X \in \mathfrak{X}(M_{Q,0})$, hence $(\mathrm{d}e_A)_(\psi_\lambda) = 0$. And as e_A is projectable, this proves that $(\mathrm{d}\epsilon_A)_{[\psi_\lambda]} = 0$. □

1.4 The geometric description of the 2-level system

As a practical application of the geometric formalism, the 2-level system is again considered. In Section 1.1.7, the properties of this system were studied in the algebraic setting. These results can be reproduced with the geometric tools presented above.

The Hilbert space associated to a 2-level system is $\mathcal{H} = \mathbb{C}^2$. Therefore, the corresponding real differentiable manifold M_Q is 4-dimensional, and there exists a global chart $\phi : M_Q \to \mathbb{R}^4$, which is determined in terms of the coordinates on $\mathbb{C}^2$ with respect to an orthonormal basis $E = \{|e_1\rangle, |e_2\rangle\}$ as follows:

$$|\psi\rangle = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} \in \mathbb{C}^2 \Rightarrow \phi_E(\psi) = (q_1, p_1, q_2, p_2) \in \mathbb{R}^4, \quad z_j = \frac{1}{\sqrt{2}}(q_j + \mathrm{i}p_j), \quad j = 1, 2. \tag{1.142}$$

The relation between elements in the basis E and coordinate vector fields is given by (1.52). Any tangent vector v to M_Q at a generic point ψ can thus be related to a vector in $\mathcal{H}$, and vice-versa.

$$u = v_1 \left.\frac{\partial}{\partial q_1}\right|_\psi + w_1 \left.\frac{\partial}{\partial p_1}\right|_\psi + v_2 \left.\frac{\partial}{\partial q_2}\right|_\psi + w_2 \left.\frac{\partial}{\partial p_2}\right|_\psi \in T_\psi M_Q \Leftrightarrow |u\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} v_1 + \mathrm{i}w_1 \\ v_2 + \mathrm{i}w_2 \end{pmatrix} \in \mathbb{C}^2. \tag{1.143}$$

It is thus possible to explicitly compute the expressions for the tensor fields. The vector field J, defined in (1.54) as $|J_\psi(v)\rangle = \mathrm{i}|v\rangle$ for any $\psi \in M_Q$, any $v \in T_\psi M_Q$, takes the form

$$J = \mathrm{d}q_1 \otimes \frac{\partial}{\partial p_1} - \mathrm{d}p_1 \otimes \frac{\partial}{\partial q_1} + \mathrm{d}q_2 \otimes \frac{\partial}{\partial p_2} - \mathrm{d}p_2 \otimes \frac{\partial}{\partial q_2}. \tag{1.144}$$

The coordinate expressions of the tensor fields g and ω can also be computed directly:

$$g = \mathrm{d}q_1 \otimes \mathrm{d}q_1 + \mathrm{d}p_1 \otimes \mathrm{d}p_1 + \mathrm{d}q_2 \otimes \mathrm{d}q_2 + \mathrm{d}p_2 \otimes \mathrm{d}p_2, \quad \omega = \mathrm{d}q_1 \wedge \mathrm{d}p_1 + \mathrm{d}q_2 \wedge \mathrm{d}p_2. \tag{1.145}$$

The vector fields that represent the linear structure, Δ and Γ, are

$$\Delta = q_1\frac{\partial}{\partial q_1} + p_1\frac{\partial}{\partial p_1} + q_2\frac{\partial}{\partial q_2} + p_2\frac{\partial}{\partial p_2}, \quad \Gamma = q_1\frac{\partial}{\partial p_1} - p_1\frac{\partial}{\partial q_1} + q_2\frac{\partial}{\partial p_2} - p_2\frac{\partial}{\partial q_2}. \tag{1.146}$$

Let us now compute the explicit expression of functions associated to observables. Recall that a basis of Herm(2) is given by the matrices $\sigma_0, \sigma_1, \sigma_2, \sigma_3$ defined in (1.38). Thus, any observable is represented by a matrix $A \in \mathrm{Herm}(2)$ of the form

$$A = \sum_{j=0}^{3} a_j \sigma_j = \begin{pmatrix} a_0 + a_3 & a_1 - \mathrm{i}a_2 \\ a_1 + \mathrm{i}a_2 & a_0 - a_3 \end{pmatrix}, \quad a_0, a_1, a_2, a_3 \in \mathbb{R}. \tag{1.147}$$

The functions associated to the matrices in the basis have the following expressions:

$$\begin{aligned}
f_{\sigma_0}(\psi) &= \langle\psi|\sigma_0|\psi\rangle = \frac{1}{2}\begin{pmatrix} q_1 - \mathrm{i}p_1, q_2 - \mathrm{i}p_2 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} q_1 + \mathrm{i}p_1 \\ q_2 + \mathrm{i}p_2 \end{pmatrix} = \frac{1}{2}(q_1^2 + p_1^2 + q_2^2 + p_2^2), \\
f_{\sigma_1}(\psi) &= \langle\psi|\sigma_1|\psi\rangle = \frac{1}{2}\begin{pmatrix} q_1 - \mathrm{i}p_1, q_2 - \mathrm{i}p_2 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} q_1 + \mathrm{i}p_1 \\ q_2 + \mathrm{i}p_2 \end{pmatrix} = q_1q_2 + p_1p_2, \\
f_{\sigma_2}(\psi) &= \langle\psi|\sigma_2|\psi\rangle = \frac{1}{2}\begin{pmatrix} q_1 - \mathrm{i}p_1, q_2 - \mathrm{i}p_2 \end{pmatrix}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}\begin{pmatrix} q_1 + \mathrm{i}p_1 \\ q_2 + \mathrm{i}p_2 \end{pmatrix} = q_2p_1 - q_1p_2, \\
f_{\sigma_3}(\psi) &= \langle\psi|\sigma_3|\psi\rangle = \frac{1}{2}\begin{pmatrix} q_1 - \mathrm{i}p_1, q_2 - \mathrm{i}p_2 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} q_1 + \mathrm{i}p_1 \\ q_2 + \mathrm{i}p_2 \end{pmatrix} = \frac{1}{2}(q_1^2 + p_1^2 - q_2^2 - p_2^2).
\end{aligned}$$

Observe that all the four function are quadratic in the coordinates, as expected. The function f_A for a general matrix of the form (1.147) is

$$f_A(\psi) = \sum_{j=0}^{3} a_j f_{\sigma_j}(\psi) = \frac{1}{2}(a_0 + a_3)(q_1^2 + p_1^2) + \frac{1}{2}(a_0 - a_3)(q_2^2 + p_2^2) + a_1q_1q_2 - a_2q_1p_2 + a_2q_2p_1 + a_1p_1p_2. \tag{1.148}$$

Generic Hamiltonian and gradient vector fields can be thus computed. The contravariant tensor fields G and Ω are

$$G = \frac{\partial}{\partial q_1} \otimes \frac{\partial}{\partial q_1} + \frac{\partial}{\partial p_1} \otimes \frac{\partial}{\partial p_1} + \frac{\partial}{\partial q_2} \otimes \frac{\partial}{\partial q_2} + \frac{\partial}{\partial p_2} \otimes \frac{\partial}{\partial p_2}, \quad \Omega = \frac{\partial}{\partial q_1} \wedge \frac{\partial}{\partial p_1} + \frac{\partial}{\partial q_2} \wedge \frac{\partial}{\partial p_2}. \tag{1.149}$$

Thus, applying the results of Proposition 1.41, it is immediate to compute the gradient and Hamiltonian vector fields associated to a generic observable A:

$$\begin{aligned} X_A = -\widehat{\Omega}(\mathrm{d}f_A) =&((a_0+a_3)p_1 + a_2q_2 + a_1p_2)\frac{\partial}{\partial q_1} - ((a_0+a_3)q_1 + a_1q_2 - a_2p_2)\frac{\partial}{\partial p_1} \\ &+ (-a_2q_1 + a_1p_1 + (a_0-a_3)p_2)\frac{\partial}{\partial q_2} - (a_1q_1 + a_2p_1 + (a_0-a_3)q_2)\frac{\partial}{\partial p_2}, \end{aligned} \tag{1.150}$$

$$\begin{aligned} Y_A = \widehat{G}(\mathrm{d}f_A) =&((a_0+a_3)q_1 + a_1q_2 - a_2p_2)\frac{\partial}{\partial q_1} + ((a_0+a_3)p_1 + a_2q_2 + a_1p_2)\frac{\partial}{\partial p_1} \\ &+ (a_1q_1 + a_2p_1 + (a_0-a_3)q_2)\frac{\partial}{\partial q_2} + (-a_2q_1 + a_1p_1 + (a_0-a_3)p_2)\frac{\partial}{\partial p_2}. \end{aligned} \tag{1.151}$$

It is immediate to check that $J(X_A) = Y_A$.

In this simple case, the result of Theorem 1.44, namely that the relation between A and f_A is a bijection, can be directly computed. Consider the points $\psi_1, \psi_2 \in M_Q$ with coordinates

$$\phi_E(\psi_1) = (1,0,0,0), \quad \phi_E(\psi_2) = (0,0,1,0). \tag{1.152}$$

The value of X_A at ψ_1 and ψ_2 is enough to determine the matrix A. For simplicity, matrix expressions are used for the tangent vectors to M_Q. The Hamiltonian vector field X_A takes the values:

$$(X_A)_{\psi_1} = \begin{pmatrix} 0 \\ -a_0 - a_3 \\ -a_2 \\ -a_1 \end{pmatrix}, \quad (X_A)_{\psi_2} = \begin{pmatrix} a_2 \\ -a_1 \\ 0 \\ -a_0 + a_3 \end{pmatrix}. \tag{1.153}$$

These values completely determine the numbers a_0, a_1, a_2, a_3. As X_A is determined by the function f_A, this proves that the relation between observables and functions associated to them is bijective.

Let us now consider a diagonal Hamiltonian, as in (1.40):

$$H = \begin{pmatrix} E_0 & 0 \\ 0 & E_1 \end{pmatrix}, \quad E_0, E_1 \in \mathbb{R} \Rightarrow f_H(\psi) = \frac{1}{2}E_0(q_1^2 + p_1^2) + \frac{1}{2}E_1(q_2^2 + p_2^2). \tag{1.154}$$

The Hamiltonian vector field X_H associated to this function is

$$X_H = E_0p_1\frac{\partial}{\partial q_1} - E_0q_1\frac{\partial}{\partial p_1} + E_1p_2\frac{\partial}{\partial q_2} - E_1q_2\frac{\partial}{\partial p_2} \tag{1.155}$$

Let $\psi(t)$ be an integral curve of X_H. The coordinates of the points along the curve satisfy the following differential equations:

$$\frac{\mathrm{d}q_1}{\mathrm{d}t} = X_H(q_1) = E_0p_1, \ \frac{\mathrm{d}p_1}{\mathrm{d}t} = X_H(p_1) = -E_0q_1, \ \frac{\mathrm{d}q_2}{\mathrm{d}t} = X_H(q_2) = E_1p_2, \ \frac{\mathrm{d}p_2}{\mathrm{d}t} = X_H(p_2) = -E_1q_2. \tag{1.156}$$

This system of differential equations can be written in matrix form as

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} q_1 \\ p_1 \\ q_2 \\ p_2 \end{pmatrix} = \begin{pmatrix} 0 & E_0 & 0 & 0 \\ -E_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_1 \\ 0 & 0 & -E_1 & 0 \end{pmatrix}\begin{pmatrix} q_1 \\ p_1 \\ q_2 \\ p_2 \end{pmatrix}. \tag{1.157}$$

By direct integration, the coordinates of points along such integral curve are

$$\begin{aligned} q_1(t) &= q_{10}\cos(E_0t) + p_{10}\sin(E_0t), \quad p_1(t) = p_{10}\cos(E_0t) - q_{10}\sin(E_0t), \\ q_2(t) &= q_{20}\cos(E_1t) + p_{20}\sin(E_1t), \quad p_2(t) = p_{20}\cos(E_1t) - q_{20}\sin(E_1t)), \end{aligned} \tag{1.158}$$

with $q_{10}, p_{10}, q_{20}, p_{20}$ being the coordinates at $t = 0$. If each point $\psi(t)$ with these coordinates is mapped onto $\mathbb{C}^2$, the result presented in (1.43) is recovered:

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} (\cos(E_0 t) - \mathrm{i}\sin(E_0 t))(q_{10} + \mathrm{i}p_{10}) \\ (\cos(E_1 t) - \mathrm{i}\sin(E_1 t))(q_{20} + \mathrm{i}p_{20}) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-\mathrm{i}E_0 t}(q_{10} + \mathrm{i}p_{10}) \\ e^{-\mathrm{i}E_1 t}(q_{20} + \mathrm{i}p_{20}) \end{pmatrix}, \tag{1.159}$$

thus recovering the algebraic solution (1.43) to the Schrödinger equation of the 2-level system.

Up to this point, the geometric formalism reproduces precisely all the aspects already presented in the algebraic approach to the Schrödinger picture. Let us now focus on the geometric description of the the manifold of states $\mathcal{P}$, which is the complex projective space of dimension 1, i.e. $\mathcal{P} = \mathbb{C}\mathrm{P}^1$ [212].

The projective manifold $\mathcal{P}$ is the set of leaves in the foliation $\mathcal{F}_{\Delta,\Gamma}$ by vector fields Δ and Γ in $M_{Q,0}$. For any element $\psi \in M_{Q,0}$, let us denote by $[\psi]$ the corresponding leaf, which is itself a point in $\mathcal{P}$. It is necessary to define coordinates in $\mathcal{P}$ in order to study its properties. As a global chart for $\mathcal{P}$ does not exist, at least two local charts are needed. In his book, Nakahara describes this atlas in the language of complex manifold. An atlas $\{(U, \xi^{\mathbb{C}}), (V, \phi^{\mathbb{C}})\}$ for $\mathbb{C}\mathrm{P}^1$ can be defined by the open sets

$$U = \mathbb{C}\mathrm{P}^1 - \{[e_1]\}, \quad V = \mathbb{C}\mathrm{P}^1 - \{[e_2]\}, \tag{1.160}$$

and the following complex coordinate functions:

$$\xi^{\mathbb{C}}([\psi]) = \frac{z_2}{z_1}, \quad [\psi] \in U; \qquad \phi^{\mathbb{C}}([\psi]) = \frac{z_1}{z_2}, \quad [\psi] \in V. \tag{1.161}$$

It is immediate to obtain from these expressions an atlas of real charts on $\mathcal{P}$ by taking the real and imaginary parts of the coordinates as

$$\xi^{\mathbb{C}} = \xi_1 + \mathrm{i}\xi_2, \quad \phi^{\mathbb{C}} = \phi_1 + \mathrm{i}\phi_2. \tag{1.162}$$

The values of these coordinates, with respect to the global coordinates (q_1, p_1, q_2, p_2) on $M_{Q,0}$, can thus be computed. The chart (U, ξ) is defined by the coordinates

$$\xi([\psi]) = (\xi_1, \xi_2), \quad \xi_1 = \frac{q_1 q_2 + p_1 p_2}{q_1^2 + p_1^2}, \quad \xi_2 = \frac{q_1 p_2 - p_1 q_2}{q_1^2 + p_1^2}. \tag{1.163}$$

In the same way, the chart (V, ϕ) on $\mathcal{P}$ has the following coordinates:

$$\phi([\psi]) = (\phi_1, \phi_2), \quad \phi_1 = \frac{q_1 q_2 + p_1 p_2}{q_2^2 + p_2^2}, \quad \phi_2 = \frac{p_1 q_2 - q_1 p_2}{q_2^2 + p_2^2}. \tag{1.164}$$

Together, they form an atlas $\{(U, \xi), (V, \phi)\}$ for the projective manifold $\mathcal{P}$. There is a clear interpretation of these coordinate charts. Observe that both U and V are obtained from $\mathcal{P}$ by removing a single point, and their corresponding coordinates map them onto the whole plane $\mathbb{R}^2$. This is precisely the same as when stereographic coordinates are taken on the sphere S^2. The complex projective space $\mathbb{C}\mathrm{P}^1$ is in fact isomorphic to the sphere S^2. Thus, it is possible to describe the pure states of a 2-level quantum system by points on the surface of a sphere. This description, presented in Figure 1.5, is known as the Bloch sphere. It was first introduced by Bloch in the context of [45]. First introduced in the study of nuclear magnetism [46], it is a useful tool in the analysis of properties of 2-level systems.

Consider thus a unit sphere S^2 embedded into the Euclidean space $\mathbb{R}^3$. In other words, the sphere S^2 is described by 3-dimensional coordinates x_1, x_2, x_3, with the constraint $x^1 + x^2 + x^3 = 1$. The relation between S^2 and $\mathbb{C}\mathrm{P}^1$ can be proved by consider the stereographic projections of the sphere. Thus, consider the stereographic projection onto the (x_1, x_2)-plane from the south pole, with coordinates ξ_1, ξ_2. A simple trigonometric computation shows that these coordinates are obtained as

$$\xi_1 = \frac{x_1}{1 + x_3}, \quad \xi_2 = \frac{x_2}{1 + x_3}, \quad x^1 + x^2 + x^3 = 1, \quad x_3 \neq -1. \tag{1.165}$$

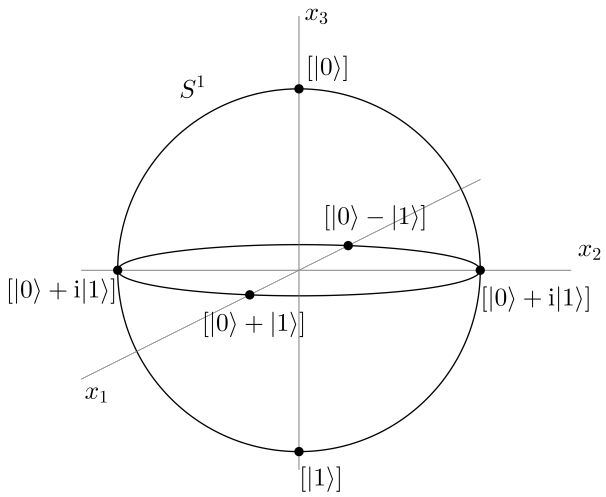


Figure 1.5: Representation on the sphere S^1 of the pure states of a 2-level system. This representation is known as the Bloch sphere. Coordinates of the points on the sphere are given by (1.166). It is possible to compute the elements $[\psi] \in \mathcal{P}$ that correspond to the intersections of the Bloch sphere with the coordinate axes. These are presented in the figure, in the basis determined by the eigenvectors of Hamiltonian (1.154). Observe that, for these energy levels, the north and south poles are respectively the ground state and the first excited state of the system. Notice also that antipodal points on the Bloch sphere correspond to orthogonal states of the system, when expressed as vectors on a Hilbert space.

The relation with the description of pure states of a 2-level system is obtained by assuming that relations (1.163) are satisfied. This proves that it is possible to map points in $M_{Q,0}$ onto $\mathbb{R}^3$ by

$$x_1 = \frac{2(q_1q_2 + p_1p_2)}{q_1^2 + p_1^2 + q_2^2 + p_2^2}, \quad x_2 = \frac{2(q_1p_2 - p_1q_2)}{q_1^2 + p_1^2 + q_2^2 + p_2^2}, \quad x_3 = \frac{q_1^2 + p_1^2 - q_2^2 - p_2^2}{q_1^2 + p_1^2 + q_2^2 + p_2^2}. \tag{1.166}$$

An identical result is obtained by assuming a stereographic projection from the north pole, with coordinates ϕ_1, ϕ_2 given by (1.164). As a consequence of relation (1.166), every point $[\psi] \in \mathbb{C}\mathrm{P}^1$ is mapped onto a point on the sphere $\mathcal{S}^1 \in \mathbb{R}^3$, being this map a bijection. It is therefore possible to describe pure states of a 2-level system as points on the sphere, as in Figure 1.5. Observe also that the coordinates thus obtained are precisely the expectation value functions of the Pauli matrices. This is a consequence of a result proved in [70], and reproduced below in Theorem 2.25, which states that it is always possible to obtain local coordinates for the projective manifold of any finite-dimensional quantum system by means of expectation values of observables.

It is immediate to compute tensor fields $\Omega_{\mathcal{P}}$ and $G_{\mathcal{P}}$, defined in (1.130), by means of relations (1.128), (1.149) and (1.166). Their values, in the given coordinates, are

$$\begin{aligned} \Omega_{\mathcal{P}} &= 2x_1 \frac{\partial}{\partial x_2} \wedge \frac{\partial}{\partial x_3} + 2x_2 \frac{\partial}{\partial x_3} \wedge \frac{\partial}{\partial x_1} + 2x_3 \frac{\partial}{\partial x_1} \wedge \frac{\partial}{\partial x_2}, \\ G_{\mathcal{P}} &= 2\left(\frac{\partial}{\partial x_1} \otimes \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} \otimes \frac{\partial}{\partial x_2} + \frac{\partial}{\partial x_3} \otimes \frac{\partial}{\partial x_3} \right) - \sum_{j,k=1}^{3} 2x_j x_k \frac{\partial}{\partial x_j} \otimes \frac{\partial}{\partial x_k}, \end{aligned} \tag{1.167}$$

with the constraint $x_1^2 + x_2^2 + x_3^2 = 1$ on the coordinates. The contractions of these tensor fields with exact 1-forms define, as usual, distributions of Hamiltonian and gradient vector fields on the sphere S^1. In order to understand the dynamics of a 2-level quantum system, consider the expectation value function ϵ_H associated to the Hamiltonian given in (1.154), whose value on the sphere is

$$\epsilon_H(x_1, x_2, x_3) = \frac{E_1 + E_0}{2} - \frac{E_1 - E_0}{2} x_3. \quad (x_1, x_2, x_3) \in S^1. \tag{1.168}$$

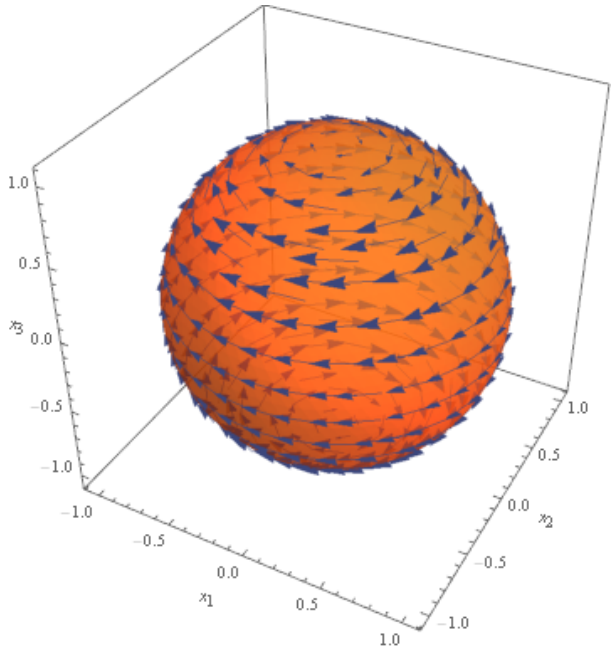


Figure 1.6: Representation of Hamiltonian vector field in (1.169) for $E_0 < E_1$. The case $E_0 > E_1$ would be obtained by inverting the arrows. The integrals curves of this vector field are the parallels of the sphere. There are two fixed points, the north and south poles. The period of rotation for non-fixed points arond the x_3-axis is given by (1.170). It is thus concluded that unitary evolution of a 2-level quantum system is represented by a rotation on the sphere S^2 with constant angular velocity.

The Hamiltonian vector field associated to this function is

$$X_{\mathcal{P},H} = -\widetilde{\Omega}_{\mathcal{P}}(\mathrm{d}\epsilon_H) = (E_1 - E_0)x_2\frac{\partial}{\partial x_1} - (E_1 - E_0)x_1\frac{\partial}{\partial x_2}. \tag{1.169}$$

Integral curves of this vector fields are the projection onto the manifold $\mathcal{P}$ of trajectories in (1.159). In other words, they are the solutions of the projection of the Schrödinger equation onto $\mathcal{P}$ for a system with Hamiltonian (1.154). The values of this vector field are represented in Figure 1.6. Observe how its integral curves are periodic orbits around the x_3-axis. A relevan difference with the analysis of dynamics on M_Q is the existence of fixed points. Vector field $X_{\mathcal{P},H}$ is zero at both north and south poles. By Figure 1.5, these points are precisely the ground and excited states of the system, as expected. Regarding periodic orbits, it is immediate that period of rotation around the x_3-axis is

$$T = \frac{2\pi}{|E_1 - E_0|}. \tag{1.170}$$

This period is independent of the initial conditions. The behaviour for any other Hamiltonian operator is similar, namely a rotation around an axis with constant period depending only on the eigenvalues of the Hamiltonian. The results presented here are obtained by direct computation and are hard to generalise to larger quantum systems. Thus, the 2-level system offers great possibilities to study the properties of projective spaces.

It is also possible to consider gradient vector fields on $\mathcal{P}$, defined by (1.138). The gradient vector field for the expectation value function ϵ_H is

$$Y_{\mathcal{P},H} = \widetilde{G}_{\mathcal{P}}(\mathrm{d}\epsilon_H) = (E_1 - E_0)\left(x_1\frac{\partial}{\partial x_1} + x_2\frac{\partial}{\partial x_2}\right) - (E_1 - E_0)(1 - x_3^2)\frac{\partial}{\partial x_3}. \tag{1.171}$$

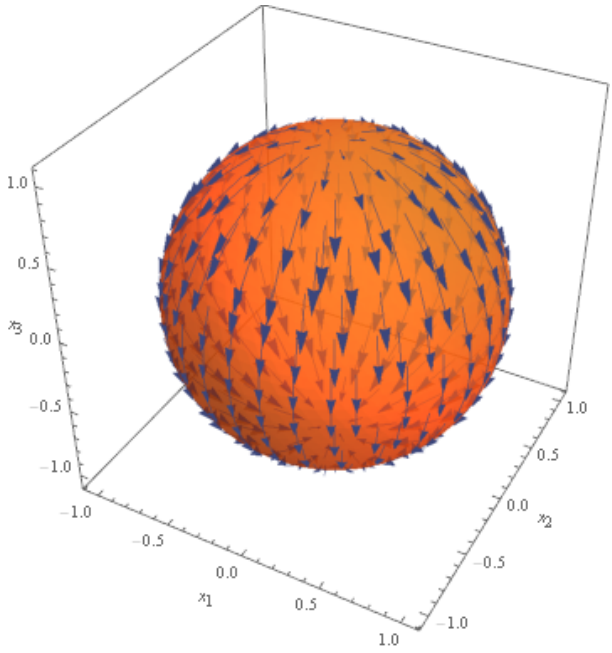


Figure 1.7: Gradient vector field (1.171) on the sphere S^2. The integral curves of this vector field are the meridians on the sphere, with the north and south poles being fixed points. Observe that it takes infinite time to reach the south pole from a generic initial state. Thus, the south pole is a stable fixed point, while the north pole is unstable.

The values of this vector field are plotted in Figure 1.7. Unlike in the case of Hamiltonian vector fields, integral curves of gradient vector fields are not periodic. Instead, there exist a stable and an unstable fixed points, which in this particular case correspond respectively to the excited and the ground state of Hamiltonian (1.154). Observe that, because of the properties of gradient vector fields, these integral curves are the projection onto $\mathcal{P}$ of the solutions of the following differential equation on $\mathcal{H}$:

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle. \tag{1.172}$$

This is, roughly speaking, the Schrödinger equation for a complex Hamiltonian $\mathrm{i}H$. These equations are use in dissipation models, as those proposed by Kaufman [173], Morrison [210] and Rajeev [225]. In the case of gradient vector field (1.171), 'dissipation' occurs from the ground state to the excited state of the system; the opposite behaviour is obtained by reversing the sign of the Hamiltonian. It is however important to notice that this is not the usual way in which dissipation occurs in nature. Firstly, dissipation is usually a probabilistic behaviour, while the evolution presented here is deterministic. Following chapters will deal with more realistic models of dissipation (see for example Section 3.4. Secondly, contrary to physical intuition, there exists an unstable fixed state (in this case, the ground state, on the north pole of the sphere). As a conclusion, the dissipation models with complex Hamiltonian should be used with care and only in situations in which dynamics is fully understood.

1.5 Analysis of the geometric characterisation of Quantum Mechanics

As a conclusion for this first chapter, let us remark the main advantages and applications of this geometric formulation. As shown, it is possible to describe the Schrödinger picture of Quantum Mechanics in a completely different way to the usual algebraic formulation. The characteristics of the theory is explicitly

determined by tensor fields, defining the Kähler structure of the quantum manifold M_Q. This description is similar to the Hamiltonian formulation of Classical Mechanics, which has proved to be useful in many different situations.

The different aspects of the theory (observables, evolution...) have been successfully described in geometric terms. Furthermore, the geometric description offers a clear advantage in the study of the projective Hilbert space $\mathcal{P}$. This is precisely the set of pure states of a quantum system, and a geometric analysis is much better adapted for its study than an algebraic one, as seen above. The manifold $\mathcal{P}$ is proved to hold also a Kähler structure, with similar structures to those obtained on M_Q.

The contravariant tensor fields defined on $\mathcal{P}$ by (1.130) are very important in the understanding of quantum systems. The Poisson tensor field $\Omega_{\mathcal{P}}$ reproduces the commutator of observables, which plays a role in many aspects of the theory. While this was achieved also at the level of the larger manifold M_Q, the properties of the symmetric tensor $G_{\mathcal{P}}$ are a new feature that boosts the importance of the study of the manifold $\mathcal{P}$. This tensor reproduces the covariance of observables, a very important quantity in the probabilistic interpretation of Quantum Mechanics. In particular, the product (ϵ_A, ϵ_A) is in direct relation with the standard derivation of the observable A, defined in (1.23):

$$G_{\mathcal{P}}(\mathrm{d}\epsilon_A, \mathrm{d}\epsilon_A)([\psi]) = 2\epsilon_{A^2}([\psi]) - 2(\epsilon_A([\psi]))^2 = 2(\Delta_\psi A)^2, \quad \forall [\psi] \in \mathcal{P}. \tag{1.173}$$

Tensor fields $\Omega_{\mathcal{P}}$ and $G_{\mathcal{P}}$ reproduce the quantum characteristics of observables. They are also the key to understand the difference between Classical and Quantum Mechanics. A classical system is described by a Poisson manifold, where observables are represented by functions on the manifold [3]. These functions form a Poisson algebra, defined with respect to the commutative, point-wise product of functions and with the natural Poisson bracket of the manifold.

The case of Quantum Mechanics is similar in some aspects, but with important differences. Quantum systems are described in terms of a Kähler manifold $\mathcal{P}$, which is a particular case of a Poisson manifold. It has therefore a richer structure, represented by the symmetric tensor field $G_{\mathcal{P}}$ and the complex structure connecting it with the Poisson tensor field $\Omega_{\mathcal{P}}$. Observables are represented by elements in a Lie-Jordan algebra of functions defined with respect to the products induced by both tensor fields.

The main difference between both theories is therefore the new tensor field $G_{\mathcal{P}}$. Its importance can be deduced from (1.131). The value of this tensor field is in direct connection with the difference between the Jordan product of functions and the point-wise products. Thus, if a classical limit of the theory were to be found, both products should become equal, hence $G_{\mathcal{P}}$ would become zero and the system would be described by a Poisson manifold, as expected. It can thus be concluded, by (1.131) and by its connection with the standard derivation of observables given in (1.173), that $G_{\mathcal{P}}$ is a fundamental ingredient in the description of quantum systems.

Applications of the geometric formalism are studied along the dissertation. Chapter 2 offers an analysis of the Schrödinger equation in terms of Lie systems. This is a powerful geometric tool in the resolution of differential equations. It will be shown that it is possible to solve the dynamics of quantum systems in this way. Chapter 5 also presents interesting applications in the study of mixed quantum-classical systems, a common problem in molecular dynamics. With this geometric formalism, it is possible to rigorously describe mixed states.

Chapter 2

Lie systems in Quantum Mechanics

A geometric description of Quantum Mechanics offers the possibility to consider quantum systems from a new perspective. Geometrical tools can be used in order to find solutions for usual problems. As an example of the huge potential of this formalism, the present chapter presents a systematic and powerful method for solving the Schrödinger equation making use of the theory of Lie systems.

Since its first conception by Newton and Leibniz, the theory of differential equations have been under study by innumerable mathematicians and scientists. Many different tools have been developed in order to deepen into their analysis. This is the case of Lie systems, particular cases of time-dependent vector fields appearing in the geometric analysis of differential equations [76, 80, 82, 190, 275]. The main characteristic defining a Lie system is the existence of a superposition rule, which gives the general solution to the system in terms of a finite number of independent particular solutions. The Lie-Scheffers theorem [82, 190] shows that a geometrical description of differential equations allows for an easy characterisation of Lie systems.

In the framework of Quantum Mechanics, consider the expression of the time-dependent Schrödinger equation:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \quad t \in \mathbb{R}. \tag{2.1}$$

This is a linear differential equation. Therefore, if the Hilbert space is n-dimensional, the general solution is obtained in terms of n functionally-independent particular solutions $|\psi_1(t)\rangle$, ..., $|\psi_n(t)\rangle$ as

$$|\psi(t)\rangle = \sum_{j=1}^{n} k_j|\psi_j(t)\rangle, \quad k_1, \ldots, k_n \in \mathbb{C}, \quad t \in \mathbb{R}. \tag{2.2}$$

Thus, there always exists a linear superposition rule for the Schrödinger equation depending on n particular solutions. This approach, however, has limitations, as non-linear superposition rules, which also exist for many problems, are not considered. Furthermore, an algebraic description cannot be extended to the set of pure states of the quantum system, namely the projective Hilbert space. A more general description is needed in order to properly describe superposition rules.

As shown recently by Cariñena, Clemente-Gallardo, de Lucas and the author, [70], a geometric description of Quantum Mechanics gives a very detailed characterisation of the problem. Schrödinger equations are, effectively, Lie systems, and as such they admit superposition rules. The additional symmetries of these systems, namely the preservation of the canonical Kähler structure, allow for the explicit computation of these superposition rules. Thus, it has been found that a Schrödinger equation on an n-dimensional Hilbert space, with $n \geq 2$ has a superposition rule depending on $n-1$ particular solutions. This is an improvement with respect to the solution presented in (2.2), albeit with an additional price. The superposition rule thus obtained is, for $n < 2$, non-linear. It is nevertheless a very important result with applications in problems such as the numerical resolution of Schrödinger equation.

Another clear advantage of this geometrical approach is the description of the projective space. As shown before, this manifold can be easily described in geometrical terms. It is in fact possible to obtain

in this way superposition rules for Schrödinger equations in finite-dimensional systems. Thus, it can be concluded that Lie systems are a powerful tool in the characterisation of the properties of quantum systems, in particular in the analysis of its unitary evolution.

This chapter presents the application of the theory of Lie systems to the study of quantum systems. It is mainly based in the results presented in the aforementioned work [70]. Section 2.1 presents a short summary of the theory of Lie systems. Sections 2.2 and 2.3 characterise geometrically the properties of Schrödinger equation as Lie-systems. Their superposition rules can be computed, as done in Section 2.4. Finally, Section 2.5 presents the particular case of 2-level systems.

2.1 Lie systems

A Lie system [76, 80, 190, 275] is a non-autonomous system of first-order differential equations whose general solution can be written in terms of a finite number of particular solutions via a function called a superposition rule. To properly present the theory of Lie systems, some preliminary definitions are needed.

Definition 2.1. *A generalized distribution D on a manifold N is a function mapping each $x \in N$ to a linear subspace $D_x \subset T_xN$. We say that D is regular at $x' \in N$ if $r : x \in N \mapsto \dim D_x \in \mathbb{N} \cup \{0\}$ is locally constant around x'. Similarly, D is said to be regular on an open $U \subset N$ when r is constant on U. Finally, a vector field Y on N takes values in D, in short $Y \in D$, if $Y_x \in D_x$ for all $x \in N$.*

Definition 2.2. *A t-dependent vector field $\mathcal{X}$ on N is a map $\mathcal{X} : (t, x) \in \mathbb{R} \times N \mapsto \mathcal{X}(t, x) \in TN$ such that $\tau_N \circ \mathcal{X} = \pi_2$, where $\pi_2 : (t, x) \in \mathbb{R} \times N \mapsto x \in N$ and τ_N is the canonical projection of the tangent bundle. A t-dependent vector field $\mathcal{X}$ on N amounts to a family of vector fields $\{\mathcal{X}_t\}_{t\in\mathbb{R}}$, with $\mathcal{X}_t : x \in N \mapsto \mathcal{X}(t, x) \in TN$ for all $t \in \mathbb{R}$.*

Definition 2.3. *The smallest Lie algebra of a t-dependent vector field $\mathcal{X}$ is the smallest real Lie algebra, $V^{\mathcal{X}}$, containing $\{\mathcal{X}_t\}_{t\in\mathbb{R}}$, namely $V^{\mathcal{X}} = \mathrm{Lie}(\{\mathcal{X}_t\}_{t\in\mathbb{R}})$.*

An integral curve of $\mathcal{X}$ is an integral curve $\gamma : \mathbb{R} \mapsto \mathbb{R} \times N$ of the so-called suspension of $\mathcal{X}$, i.e. the vector field $\mathcal{X}(t, x) + \partial/\partial t$ on $\mathbb{R} \times N$ [3]. The curve γ always admits a reparametrisation $\bar{t} = \bar{t}(t)$ such that

$$\frac{\mathrm{d}(\pi_2 \circ \gamma)}{\mathrm{d}\bar{t}}(\bar{t}) = (\mathcal{X} \circ \gamma)(\bar{t}). \tag{2.3}$$

This system is referred to as the associated system of $\mathcal{X}$. Conversely, a system of first-order differential equations in normal form is always the associated system of a unique t-dependent vector field. This induces a bijection between t-dependent vector fields and systems of first-order differential equations in normal form. This justifies to denote by $\mathcal{X}$ both a t-dependent vector field and its associated system.

Definition 2.4. *A superposition rule depending on m particular solutions for a system $\mathcal{X}$ on N is a function $\Phi : (u_{(1)}, \ldots, u_{(m)}; \lambda) \in N^m \times N \mapsto \Phi(u_{(1)}, \ldots, u_{(m)}; \lambda) \in N$ such that the general solution, $x(t)$, of $\mathcal{X}$ can be brought into the form $x(t) = \Phi(x_{(1)}(t), \ldots, x_{(m)}(t); \lambda)$, where $x_{(1)}(t), \ldots, x_{(m)}(t)$ is a generic set of particular solutions to $\mathcal{X}$ and $\lambda \in N$.*

Theorem 2.5 (The Lie-Scheffers Theorem [80, 190]). *A system $\mathcal{X}$ on N admits a superposition rule if and only if $\mathcal{X} = \sum_{\alpha=1}^{r} b_\alpha(t) X_\alpha$ for a family $b_1(t), \ldots, b_r(t)$ of t-dependent functions and a basis $X_1, \ldots, X_r$ of a real Lie algebra of vector fields on N.*

If $\mathcal{X}$ possesses a superposition rule, then $\mathcal{X}$ is called a Lie system. The associated real Lie algebra of vector fields $\langle X_1, \ldots, X_r \rangle$ is called a Vessiot-Guldberg Lie algebra of $\mathcal{X}$. The Lie-Scheffers theorem amounts to saying that $\mathcal{X}$ is a Lie system if and only if $V^{\mathcal{X}}$ is finite-dimensional. This fact is the keystone of the theory of Lie systems. From a practical point of view, superposition rules make possible the resolution of differential equations by means of linear algebra. Because of this, solutions of Lie systems can be obtained in many cases, either analytically or with help of numerical tools.

2.1.1 The superposition rule

One of the most important characteristics of Lie systems is the existence of superposition rules. These functions, as mentioned, give an algebraic solution to a differential problem. The computation of their superposition rules has been thoroughly studied [80, 82, 275]. It is possible to obtain the superposition rule of a Lie system by means of its diagonal prolongations, as proved below.

In the following, let N be a differentiable manifold. For any natural number $m \geq 1$, the product set $N^m = N \times \cdots \times N$ (m times) is also a differentiable manifold. Each copy of the initial manifold N in the product manifold N^m is indexed as $N^{(r)}$, with r from 0 to $m-1$. The same notation is used for points, functions and geometrical objects. Points in N^m take the form $(x^{(0)}, x^{(1)}, \ldots, x^{(m-1)}) \in N^m$. Regarding coordinate functions, if N is an n-dimensional manifold with coordinates $(x_1, \ldots, x_n)$, then N^m is an mn-dimensional manifold with coordinates $(x_1^{(0)}, \ldots, x_n^{(0)}, x_1^{(1)}, \ldots, x_n^{(1)}, \ldots, x_1^{(m-1)}, \ldots, x_n^{(m-1)})$.

Definition 2.6. *Let $(E, N, \tau : E \to N)$ be a vector bundle. Its diagonal prolongation to N^m is a vector bundle $(E^{[m]}, N^m, \tau^{[m]} : E^{[m]} \to N^m)$, where $E^{[m]} := E \times \cdots \times E$ (m-times) and $\tau^{[m]}$ is the only map satisfying that $\pi_{N,j} \circ \tau^{[m]} = \tau \circ \pi_{E,j}$ for $j = 0, 1, \ldots, m-1$, with $\pi_{E,j} : E^{[m]} \to E$ and $\pi_{N,j} : N^m \to N$ being the natural projections of $E^{[m]}$ and N^m into the j-th copy of E and N within $E^{[m]}$ and N^m, respectively.*

Definition 2.7. *Given a section $e : N \to E$ of (E, N, τ), its diagonal prolongation to N^m is the section $e^{[m]}$ of $(E^{[m]}, N^m, \tau^{[m]})$ given by*

$$e^{[m]} := e^{(0)} + \cdots + e^{(m-1)}. \tag{2.4}$$

Observe that the diagonal prolongation to N^m of a section $e : N \to E$ is the only section $e^{[m]} : N^m \to E^{[m]}$ satisfying that $\pi_{E,j} \circ e^{[m]} = e \circ \pi_{N,j}$ for $j = 0, 1, \ldots, m-1$. A particular case of diagonal prolongations is that of functions. Given a function f on N, the function $f^{[m]}$ on N^m takes the value

$$f^{[m]}(x^{(0)}, x^{(1)}, \ldots, x^{(m-1)}) = f(x^{(0)}) + f(x^{(1)}) + \cdots + f(x^{(m-1)}), \quad (x^{(0)}, x^{(1)}, \ldots, x^{(m-1)}) \in N^m. \tag{2.5}$$

There exists a natural symmetry in the study of diagonal prolongations given by the interchange of copies of the initial manifold N. In particular, given the diagonal prolongation to N^m of a vector bundle over N, the interchange of any two copies of the manifold implies a change in its sections that has to be properly described.

Proposition 2.8. *Let $(E, N, \tau : E \to N)$ be a vector bundle and $\epsilon : N^m \to E^{[m]}$ a section of its diagonal prolongation to N^m. For any $r = 0, 1, \ldots, m-1$, there exists a unique section $\epsilon_r : N \to E$ such that $\pi_{E,r} \circ \epsilon = \epsilon_r \circ \pi_{N,r}$. These sections completely determine the value of ϵ:*

$$\epsilon = \epsilon_0^{(0)} + \epsilon_1^{(1)} + \cdots + \epsilon_{m-1}^{(m-1)} = \sum_{r=0}^{m-1} \epsilon_r^{(r)}. \tag{2.6}$$

In particular, given a section $e : N \to E$ and its diagonal prolongation $e^{[m]}$, then $e_r^{[m]} = e$ for every $r = 0, 1, \ldots, m-1$.

Definition 2.9. *Let $(E, N, \tau : E \to N)$ be a vector bundle. For any $s, s' = 0, 1, \ldots, m-1$, let $S_{ss'}^E$ be the endomorphism of the set of sections of $(E^{[m]}, N^m, \tau^{[m]} : E^{[m]})$ defined as*

$$S_{ss'}^E(\epsilon) = \sum_{\substack{r=0 \\ r \neq s, s'}}^{m-1} \epsilon_r^{(r)} + \epsilon_s^{(s')} + \epsilon_{s'}^{(s)}. \tag{2.7}$$

The applications thus defined interchange two of the terms of a section ϵ given as in (2.6). Observe that $S_{ss'}^E$ is symmetric under the interchange of its indexes, and that it is the identity application for $s = s'$. Also, if $e^{[m]}$ is the diagonal prolongation of a section $e : N \to E$, then $S_{ss'}^E(e^{[m]}) = e^{[m]}$ for any $s, s' = 0, 1, \ldots, m-1$.

Diagonal prolongations pay a key role in the resolution of Lie systems. The following result gives the number of particular solutions that are needed in order to obtain the general solution of a Lie system by means of a superposition rule.

Theorem 2.10. [80, 82] *Let $\mathcal{X}$ be a Lie system on an n-dimensional manifold N and V its Vessiot-Guldberg Lie algebra. The number m of particular solutions needed to obtain the general solution to $\mathcal{X}$ by means of a superposition rule is the minimum integer such that the diagonal prolongations of elements in V to N^m span at every point a distribution of rank* $\dim V$.

The superposition rule is obtained by means of the implicit function theorem. Let $I_1, \ldots, I_n \in \mathcal{F}(N^{m+1})$ be n common first integrals of the diagonal prolongations of elements in V to N^{m+1} satisfying the condition

$$\det\left(\frac{\partial I_j}{\partial x_k^{(0)}}\right) \neq 0. \tag{2.8}$$

Then, it is possible to solve, at least in the neighbourhood of a point $x \in N^{m+1}$, for the values of $x_1^{(0)}, \ldots, x_n^{(0)}$ in terms of the remaining coordinates and the values $k_1, \ldots, k_n$ that the first integrals $I_1, \ldots, I_n$ take in such point:

$$\Phi(x^{(1)}, \ldots, x^{(m)}, k_1, \ldots, k_n) = x^{(0)}. \tag{2.9}$$

By replacing the arguments of Φ by independent particular solution $x^1(t), \ldots, x^m(t)$ to $\mathcal{X}$, the general solution $x(t)$ is obtained:

$$\Phi(x^1(t), \ldots, x^m(t), k_1, \ldots, k_n) = x(t). \tag{2.10}$$

This procedure to obtain the superposition rule is therefore based in the first integrals of some vector fields. Here is where the additional structures that appear in particular cases of Lie systems play an important role. The properties of Lie systems can be exploit to obtain in a systematic way the first integrals that determine the superposition rule.

2.1.2 Additional structures in Lie systems

As noted above, the existence of additional structures in a manifold makes possible for Lie systems to have richer properties, leading to simplified procedures to solve their integral curves. This is the case of Lie-Hamilton systems in symplectic, Poisson or Dirac manifolds [36, 75, 106, 130, 131, 194]. When $V^{\mathcal{X}}$ consists of Hamiltonian vector fields relative to some geometric structure, much more powerful methods can be devised to study Lie systems.

Definition 2.11. *A system $\mathcal{X}$ on N is said to be a Lie-Hamilton system if $V^{\mathcal{X}}$ is a Vessiot-Guldberg Lie algebra of Hamiltonian vector fields relative to some Poisson bivector field on N.*

Definition 2.12. *A Lie-Hamiltonian structure is a triple (N, Ω, h), where Ω is a Poisson bivector on N and $h : (t, x) \in \mathbb{R} \times N \mapsto h_t(x) := h(t, x) \in \mathbb{R}$ is such that* $\mathrm{Lie}(\{h_t\}_{t\in\mathbb{R}}, \{\cdot,\cdot\}_\Omega)$*, with $\{\cdot,\cdot\}_\Omega$ being the Lie bracket induced by Ω [265], is finite-dimensional.*

The following theorem, presented in [84], gives a characterisation of Lie-Hamilton systems.

Theorem 2.13. *A system $\mathcal{X}$ on N is a Lie-Hamilton system if and only if there exists a Lie-Hamiltonian structure (N, Ω, h) such that $\mathcal{X}_t$ is a Hamiltonian vector field for the function h_t for each $t \in \mathbb{R}$. We say that* $\mathrm{Lie}(\{h_t\}_{t\in\mathbb{R}}, \{\cdot,\cdot\}_\Omega)$ *is a Lie-Hamilton algebra of $\mathcal{X}$.*

Following this idea, the existence of a Kähler structure makes possible to define a new type of Lie systems, the so called Lie-Kähler systems [70]. They are defined as those Lie systems on the manifold such that the Kähler structure is preserved along the evolution. As a consequence, the superposition rule can be determined by the Kähler structure.

Definition 2.14. *A system $\mathcal{X}$ on a Kähler manifold (M, ω, g, J) is called a Lie-Kähler system if it is a Lie-Hamilton structure with respect to the Poisson bivector determined by the symplectic form ω and preserves the complex structure, i.e. $\mathcal{L}_{\mathcal{X}_t} J = 0$ for any $t \in \mathbb{R}$.*

Proposition 2.15. *If $\mathcal{X}$ is a Lie-Kähler system on a Kähler manifold (M, ω, g, J), then for any $t \in \mathbb{R}$, the vector field $\mathcal{X}_t$ is a Killing vector field with respect to the metric tensor g.*

Proof. Tensor fields ω, g and J are related by (1.66). If both ω and J are symmetries for a certain vector field, then g is also a symmetry. The proposition follows as a consequence. □

The following result could be restated in order to use it as an alternate definition of Lie-Kähler systems.

Proposition 2.16. *If $\mathcal{X}$ is a Lie-Kähler system on a Kähler manifold (M, ω, g, J), then any vector field in its Vessiot-Guldberg Lie algebra is a symmetry of the Kähler structure on M.*

Proof. This result is evident as a consequence of the definition of Lie-Kähler systems and Proposition 2.15. □

The existence of symmetries for Lie systems is a key property in order to obtain the superposition rule. As it will be detailed in following sections, Lie-Kähler systems can be solved with help of these symmetries.

2.2 Lie-Kähler systems in Quantum Mechanics

It is known that Lie systems appear in the geometric study of time-dependent Schrödinger equations [44, 83, 85, 86]. The expression of this equation in natural units (with $\hbar = 1$) is

$$\mathrm{i}\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \quad t \in \mathbb{R}, \tag{2.11}$$

where $H(t)$ is a Hermitian operator on $\mathcal{H}$ for every t. This operator is called the time-dependent Hamiltonian of the system. The aim of this section is to prove that, for finite-dimensional systems, it is possible to describe such an equation in terms of a Lie system.

Definition 2.17. *A time-dependent Hamiltonian $H(t)$ is called a quantum Lie system if there exists a set of r real differentiable functions $b_1, \ldots, b_r$ such that*

$$H(t) = \sum_{j=1}^{r} b_j(t) H_j, \tag{2.12}$$

where the Hermitian operators $H_1, \ldots, H_r$ close a finite-dimensional Lie algebra V^H, called the quantum Vessiot-Guldberg Lie algebra of $H(t)$.

Proposition 2.18. *Any time-dependent Hamiltonian on a finite-dimensional Hilbert space is a quantum Lie system.*

Proof. If the Hilbert space $\mathcal{H}$ is finite-dimensional, any basis $\{H_1, \ldots, H_n\}$ for $\mathrm{Herm}(\mathcal{H})$ makes possible to write a generic time-dependent Hamiltonian $H(t)$ in the form of (2.12). For particular cases, it may be possible to find smaller quantum Vessiot-Guldberg Lie algebras for $H(t)$. □

Theorem 2.19. *Consider a quantum Lie system $H(t)$ on a finite-dimensional Hilbert space $\mathcal{H}$, with $V^H = \mathrm{Lie}(H_1, \ldots, H_r)$ its quantum Vessiot-Guldberg Lie algebra. The time-dependent vector field $\mathcal{X}^H$ on the differentiable manifold M_Q defined as*

$$\mathcal{X}^H_t = \sum_{j=1}^{r} b_j(t) X_j, \tag{2.13}$$

with $X_j := X_{H_j}$ being the Hamiltonian vector field on M_Q associated to the Hermitian operator H_j, for $j = 1, \ldots, r$, is a Lie-Kähler system on M_Q. The associated system of $\mathcal{X}^H$ is the time-dependent Schrödinger equation.

Proof. Hamiltonian vector fields satisfy the commutation relation (1.91). If the Lie bracket of V^H is $[\![H_j, H_k]\!] = \sum_l c_{jkl} H_l$, then

$$[X_j, X_k] = -X_{[\![H_j, H_k]\!]} = -\sum_{l=1}^{r} c_{jkl} X_l, \quad j, k = 1, 2, \ldots, r.$$

Therefore, $\mathrm{Lie}(X_1, \ldots, X_r)$ is a finite-dimensional Lie algebra isomorphic to V^H. As a consequence of the Lie-Scheffers Theorem 2.5, $\mathcal{X}^H$ is a Lie system with $\mathrm{Lie}(X_1, \ldots, X_r)$ as its Vessiot-Guldberg Lie algebra.

For each $t \in \mathbb{R}$, the vector field $\mathcal{X}^H_t$ is Hamiltonian with respect to the function on M_Q associated with the operator $\sum_j b_j(t) H_j = H(t)$. Because of Theorem 1.48, its associated differential equation is (2.11), thus proving the relation between Lie systems and the time-dependent Schrödinger equation. □

2.2.1 2-level Lie systems

The above result can be exemplified by studying a 2-level quantum system. The algebraic and geometric descriptions of 2-level systems have been presented in sections 1.1.7 and 1.4, respectively. The Hilbert space of the system is isomorphic to $\mathbb{C}^2$, and observables are represented by matrices in Herm(2). The time-dependent Schrödinger equation is therefore the particularisation of (2.11) to the 2-level system:

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = -\mathrm{i}H(t)|\psi(t)\rangle, \quad H(t) \in \mathrm{Herm}(2), \quad \forall t \in \mathbb{R}. \tag{2.14}$$

A basis for Herm(2) is given by matrices $\sigma_0, \sigma_1, \sigma_2, \sigma_3$, defined in Definition 1.38. A generic Hermitian matrix takes the form

$$A = \sum_{j=0}^{3} a_j \sigma_j = a_0 \sigma_0 + \sum_{j=1}^{3} a_j \sigma_j = \begin{pmatrix} a_0 + a_3 & a_1 - i a_2 \\ a_1 + i a_2 & a_0 - a_3 \end{pmatrix}, \quad a_0, a_1, a_2, a_3 \in \mathbb{R}, \tag{2.15}$$

A time-dependent Hamiltonian can thus be written as

$$H(t) = B_0(t)\sigma_0 + \sum_{j=1}^{3} B_j(t)\sigma_j. \tag{2.16}$$

Physically, this Hamiltonian models a $\frac{1}{2}$-spin system coupled with a time-dependent magnetic field $(B_1(t), B_2(t), B_3(t))$. The time-dependent Hamiltonian $H(t)$ is therefore a quantum Lie system. It determines a Schrödinger equation of the form (2.14) in $\mathbb{C}^2$ [80].

Consider now the geometric formalism presented in the previous chapter. As detailed in Section 1.4, the Hilbert space $\mathcal{H} \cong \mathbb{C}^2$ is replaced by a 4-dimensional differentiable manifold M_Q, provided with a global chart with coordinates (q_1, p_1, q_2, p_2). These coordinates, as presented in (1.49), are

$$z_1 = \frac{1}{\sqrt{2}}(q_1 + \mathrm{i}p_1), \quad z_2 = \frac{1}{\sqrt{2}}(q_2 + \mathrm{i}p_2). \tag{2.17}$$

The quantum Lie system $H(t)$ defines a Lie-Kähler system $\mathcal{X}^H$ on M_Q with expression:

$$\mathcal{X}^H = \sum_{j=0}^{3} B_j(t) X_j, \tag{2.18}$$

The associated system of $\mathcal{X}^H$ is the geometrical equivalent of the Schrödinger equation (2.14). Its coordinate expression is

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} q_1 \\ p_1 \\ q_2 \\ p_2 \end{pmatrix} = \begin{pmatrix} 0 & B_0(t)+B_3(t) & -B_2(t) & B_1(t) \\ -B_0(t)-B_3(t) & 0 & -B_1(t) & -B_2(t) \\ B_2(t) & B_1(t) & 0 & B_0(t)-B_3(t) \\ -B_1(t) & B_2(t) & B_3(t)-B_0(t) & 0 \end{pmatrix}\begin{pmatrix} q_1 \\ p_1 \\ q_2 \\ p_2 \end{pmatrix}. \tag{2.19}$$

The vector fields X_0, X_1, X_2, X_3 span the Vessiot-Guldberg Lie algebra of $\mathcal{X}^H$. The commutation relations can be directly computed by their coordinate expressions:

$$\begin{aligned} X_0 &= p_1\frac{\partial}{\partial q_1} - q_1\frac{\partial}{\partial p_1} + p_2\frac{\partial}{\partial q_2} - q_2\frac{\partial}{\partial p_2}, & X_1 &= p_2\frac{\partial}{\partial q_1} - q_2\frac{\partial}{\partial p_1} + p_1\frac{\partial}{\partial q_2} - q_1\frac{\partial}{\partial p_2}, \\ X_2 &= -q_2\frac{\partial}{\partial q_1} - p_2\frac{\partial}{\partial p_1} + q_1\frac{\partial}{\partial q_2} + p_1\frac{\partial}{\partial p_2}, & X_3 &= p_1\frac{\partial}{\partial q_1} - q_1\frac{\partial}{\partial p_1} - p_2\frac{\partial}{\partial q_2} + q_2\frac{\partial}{\partial p_2}, \end{aligned} \tag{2.20}$$

As expected, these vector fields span a 4-dimensional Lie algebra isomorphic to Herm(2):

$$[X_0, \cdot] = 0, \quad [X_1, X_2] = -X_3, \quad [X_2, X_3] = -X_1, \quad [X_3, X_1] = -X_2. \tag{2.21}$$

Recall that M_Q admits a Kähler structure composed of a symplectic form ω, a metric g and an almost-complex structure J. Their coordinate expressions are given in (1.144) and (1.145). The vector fields X_0, X_1, X_2, X_3 are Hamiltonian with respect to ω. Their Hamiltonian functions are

$$\begin{aligned} h_0(\psi) &= \langle\psi|\sigma_0|\psi\rangle = \frac{1}{2}(q_1^2+p_1^2+q_2^2+p_2^2), & h_1(\psi) &= \langle\psi|\sigma_1|\psi\rangle = q_1q_2+p_1p_2, \\ h_2(\psi) &= \langle\psi|\sigma_2|\psi\rangle = q_1p_2-p_1q_2, & h_3(\psi) &= \langle\psi|\sigma_3|\psi\rangle = \frac{1}{2}(q_1^2+p_1^2-q_2^2-p_2^2), \end{aligned} \tag{2.22}$$

with $\iota_{X_\alpha}\omega = \mathrm{d}h_\alpha$ for $\alpha = 0,1,2,3$. These Hamiltonian functions span a Lie algebra isomorphic to Herm(2):

$$\{h_0, \cdot\} = 0, \qquad \{h_1, h_2\} = h_3, \qquad \{h_2, h_3\} = h_1, \qquad \{h_3, h_1\} = h_2. \tag{2.23}$$

Notice that h_1, h_2, h_3 are functionally independent, but $h_0^2 = 4(h_1^2+h_2^2+h_3^2)$.

The t-dependent Schrödinger equation (2.14) enjoys an additional property. Vector fields X_0, X_1, X_2 and X_3 are Killing vector fields with respect to g, namely $\mathcal{L}_{X_\alpha}g = 0$ for $\alpha = 0,1,2,3$. Using this, it can be proved in an intrinsic geometric way that

$$I_1 = g(X_0, X_0), \qquad I_2 = g(X_1, X_1)+g(X_2, X_2)+g(X_3, X_3), \qquad I_3 = h_1^2+h_2^2+h_3^2, \qquad I_4 = h_0 \tag{2.24}$$

are constants of the motion for X. This example is relevant because it illustrates how to define the above constants of the motion geometrically in terms of g and the Hamiltonian functions due to ω.

Note also that the description in terms of real coordinates comes from a linear complex differential equation. This gives rise to a symmetry $(q_1, p_1, q_2, p_2) \in M_Q \mapsto (-p_1, q_1, -p_2, q_2) \in M_Q$ of system (2.19), which is the counterpart of the multiplication by the imaginary unit in $\mathbb{C}^2$. Therefore, the Lie system preserves the complex structure J in M_Q.

2.2.2 Schrödinger equations and Lie-Kähler systems

The results obtained for the 2-level system can be generalised to larger systems. Lie systems appearing in Quantum Mechanics have the property of preserving the natural Kähler structure. This in turn facilitates the computation of symmetries, key ingredients in the computation of superposition rules.

Theorem 2.20. *Every time-dependent Schrödinger equation on a finite-dimensional Hilbert space $\mathcal{H}$ defines a Lie-Kähler system on the associated Kähler manifold M_Q, whose Vessiot-Guldberg Lie algebra is isomorphic to a subalgebra of* Herm($\mathcal{H}$).

Proof. It is clear by Theorem 2.19 the relation between time-dependent Schrödinger equations on $\mathcal{H}$ and Lie systems on M_Q. The Vessiot-Guldberg Lie algebra of $\mathcal{X}^H$ is isomorphic to the quantum Vessiot-Guldberg Lie algebra V^H of $H(t)$, which in turn is a subalgebra of $\mathrm{Herm}(\mathcal{H})$, as proved in Proposition 2.18. The preservation of the Kähler structure of M_Q remains to be proved.

Consider the natural action $\varphi_{\mathcal{H}} : U(\mathcal{H}) \times \mathcal{H} \to \mathcal{H}$ of the unitary Lie group $U(\mathcal{H})$ on the Hilbert space $\mathcal{H}$. By definition, this action preserves Hermitian product on $\mathcal{H}$. Due to linearity properties, the action also preserves the multiplication by scalar, in particular by the imaginary unit.

$$\langle U\phi|U\chi\rangle = \langle\phi|\chi\rangle, \quad U(\mathrm{i}|\phi\rangle) = \mathrm{i}U|\phi\rangle, \quad \forall U \in U(\mathcal{H}), \quad \forall|\phi\rangle, |\chi\rangle \in \mathcal{H}. \tag{2.25}$$

The action $\varphi_{\mathcal{H}}$ defines additionally an action $\varphi_M : U(\mathcal{H}) \times M_Q \to M_Q$ on the differentiable manifold M_Q. The Hermitian and complex structures on $\mathcal{H}$ are replaced by the Kähler structure on M_Q, which therefore is preserved by this action.

As proved in the previous chapter, the action φ_M is generated by Hamiltonian vector fields. Thus, as every vector in the Vessiot-Guldberg Lie algebra of $\mathcal{X}^H$ is Hamiltonian, it preserves the Kähler structure, hence $\mathcal{X}^H$ is a Lie-Kähler system. □

Proposition 2.21. *The space $I^{\mathcal{X}}$ of time-independent constants of motion for a Lie-Kähler system $\mathcal{X}$ is a Poisson algebra with respect to the Poisson bracket of the Kähler structure and a commutative algebra relative to the bracket induced by the Riemannian structure.*

Proof. This proposition is a consequence of simple computation of differential geometry. Lie derivatives and contractions satisfy the following relation [104, 177]:

$$[\mathcal{L}_X, \iota_Y] = \iota_{[X,Y]}, \tag{2.26}$$

for any pair of vector fields X, Y.

Any time-independent constant of motion $f \in I^{\mathcal{X}}$ satisfies $\mathcal{X}_t(f) = \mathcal{L}_{\mathcal{X}_t}(f) = 0$ for any $t \in \mathbb{R}$. On the other hand, the Hamiltonian vector field X_f associated to f satisfies $\mathrm{d}f = \iota_{X_f}\omega$, with ω the symplectic structure on the Kähler manifold. The two relation combined yield the following result:

$$\mathrm{d}(\mathcal{L}_{\mathcal{X}_t}(f)) = \mathcal{L}_{\mathcal{X}_t}(\mathrm{d}f) = 0 \Rightarrow \mathcal{L}_{\mathcal{X}_t}(\iota_{X_f}\omega) = 0 \Rightarrow \iota_{[\mathcal{X}_t, X_f]}\omega = 0,$$

where the fact that $\mathcal{X}$ is a Lie-Kähler system, hence $\mathcal{L}_{\mathcal{X}_t}\omega = 0$, has been considered.

The Poisson bracket of any two functions f, f' is defined as $\{f, f'\} = \omega(X_f, X_{f'})$. Its Lie derivative with respect to a vector field $Y \in \mathfrak{X}(M_Q)$ satisfies the following relation:

$$\mathcal{L}_Y(\{f, f'\}) = \mathcal{L}_Y(\omega(X_f, X_{f'}) = (\mathcal{L}_Y\omega)(X_f, X_{f'}) - \omega([Y, X_f], X_{f'}) - \omega(X_f, [Y, X_{f'}]).$$

In particular, this relation is held for $Y = \mathcal{X}_t$. If f and f' are constants of motion, then the right-hand side of the equality is zero, hence

$$\mathcal{L}_{\mathcal{X}_t}(\{f, f'\}) = 0, \quad f, f' \in I^{\mathcal{X}}. \tag{2.27}$$

Therefore $\{f, f'\}$ is also a constant of motion. Likewise, the symmetric product defined by the metric g provided by the Kähler structure satisfies a similar relation. □

The presence of a Kähler structure makes possible to devise techniques in order to obtain constants of the motion and superposition rules for Lie-Kähler systems, as hinted for the 2-level system. If two vector fields Y_1, Y_2 commute with all the elements of the Vessiot-Guldberg Lie algebra of a Lie-Kähler system $\mathcal{X}$, then $g(Y_1, Y_1)$, $g(Y_2, Y_2)$, $g(Y_1, Y_2)$ and $\omega(Y_1, Y_2)$ are constants of motion for $\mathcal{X}$.

2.3 Lie systems on the quantum quotient manifolds

As fully explained in Section 1.3, the proper description of the states of quantum systems requires an analysis of the fibration $\mathcal{F}_{\Delta\Gamma}$ of M_Q generated by vector fields Γ and Δ. This fibration is regular on $M_{Q,0} = M_Q - \{0\}$, and a projection onto the manifold of leaves of the foliation can be determined. Furthermore, as these vector fields commute, the projection can be decomposed in two steps, and carried out in any order.

As a result, different quotient manifolds $\mathcal{R}$, $\mathcal{Q}$ and $\mathcal{P}$ are obtained. They are collectively referred to as the quantum quotient manifolds. The diagram in Figure 2.1 reproduces the existing maps and inclusions. Also, the relevant structures in each manifold are indicated. The following sections consider the properties of Lie systems determined by time-dependent Schrödinger equations on each of the quantum quotient manifolds.

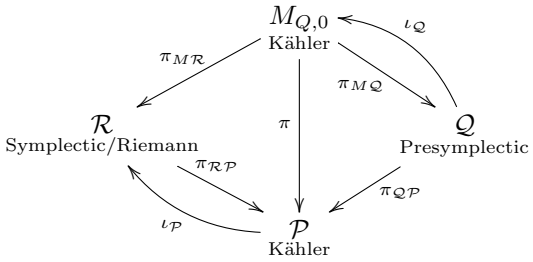


Figure 2.1: The diagram illustrates the differentiable manifolds appearing in the study of quantum systems. The projections and natural inclusions are indicated. Each manifold is labelled according to the relevant geometric structure it possesses. These structures are useful in the determination of superposition rules for Lie systems.

2.3.1 Lie systems on the manifold $\mathcal{Q}$

Consider the inclusion $\iota_{\mathcal{Q}} : \mathcal{Q} \to M_{Q,0}$, as indicated in Figure 2.1. Since the unitary evolution in $\mathcal{H}$ determined by the Schrödinger equation preserves the norm of vector, its geometrical counterpart on $M_{Q,0}$ leaves $\iota_{\mathcal{Q}}(\mathcal{Q})$ invariant. Thus, it seems natural at first to restrict the associate Lie-Kähler system to the unity sphere $\mathcal{Q}$. Nevertheless, as shown below, such a restriction is generally no longer neither a Lie-Kähler system nor a Lie-Hamilton one.

Proposition 2.22. *Consider the Lie-Kähler system $\mathcal{X}^H$ on $M_{Q,0}$ determined by a quantum Lie system $H(t)$. It can be projected to $\mathcal{Q}$ giving rise to a Lie system $\mathcal{X}^H_{\mathcal{Q}}$ possessing a Vessiot-Guldberg Lie algebra $V_{\mathcal{Q}}$ of Hamiltonian vector fields with respect to the presymplectic form $\omega_{\mathcal{Q}} := \iota^*_{\mathcal{Q}}\omega$ with $\iota_{\mathcal{Q}} : \mathcal{Q} \to M_Q$. If $V^{\mathcal{X}^H_{\mathcal{Q}}} = V_{\mathcal{Q}}$, then $\mathcal{X}^H_{\mathcal{Q}}$ is not a Lie-Hamilton system.*

Proof. For a generic quantum Lie system $H(t)$, the Vessiot-Guldberg Lie algebra $V^{\mathcal{X}^H}$ of $\mathcal{X}^H$ is the Lie algebra of fundamental vector fields of the unitary action on M_Q, namely $\varphi_M : U(\mathcal{H}) \times M_Q \to M_Q$, as proved in Proposition 2.18. Recall that unitary action preserves the Hermitian product in $\mathcal{H}$. Hence, the norm $\|\psi\|$ defined by the metric g is invariant under φ_M and, in consequence, a first-integral of its fundamental vector fields, which span $V^{\mathcal{X}^H}$. The restrictions of the elements of $V^{\mathcal{X}^H}$ to $\mathcal{Q}$ become tangent to $\iota_{\mathcal{Q}}(\mathcal{Q})$ and therefore they span a finite-dimensional Lie algebra of vector fields $V_{\mathcal{Q}}$ on $\mathcal{Q}$. The Lie-Kähler system $\mathcal{X}^H$, being generated by the elements in $V^{\mathcal{X}^H}$, can also be restricted to $\iota_{\mathcal{Q}}(\mathcal{Q})$. It gives rise to a Lie system $\mathcal{X}^H_{\mathcal{Q}}$ on $\mathcal{Q}$ admitting a Vessiot-Guldberg Lie algebra $V_{\mathcal{Q}}$.

The embedding $\iota_{\mathcal{Q}} : \mathcal{Q} \to M_Q$ gives rise to a presymplectic structure $\omega_{\mathcal{Q}} = \iota^*_{\mathcal{Q}}\omega$ on $\mathcal{Q}$, where ω is the natural symplectic structure on M_Q. Since the elements of $V^{\mathcal{X}^H}$ are Hamiltonian vector fields on M_Q with Hamiltonian functions $h_H(\psi) = \frac{1}{2}\langle\psi|H|\psi\rangle$ with $H \in \mathrm{Herm}(\mathcal{H})$, their restrictions to $\mathcal{Q}$ are

Hamiltonian relative to the presymplectic form $\omega_{\mathcal{Q}}$ with Hamiltonian functions $\iota_{\mathcal{Q}}^* h_H$. Therefore, the algebra $V_{\mathcal{Q}}$ on $\mathcal{Q}$ is composed of Hamiltonian vector fields relative to the presymplectic structure $\omega_{\mathcal{Q}}$.

As $\mathcal{Q}$ is an orbit of φ_M, then $T\mathcal{Q} = D^{V^{\mathcal{X}^H}}|_{\mathcal{Q}}$, which is an odd $(2n-1)$-dimensional distribution on $\mathcal{Q}$. From assumption, $V^{X_{\mathcal{Q}}} = V_{\mathcal{Q}}$, and hence $D^{X_{\mathcal{Q}}} = D^{V_{\mathcal{Q}}} = D^{V^{\mathcal{X}^H}}|_{\mathcal{Q}} = T\mathcal{Q}$. The so-called no-go Theorem for Lie-Hamilton systems (see [84]) states that previous conditions are enough to ensure that $\mathcal{X}_{\mathcal{Q}}^H$ is not a Lie-Hamilton system. □

A Dirac structure is a generalisation of presymplectic and Poisson manifolds. In fact, presymplectic and Poisson manifolds can be naturally attached to Dirac structures whose Hamiltonian vector fields are exactly the Hamilton vector fields of the structures originating them (see [75] for details). This fact makes possible to prove the following.

Corollary 2.23. *The Lie system $\mathcal{X}_{\mathcal{Q}}^H$ on $\mathcal{Q}$ determined by a quantum Lie system $H(t)$ is a Dirac-Lie system with respect to the Dirac structure induced by $\omega_{\mathcal{Q}}$.*

2.3.2 Lie systems on the manifold $\mathcal{R}$

The next results prove that the projection of the restriction of the Lie-Kähler system $\mathcal{X}^H$ to $M_{Q,0}$ onto $\mathcal{R}$ exists and it is a Lie-Hamilton system. It can be endowed with a natural coordinate system coming from this fact. Some preliminary results are given in the form of lemmas.

Lemma 2.24. *The manifold $\mathcal{R}$ satisfies the following relation:*

$$\mathcal{R} := M_{Q,0}/U(1) \cong \frac{SU(n)}{U(n-1)} \times \mathbb{R}_+. \tag{2.28}$$

Proof. Recall from Section 1.3.2 that $\mathcal{Q}$ is obtained as the set of leaves of the foliation by Δ of $M_{Q,0}$. As Δ is the infinitesimal generator of the group action of $\mathbb{R}_+$ on the manifold, then it is clear that $M_{Q,0} \cong \mathcal{Q} \times \mathbb{R}_+$. If $\mathcal{H}$ is the Hilbert space of an n-level system, then the Lie group $U(\mathcal{H})$ acts naturally on $\mathcal{Q}$ transitively. The isotropy group of an element $\psi \in \mathcal{Q}$ is given by the special unitary transformations leaving ψ invariant, i.e. $U(n-1)$. Hence $\mathcal{Q} \cong U(n)/U(n-1)$. Consider the natural group morphism

$$\mathcal{K} : A \in U(1) \mapsto \mathrm{diag}(\overbrace{1, \ldots, 1}^{(n-1)-\text{times}}, \det A) \in U(n).$$

The Lie group $\mathcal{K}(U(1))$ acts on $SU(n)$ by inner automorphisms giving rise to a semidirect product $U(1) \ltimes SU(n)$. Moreover, there exists a Lie group isomorphism $A \in U(n) \mapsto (\mathcal{K}(\det A), \mathcal{K}(\det{}^{-1} A)A) \in U(1) \ltimes SU(n)$. Therefore,

$$\mathcal{R} \simeq \frac{\mathcal{Q}}{U(1)} \times \mathbb{R}_+ \simeq \frac{U(n)/U(1)}{U(n-1)} \times \mathbb{R}_+ \simeq \frac{SU(n)}{U(n-1)} \times \mathbb{R}_+, \tag{2.29}$$

as proposed. □

Lemma 2.25. *The manifold $\mathcal{R}$ admits a local coordinate system on a neighbourhood of each point given by $2n-1$ functions $f_\alpha(\psi) = \frac{1}{2}\langle\psi|H_\alpha|\psi\rangle$, for $\alpha = 1, 2, \ldots, 2n-1$, for certain traceless observables $H_\alpha \in \mathrm{Herm}(\mathcal{H})$.*

Proof. For $n > 1$ any two elements of $M_{Q,0}$ with the same norm can be connected by the action of an element of $SU(n)$. Hence, the special unitary action $SU(n) \times M_{Q,0} \to M_{Q,0}$, with $n > 1$, has $(2n-1)$-dimensional orbits, which are embedded submanifolds of $M_{Q,0}$. Since $\dim SU(n) = n^2 - 1 \geq 2n - 1$ for $n > 1$, for any point of $M_{Q,0}$ there exists an open neighbourhood A_0 where $2n-1$ fundamental vector fields of φ are linearly independent at each point. As they are also Hamiltonian vector fields, their Hamiltonian functions, which can be taken of the form $f_\alpha(\psi) = \frac{1}{2}\langle\psi|H_\alpha|\psi\rangle$, with $H_\alpha \in \mathrm{Herm}(\mathcal{H})$ traceless observables and $\alpha = 1, 2, \ldots, 2n-1$, are functionally independent on A_0. These functions are invariant

under the natural action of $U(1)$ on $M_{Q,0}$, and give rise to well-defined functions $f_1|_{\mathcal{R}}, \ldots, f_{2n-1}|_{\mathcal{R}}$, on an open subset of $\mathcal{R}$. As $f_1, \ldots, f_{2n-1}$ are functionally independent on $A_0 \subset M_{Q,0}$, then $f_1|_{\mathcal{R}}, \ldots, f_{2n-1}|_{\mathcal{R}}$ are functionally independent and provide a local coordinate system on $\mathcal{R}$. □

This lemma provides a method to obtain coordinates on the quantum quotient manifold $\mathcal{R}$ of any finite-dimensional quantum system. To illustrate this result, the 2-level system is characterised. Recall that a 2-level system is described by a 4-dimensional manifold M_Q with coordinates (q_1, p_1, q_2, p_2), as described in Section 1.4. The time-dependent Schrödinger equation has already been discussed in Section 2.2.1, which in turn defines the following Lie-Kähler system

$$\mathcal{X}_t^H = \sum_{j=0}^{3} B_j(t) X_j, \tag{2.30}$$

The vector fields X_0, X_1, X_2, X_3, given in (2.20), are Hamiltonian vector fields with respect to the natural symplectic structure on M_Q. Their Hamiltonian functions h_0, h_1, h_2, h_3 are given in (2.22).

Functions h_1, h_2, h_3 satisfy the conditions of Lemma 2.25, as they are the functions associated to the traceless observables $\sigma_1, \sigma_2, \sigma_3 \in \mathrm{Herm}(2)$. As any other traceless observable is a linear combination of them, it can be concluded by Lemma 2.25 that these functions define a coordinate system on $\mathcal{R}$. To verify it, consider the map $\phi_\sigma : M_{Q,0} \to \mathbb{R}_0^3$ given by

$$\phi_\sigma(\psi) = (h_1(\psi), h_2(\psi), h_3(\psi)) = (x, y, z) \in \mathbb{R}^3 \Rightarrow \begin{cases} x = q_1 q_2 + p_1 p_2 = \mathrm{Re}\,(z_1^* z_2), \\ y = q_1 p_2 - q_2 p_1 = \mathrm{Im}\,(z_1^* z_2), \\ z = \dfrac{1}{2}(q_1^2 + p_1^2 - q_2^2 - p_2^2) = \dfrac{1}{2}(|z_1|^2 - |z_2|^2). \end{cases} \tag{2.31}$$

where the complex notation $(z_1, z_2) = (q_1 + ip_1, q_2 + ip_2)$ is used. Observe that

$$x^2 + y^2 + z^2 = \frac{1}{4}(|z_1|^2 + |z_2|^2)^2. \tag{2.32}$$

The manifold $\mathcal{R}$ is defined as the set of equivalence classes under the natural action of $U(1)$. With this complex notation, this action is simply $(e^{i\alpha}, (z_1, z_2)) \mapsto (e^{i\alpha} z_1, e^{i\alpha} z_2)$. Hence, x, y, z are constant along these equivalence classes. Furthermore, if $\psi, \psi' \in M_{Q,0}$ belong to the same equivalence class, then $\phi_\sigma(\psi) = \phi_\sigma(\psi')$. This implication works on both directions. Indeed, consider two points $\psi = (z_1, z_2)$ and $\psi' = (z_1', z_2')$ such that $\phi_\sigma(\psi) = \phi_\sigma(\psi')$. Then, because of (2.31) and (2.32):

$$|z_1| = |z_1'|, \quad |z_2| = |z_2'|, \quad z_1^* z_2 = (z_1')^* z_2'. \tag{2.33}$$

In view of this, $(z_1, z_2) = e^{i\alpha}(z_1', z_2')$ for some $\alpha \in \mathbb{R}$. Thus, if $\phi_\sigma^{-1}(x, y, z)$ is not empty, it gives rise to an equivalence class of $\mathcal{R}$.

It remains to be proved that ϕ_σ is a surjection. For every $(x, y, z) \in \mathbb{R}_0^3$, it can be verified that

$$\phi_\sigma\left(\sqrt{2(\sqrt{x^2+y^2+z^2}+z)},\ e^{i\Theta}\sqrt{2(\sqrt{x^2+y^2+z^2}-z)}\right) = (x, y, z), \tag{2.34}$$

where $\Theta \in [0, 2\pi)$ is the unique angle satisfying

$$\frac{x}{\sqrt{x^2+y^2}} = \cos\Theta, \qquad \frac{y}{\sqrt{x^2+y^2}} = \sin\Theta.$$

The above expressions show that ϕ_σ is surjective. Therefore, $\phi_\sigma^{-1}(x, y, z)$ is the equivalence class of an element of $\mathcal{R}$ for every $(x, y, z) \in \mathbb{R}_0^3$ and $\mathcal{R} \cong \mathbb{R}_0^3$.

Once defined an appropriate differentiable structure on the manifold $\mathcal{R}$, the following results show the properties of the Lie systems representing the time-dependent Schrödinger equation on this manifold.

Proposition 2.26. *The time-dependent Schrödinger equation, when restricted to $M_{Q,0}$, can be projected onto $\mathcal{R}$ originating a Lie-system $\mathcal{X}^H_{\mathcal{R}}$ possessing a Vessiot-Guldberg Lie algebra $V_{\mathcal{R}} \simeq \mathfrak{su}(\mathcal{H})$ of Hamiltonian vector fields with respect to the projection of Ω on $M_{Q,0}$ onto $\mathcal{R}$.*

Proof. The $\mathbb{C}$-linear Lie group action $\varphi_M : U(\mathcal{H}) \times M_{Q,0} \to M_{Q,0}$ induces, due to its $\mathbb{C}$-linearity, an action $\phi_{\mathcal{R}}$ on $\mathcal{R}$ such that the map $\pi_{M\mathcal{R}}$ is equivariant, as follows:

$$\begin{array}{rccc} \varphi_{\mathcal{R}} : & U(\mathcal{H}) \times \mathcal{R} & \longrightarrow & \mathcal{R}, \\ & (g, [\psi]_{\mathcal{R}}) & \longmapsto & [\varphi_M(g, \psi)]_{\mathcal{R}}. \end{array} \tag{2.35}$$

Let V_M denote the algebra of fundamental vector fields of φ_M As a consequence of (2.35), vectors in V_M project onto $\mathcal{R}$ giving rise to a new finite-dimensional Lie algebra of vector fields $V_{\mathcal{R}}$. The projection map $\pi_{M\mathcal{R}} : M_{Q,0} \to \mathcal{R}$ induces a Lie algebra morphism $\pi_{M\mathcal{R}*}|_{V_M} : V_M \to V_{\mathcal{R}}$. Then, the restriction to $M_{Q,0}$ of the Lie-Kähler system $\mathcal{X}^H$ describing Schrödinger equation also projects onto $\mathcal{R}$, giving rise to a Lie system $\mathcal{X}^H_{\mathcal{R}}$.

It can be proved that $\mathcal{X}^H_{\mathcal{R}}$ admits a Vessiot-Guldberg Lie algebra isomorphic to $\mathfrak{su}(\mathcal{H})$. As $V_M \simeq \mathfrak{u}(\mathcal{H}) \simeq \mathbb{R} \oplus \mathfrak{su}(\mathcal{H})$, the kernel of $\pi_{M\mathcal{R}*}|_{V_M}$, which is an ideal of V_M, may be either zero, isomorphic to $\mathbb{R}$, to $\mathfrak{su}(\mathcal{H})$ or to $\mathfrak{u}(\mathcal{H})$. The one-parameter group of diffeomorphism induced by the vector field Γ is given by $\Phi^{\Gamma}_t : \psi \in M_{Q,0} \mapsto e^{it}\psi \in M_{Q,0}$. Hence, $\pi_{M\mathcal{R}*}(\Gamma) = 0$ and Γ belongs to the center of V_M. As $V_{\mathcal{R}} \neq 0$ and in view of the decomposition of V_M, then $\ker \pi_{M\mathcal{R}*} \simeq \langle \Gamma \rangle$ and $\operatorname{Im} \pi_{M\mathcal{R}*}|_{V_M} \simeq \mathfrak{su}(\mathcal{H})$. Thus, the projection of the Lie-Kähler system $\mathcal{X}^H$ onto $\mathcal{R}$ admits a Vessiot-Guldberg Lie algebra $V_{\mathcal{R}} \simeq \mathfrak{su}(\mathcal{H})$. □

In the case of 2-level systems, a simple computation shows that there exist vector fields Y_α on $\mathcal{R}$ such that $\pi_{M\mathcal{R}*}(X_\alpha) = Y_\alpha$ for $\alpha = 1, 2, 3$. Indeed,

$$Y_1 = -z\frac{\partial}{\partial y} + y\frac{\partial}{\partial z}, \quad Y_2 = z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}, \quad Y_3 = -y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}. \tag{2.36}$$

The Lie brackets between these vector fields read

$$[Y_1, Y_2] = -Y_3, \quad [Y_2, Y_3] = -Y_1, \quad [Y_3, Y_1] = -Y_2 \quad \Longrightarrow \quad [Y_j, Y_k] = -\sum_{l=1}^{3} \epsilon_{jkl} Y_l, \quad j, k = 1, 2, 3 \tag{2.37}$$

The projection of the Lie-Kähler system $\mathcal{X}^H$ given in (2.13) onto $\mathcal{R}$, i.e. the t-dependent vector field $\mathcal{X}^H_{\mathcal{R}}$ on $\mathcal{R}$ satisfying $(\mathcal{X}^H_{\mathcal{R}})_t = \pi_{M\mathcal{R}*}(X_t)$, becomes

$$\mathcal{X}^H_{\mathcal{R}} = \sum_{j=1}^{3} B_j(t) Y_j, \quad t \in \mathbb{R}. \tag{2.38}$$

Comparison between (1.39) and (2.37) shows that the Vessiot-Guldberg Lie algebra of $\mathcal{X}^H_{\mathcal{R}}$ is isomorphic to $\mathrm{Herm}(2) \cong \mathfrak{su}^*(2)$. Therefore, $\mathcal{X}^H_{\mathcal{R}}$ is a Lie system. Observe that Y_1, Y_2, Y_3 span a two-dimensional distribution on $\mathcal{R}$.

Returning to the general case, the following proposition shows that $\mathcal{R}$ can be endowed with a Poisson structure, turning $V_{\mathcal{R}}$ into a Lie algebra of Hamiltonian vector fields.

Proposition 2.27. *The Lie system $\mathcal{X}^H_{\mathcal{R}}$ is a Lie-Hamilton system with respect to the bivector field $\pi_{M\mathcal{R}*}(\Omega)$, which is a Poisson tensor.*

Proof. Since $\mathcal{L}_\Gamma \Omega = 0$, the Poisson bivector Ω on $M_{Q,0}$ can be projected onto $\mathcal{R}$. Additionally,

$$\pi_{M\mathcal{R}*}([\Omega, \Omega]_{SN}) = [\pi_{M\mathcal{R}*}(\Omega), \pi_{M\mathcal{R}*}(\Omega)]_{SN}, \tag{2.39}$$

with $[\cdot, \cdot]_{SN}$ being the Schouten-Nijenhuis bracket [265]. Thus, $\pi_{M\mathcal{R}*}(\Omega)$ is a Poisson bivector on $\mathcal{R}$. The vector fields X_α spanning the Vessiot-Guldberg Lie algebra V_M of $\mathcal{X}^H$ are Hamiltonian relative to the restrictions to $M_{Q,0}$ of the functions h_α in (2.22). Such Hamiltonian functions are invariant with respect to the action of $U(1)$ on $M_{Q,0}$ and hence projectable onto $\mathcal{R}$. The projections $\pi_{M\mathcal{R}*}(X_\alpha)$ are thus Hamiltonian vector fields with Hamiltonian functions x_α such that $h_\alpha = \pi^*_{M\mathcal{R}}(x_\alpha)$. Therefore, the Vessiot-Guldberg Lie algebra $V_{\mathcal{R}}$ on $\mathcal{R}$ consists of Hamiltonian vector fields relative to $\pi_{M\mathcal{R}*}(\Omega)$. □

Proposition 2.28. *The Vessiot-Guldberg Lie algebra of the Lie system $\mathcal{X}^H_{\mathcal{R}}$ consists of Killing vector fields with respect to the metric induced by the projection of the tensor field G onto $\mathcal{R}$.*

Proof. As shown in (1.115), the Lie derivative of G with respect to Γ is zero. Hence, G projects onto $\mathcal{R}$. Since G is Riemannian, it is non-degenerate, and so is its projection onto $\mathcal{R}$. giving rise to a Riemannian metric on $\mathcal{R}$. The vector fields of V_M are Killing relative to G and projectable under $\pi_{M\mathcal{R}*}$. Therefore, their projections, namely the elements of $V_{\mathcal{R}}$, are also Killing vector fields relative to the projection of G onto $\mathcal{R}$ and span a Vessiot-Guldberg Lie algebra $V_{\mathcal{R}}$ of Killing vector fields. □

The projections of the contravariant tensor fields Ω and G onto $\mathcal{R}$ can be easily computed for the 2-level system. For example, the Poisson bivector Ω on M_Q projects onto $\mathcal{R}$ giving rise to the Poisson bivector

$$\pi_{M\mathcal{R}*}(\Omega) = z\frac{\partial}{\partial x}\wedge\frac{\partial}{\partial y} + x\frac{\partial}{\partial y}\wedge\frac{\partial}{\partial z} + y\frac{\partial}{\partial z}\wedge\frac{\partial}{\partial x}, \tag{2.40}$$

in the coordinate system given in (2.31). Similarly, the tensor field G on M_Q projects onto $\mathcal{R}$ giving rise to the tensor field

$$\pi_{M\mathcal{R}*}(G) = (x^2+y^2+z^2)^{1/2}\left(\frac{\partial}{\partial x}\otimes\frac{\partial}{\partial x} + \frac{\partial}{\partial y}\otimes\frac{\partial}{\partial y} + \frac{\partial}{\partial z}\otimes\frac{\partial}{\partial z}\right). \tag{2.41}$$

This tensor field naturally defines a Riemannian metric $g_{\mathcal{R}}$ on $\mathcal{R}$ given by

$$g_{\mathcal{R}} = \frac{\mathrm{d}x\otimes\mathrm{d}x + \mathrm{d}y\otimes\mathrm{d}y + \mathrm{d}z\otimes\mathrm{d}z}{(x^2+y^2+z^2)^{1/2}}. \tag{2.42}$$

It is immediate to check that the Lie derivatives of these tensor fields with respect to the vector fields (2.36) are zero, in agreement with Propositions 2.27 and 2.28.

2.3.3 Lie-Kähler system on the projective manifold $\mathcal{P}$

As proved above, it is possible to project the Lie-Kähler system $\mathcal{X}^H$ associated to a quantum Lie system $H(t)$ onto the projective manifold $\mathcal{P}$. Additionally, this manifold presents a Kähler structure that is preserved along the evolution. Thus, the time-dependent vector field representing the projective time-dependent Schrödinger equation happens to be again a Lie-Kähler system.

Lemma 2.29. *The Lie-Kähler system $\mathcal{X}^H$ on $M_{Q,0}$ related to a time-dependent Schrödinger equation is projectable under $\pi : M_{Q,0}\to\mathcal{P}$ onto a Lie system $\mathcal{X}^H_{\mathcal{P}}$.*

Proof. Let $\varphi_M : U(\mathcal{H})\times M_{Q,0}\to M_{Q,0}$ be the action the unitary group on $M_{Q,0}$. There exists a natural action of $U(\mathcal{H})$ onto $\mathcal{P}$ given by

$$\begin{array}{rccc} \varphi_{\mathcal{P}}: & U(\mathcal{H})\times\mathcal{P} & \to & \mathcal{P}, \\ & (g,[\psi]_{\mathcal{P}}) & \mapsto & [\varphi_M(g,\psi)]_{\mathcal{P}}. \end{array} \tag{2.43}$$

Then, the map $\pi : M_{Q,0}\to\mathcal{P}$ is equivariant. Let V_M and $V_{\mathcal{P}}$ denote the Lie algebras of fundamental vector fields of φ_M and $\varphi_{\mathcal{P}}$, respectively. Each vector field of V_M projects onto a fundamental vector field of $\varphi_{\mathcal{P}}$. As $\mathcal{X}^H$ takes values in V_M, this ensures $\mathcal{X}^H_{\mathcal{P},t} = \pi_*(\mathcal{X}^H_t)$ to exist for each $t\in\mathbb{R}$. Thus, $\mathcal{X}^H_{\mathcal{P}}$ is a Lie system whose Vessiot-Guldberg Lie algebra is $V_{\mathcal{P}}$. □

Definition 2.30. *Given a Schrödinger equation (2.11), with $\mathcal{X}^H$ its corresponding Lie-Kähler system on M_Q, the projective Schrödinger equation on $\mathcal{P}$ is the system of differential equations*

$$\frac{\mathrm{d}\xi}{\mathrm{d}t} = \mathcal{X}^H_{\mathcal{P}}(t,\xi), \quad \xi\in\mathcal{P}, \quad \forall t\in\mathbb{R}, \tag{2.44}$$

where $\mathcal{X}^H_{\mathcal{P}}$ is the projection onto $\mathcal{P}$ of $\mathcal{X}^H$ under $\pi : M_{Q,0}\to\mathcal{P}$.

Theorem 2.31. *The system (2.44) is a Lie-Kähler system with respect to the natural Kähler structure on $\mathcal{P}$. Its Vessiot-Guldberg Lie algebra is, in general, isomorphic to $\mathfrak{su}(\mathcal{H})$.*

Proof. In view of Theorem 2.20, the vector fields of V_M leave invariant G and Ω, i.e. $\mathcal{L}_X\Omega = \mathcal{L}_X G = 0$ for every $X \in V_M$. Since this vectors are projectable onto $\mathcal{P}$, they span a Vessiot-Guldberg Lie algebra $V_{\mathcal{P}}$ for $\mathcal{X}^H_{\mathcal{P}}$ of Kähler vector fields relative to the natural Kähler structure on $\mathcal{P}$.

The natural projection map $\pi : M_{Q,0} \to \mathcal{P}$ induces a Lie algebra morphism $\pi_*|_{V_M} : V_M \to V_{\mathcal{P}}$. As $V_M \simeq \mathfrak{u}(\mathcal{H}) \simeq \mathbb{R} \oplus \mathfrak{su}(\mathcal{H})$, the kernel of $\pi_*|_{V_M}$, which is an ideal of V_M, may be either zero, isomorphic to $\mathbb{R}$, to $\mathfrak{su}(\mathcal{H})$ or to $\mathfrak{u}(\mathcal{H})$. The one-parameter group of diffeomorphism induced by the vector field Γ on $M_{Q,0}$ is given by $\Phi^\Gamma_t : \psi \in M_{Q,0} \mapsto e^{it}\psi \in M_{Q,0}$. Hence, $\pi_*(\Gamma) = 0$ and Γ belongs to the kernel. Since $V_{\mathcal{P}} \neq \{0\}$ and in view of the decomposition of V_M, then $\ker \pi_* \simeq \langle \Gamma \rangle$ and $\operatorname{Im} \pi_*|_{V_M} \simeq \mathfrak{su}(\mathcal{H})$. Thus, $V_{\mathcal{P}} \simeq \mathfrak{su}(\mathcal{H})$. □

2.4 Superposition rules for Schrödinger equations

The previous section has proved the equivalence between Schrödinger equation and Lie systems. Thus, the tools developed for the study of Lie systems can be employed in order to describe quantum evolution. In particular, it is possible to devise superposition rules that give as a result the general solution to the Schrödinger equation, either on M_Q or on any of the quantum quotient manifolds.

As explained in the beginning of the present chapter, the existence of superposition rules in Quantum Mechanics is not a new discovery. Consider a Schrödinger equation on a finite-dimensional Hilbert space $\mathcal{H}$,

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \quad t \in \mathbb{R}. \tag{2.45}$$

The general solution for this differential equation can be obtained, due to the linear nature of $\mathcal{H}$, as

$$|\psi(t)\rangle = \sum_{j=1}^{n} k_j |\psi_j(t)\rangle, \quad k_1, \ldots, k_n \in \mathbb{C}, \quad n = \dim_{\mathbb{C}} \mathcal{H}, \quad t \in \mathbb{R}, \tag{2.46}$$

with $|\psi_1(t)\rangle$, ..., $|\psi_n(t)\rangle$ linearly independent particular solutions. A similar expression cannot be found on the projective Hilbert space, as it is not a linear space. Lie systems, not being bounded to linearity conditions, generalise this idea. As shown in the following theorems, it is possible to derive a superposition rule on M_Q and also on the quantum quotient manifolds. It is proved below that the superposition rule on M_Q thus obtained depends only on $n-1$ particular solution; however, unlike (2.46), it is non-linear for $n < 2$.

2.4.1 Particular solutions of the Schrödinger equation

It is possible to determine, for each manifold, the necessary number of particular solutions in order to derive the superposition rule. The algorithm that gives the number of necessary particular solution has been presented in [80,82], and summarised in Section 2.1.1. The aim of the present section is to apply this algorithm to the Lie-Kähler system on M_Q. In order to obtain a relevant result, physical considerations have to be made. Due to the expression (2.12) of quantum Lie systems, the general Vessiot-Guldberg Lie algebra of a generic Lie-Kähler system on M_Q is isomorphic to $\mathcal{O} = \mathrm{Herm}(\mathcal{H})$. From a physical perspective, however, only vector fields with non-zero projection onto $\mathcal{P}$ are relevant. This is no the case of the Hamiltonian vector field X_I associated with the identity observable. This element, and any one proportional to it, can thus been taken out of the Vessiot-Guldberg algebra of the Lie-Kähler system. The result is isomorphic to the algebra of traceless Hermitian operators on $\mathcal{H}$, which is itself isomorphic to $\mathfrak{su}(\mathcal{H})$. This is the algebra of traceless skew-Hermitian operators on $\mathcal{H}$, and the Lie algebra associated to the Lie group $SU(\mathcal{H})$ of special unitary transformations on $\mathcal{H}$. Because of this physical property, an interesting result can be obtained, as seen next.

Theorem 2.32. *Every Lie-Kähler system $\mathcal{X}^H$ on M_Q with a Vessiot-Guldberg Lie algebra V^H isomorphic to $\mathfrak{su}(\mathcal{H})$ admits a superposition rule depending on $n-1$ particular solutions.*

Proof. Consider a traceless quantum Lie-system $H(t)$ on $\mathcal{H}$ and its corresponding Lie system $\mathcal{X}^H$ on M_Q. In light of Theorem 2.20, this system admits a Vessiot-Guldberg Lie algebra V of Kähler vector fields isomorphic to $\mathfrak{su}(\mathcal{H})$. The first step to derive a superposition rule is the determination of the smallest $m \in \mathbb{N}$ so that the diagonal prolongations to M_Q^m of the vector fields of V^H span a distribution of rank $\dim V^H$ at a generic point. Since $V^H \subset V_M$ and $V^H \simeq \mathfrak{su}(\mathcal{H})$, the elements of V are fundamental vector fields of the standard linear action of $SU(\mathcal{H})$ on M_Q (thought of as a $\mathbb{C}$-linear space). The diagonal prolongations of V to M_Q^m span the tangent space to the orbits of the Lie group action

$$\begin{array}{rccc} \varphi_M^m : & SU(\mathcal{H}) \times M_Q^m & \longrightarrow & M_Q^m \\ & (U; \psi_1, \ldots, \psi_m) & \longmapsto & (U\psi_1, \ldots, U\psi_m). \end{array} \tag{2.47}$$

The fundamental vector fields of this action span a distribution of rank $\dim V$ at $\xi \in M_Q^m$ if and only if its isotropy group $\mathcal{O}_\xi$ at $\xi \in M_Q^m$ is discrete. With the hypothesis $m = n-1$, the elements $U \in \mathcal{O}_\xi$, with $\xi := (\psi_1, \ldots, \psi_{n-1}) \in M_Q^{n-1}$, satisfy

$$U\psi_j = \psi_j, \quad j = 1, 2, \ldots, n-1. \tag{2.48}$$

At a generic point of M_Q^{n-1}, the components $\psi_1, \ldots, \psi_{n-1}$ can be assumed to be linearly independent elements (over $\mathbb{C}$). Then, the knowledge of the action of U on these elements fixes U on $\langle \psi_1, \ldots, \psi_{n-1} \rangle_{\mathbb{C}} \subset M_Q$, where it acts as the identity map. If ψ is orthogonal to $\langle \psi_1, \ldots, \psi_{n-1} \rangle_{\mathbb{C}}$ with respect to the natural Hermitian product on $\mathcal{H}$, then $U\psi$ must also be orthogonal to $\langle \psi_1, \ldots, \psi_{n-1} \rangle_{\mathbb{C}}$ because of (2.48) and the unitarity of U. Therefore, $U\psi$ is proportional to ψ. Since $U \in SU(\mathcal{H})$, then $U\psi = \psi$ and $U = \mathrm{Id}$. Therefore, the isotropy group of φ^m is trivial at a generic point of M_Q^{n-1}, the fundamental vector fields of φ^m are linearly independent over $\mathbb{R}$ and there exists a superposition rule depending on $n-1$ particular solutions. □

It is worth noting that, if $m < n-1$, then the isotropy group for φ^m is not trivial at any point of M_Q^m. Given m linearly independent elements $(\psi_1, \ldots, \psi_m)$ over $\mathbb{C}$, there exist special unitary transformations on M_Q acting as the identity on $\langle \psi_1, \ldots, \psi_m \rangle_{\mathbb{C}}$ and leaving stable its orthogonal complement. Hence, the isotropy group on any point of M_Q^m is not discrete.

Since the elements of $U(\mathcal{H})$ act on M_Q preserving the norm relative to the Kähler structure, the Lie group action φ_M^m given in the proof of the previous theorem can be restricted to $\mathcal{Q}^m$. In view of this, the previous proof can be slightly modified to prove that the restriction of φ_M^m to $\mathcal{Q}^m$ have a trivial isotropy group at a generic point for $m = n-1$. This proves the following corollary.

Corollary 2.33. *Every Lie system $\mathcal{X}_\mathcal{Q}^H$ on $\mathcal{Q}$ with a Vessiot-Guldberg Lie algebra $V^H \subset V_\mathcal{Q}$ isomorphic to $\mathfrak{su}(\mathcal{H})$ admits a superposition rule depending on $n-1$ particular solutions.*

Similar results can be proved for the Lie systems on the remaining quantum quotient manifold $\mathcal{R}$ and $\mathcal{P}$, as seen next.

Theorem 2.34. *Every Lie system $\mathcal{X}_\mathcal{R}^H$ on $\mathcal{R}$ admits a superposition rule depending on n particular solutions.*

Proof. In view of Proposition 2.26, the Lie system $\mathcal{X}_\mathcal{R}^H$ admits a Vessiot-Guldberg Lie algebra $V_\mathcal{R}$ of fundamental vector fields isomorphic to $\mathfrak{su}(\mathcal{H})$. Also the proof of Proposition 2.26 shows that the diagonal prolongation of the elements of $V_\mathcal{R}$ to $\mathcal{R}^m$ are the fundamental vector fields of the Lie group action

$$\begin{array}{rccc} \varphi_\mathcal{R}^m : & SU(\mathcal{H}) \times \mathcal{R}^m & \to & \mathcal{R}^m \\ & (U; [\psi_1]_\mathcal{R}, \ldots, [\psi_m]_\mathcal{R}) & \mapsto & ([U\psi_1]_\mathcal{R}, \ldots, [U\psi_m]_\mathcal{R}). \end{array} \tag{2.49}$$

The derivation of a superposition rule for $\mathcal{X}_\mathcal{R}^H$ requires the determination of the needed number m of particular solutions. This number is the smallest positive integer so that the diagonal prolongations of

vector fields in $V_{\mathcal{R}}$ become linearly independent at a generic point. This occurs at $\xi \in \mathcal{R}^m$ if and only if the isotropy group of this action at ξ is discrete. If $m = n$, then the elements of the isotropy group of $\varphi^n_{\mathcal{R}}$ at a generic point $(\psi_1, \ldots, \psi_n) \in \mathcal{R}^n$ satisfy

$$U[\psi_j]_{\mathcal{R}} = [\psi_j]_{\mathcal{R}}, \quad j = 1, 2, \ldots, n. \tag{2.50}$$

At a generic point of $\mathcal{R}^n$, the components $\psi_1, \ldots, \psi_n$ are linearly independent elements (over $\mathbb{C}$). In view of (2.50), the operator U diagonalises on the basis $\psi_1, \ldots, \psi_n$. Since $U \in U(\mathcal{H})$, then $\langle U\psi_i, U\psi_j \rangle = \langle \psi_i, \psi_j \rangle$ for $i, j = 1, 2, \ldots, n$ and all factors in the diagonal of the matrix representation of U must be equal. As $U \in SU(\mathcal{H})$, the multiplication of such diagonal elements must be equal to 1. This fixes $U = e^{i2\pi k/n}$ for $k \in \mathbb{Z}$. Therefore, the stability group of $\varphi^n_{\mathcal{R}}$ is discrete at a generic point of $\mathcal{R}^n$, the fundamental vector fields of $\varphi^n_{\mathcal{R}}$ are linearly independent over $\mathbb{R}$ at a generic point and $\mathcal{X}^H_{\mathcal{R}}$ admits a superposition rule depending on n particular solutions. □

As presented in Figure 2.1, the projective manifold that $\mathcal{P}$ can be embedded naturally within $\mathcal{R}$. Additionally, the projection $\pi_{\mathcal{RP}} : \mathcal{R} \to \mathcal{P}$ is equivariant relative to the the Lie group action of $SU(\mathcal{H})$ on $\mathcal{R}$ and the action $\varphi_{\mathcal{P}}$ of $SU(\mathcal{H})$ on $\mathcal{P}$. Following the same line of reasoning as in Corollary 2.33, the following result can be proved.

Corollary 2.35. *Every Lie-Kähler system on $\mathcal{P}$ admits a superposition rule depending on n particular solutions.*

2.4.2 Constants of motion and superposition rules

The next step in order to obtain the superposition rules for Schrödinger equations is the computation of constants of motion. The characterisation of Lie systems on the relevant manifold, that has been carried out along the chapter, makes this task easier. As shown next, it is possible to describe a general method in order to obtain constant of motion for Lie-Kähler systems. This method could have interesting applications in order to obtain solutions for the Schrödinger equation, as it can be easily implemented in numerical computations. Thus, Lie systems prove to be a powerful tool in the computation of the dynamics of quantum systems.

Firstly, this section describes the procedure to obtain a superposition rule for a Lie-Kähler system $\mathcal{X}^H$ on M_Q, determined by a traceless quantum Lie system $H(t)$, as given by (2.13):

$$H(t) = \sum_{j=1}^{r} b_j(t) H_j \quad \Longrightarrow \quad \mathcal{X}^H_t = \sum_{j=1}^{r} b_j(t) X_j, \quad X_j := X_{H_j} \tag{2.51}$$

As shown by Theorem 2.32, this superposition rule depends on $n - 1$ particular solutions, one less than the linear one (2.46). In contrast, the new superposition rule is not linear (except in the case of 2-level systems; see next section).

The superposition rule is derived through a number of constant of motions of the diagonal extension of the Lie system to $(M_Q)^n$. The number of necessary functions is equal to the dimension of the manifold M_Q. Thus, the superposition rule for the Schrödinger equation on M_Q is obtained in terms of $2n$ functions on $(M_Q)^n$. These functions are first integrals for the diagonal prolongation $\mathcal{X}^{H[n]}$, and hence for all the diagonal prolongations $X^{[n]}_\alpha$, with $\alpha = 1, 2, \ldots, r$, of the vector fields spanning the Vessiot-Guldberg Lie algebra of $\mathcal{X}^H$.

Lemma 2.36. *Consider the volume form $\Omega_{\mathcal{H}}$ on the complex Hilbert space $\mathcal{H}$ defined in the given coordinate system as*

$$\Omega_{\mathcal{H}} := \mathrm{d}z_1 \wedge \cdots \wedge \mathrm{d}z_n. \tag{2.52}$$

Let Ω_R, Ω_I be the n-forms on M_Q defined as in terms of the real and imaginary parts of $\Omega_{\mathcal{H}}$:

$$(\Omega_R)_\psi(v_1, \ldots, v_n) := \sqrt{n}\, \mathrm{Re}\, \Omega_{\mathcal{H}}\left(|v_1\rangle, \ldots, |v_n\rangle\right), \quad (\Omega_I)_\psi(v_1, \ldots, v_n) := \sqrt{n}\, \mathrm{Im}\, \Omega_{\mathcal{H}}\left(|v_1\rangle, \ldots, |v_n\rangle\right), \tag{2.53}$$

for any $\psi \in M_Q$ and any set $v_1, \ldots, v_n \in T_\psi M_Q$. These n-forms are symmetries of Lie-Kähler systems associated with traceless quantum Lie systems.

Proof. The rate of change in volume in $\mathcal{H}$ for a unitary evolution is proportional to the trace of the generator of such evolution. Thus, traceless generators define evolutions that preserve the volume. When transported to M_Q, these evolutions preserve both Ω_R and Ω_I. □

The value $\Omega_{\mathcal{H}}$ value on a set of vectors $|\psi^1\rangle, \ldots, |\psi^n\rangle \in \mathcal{H}$ can be directly computed by the determinant of their coordinates as

$$\Omega_{\mathcal{H}}(|\psi^1\rangle, \ldots, |\psi^n\rangle) = \det \begin{pmatrix} \psi_1^1 & \cdots & \psi_n^1 \\ \vdots & \ddots & \vdots \\ \psi_1^n & \cdots & \psi_n^n \end{pmatrix}, \tag{2.54}$$

with $\psi_1^j, \ldots, \psi_n^j \in \mathbb{C}$ the coordinates of $|\psi^j\rangle$ in the given basis, for $j = 1, 2, \ldots, n$. The real and imaginary parts of this determinant yield the values of Ω_R and Ω_I. In particular, this expression is useful to compute their coordinate expressions. For the 2-level system, their expressions are

$$\Omega_R = \mathrm{d}q_1 \wedge \mathrm{d}q_2 - \mathrm{d}p_1 \wedge \mathrm{d}p_2, \qquad \Omega_I = \mathrm{d}q_1 \wedge \mathrm{d}p_2 + \mathrm{d}p_1 \wedge \mathrm{d}q_2. \tag{2.55}$$

Larger expressions are obtained for systems with greater dimension.

Lemma 2.37. *The functions $I_1^c, I_1^s, \ldots, I_n^c, I_n^s : (M_Q)^n \to \mathbb{R}$ defined as*

$$\begin{aligned} I_j^c &:= g^{[n]}(\Delta^{(0)}, S_{0j}(\Delta^{(j)})) = \sum_{k=1}^n (q_k^{(0)} q_k^{(j)} + p_k^{(0)} p_k^{(j)}), \\ I_j^s &:= g^{[n]}(\Gamma^{(0)}, S_{0j}(\Delta^{(j)})) = \sum_{k=1}^n (q_k^{(0)} p_k^{(j)} - p_k^{(0)} q_k^{(j)}), \end{aligned} \qquad j = 1, \ldots, n-1; \tag{2.56}$$

$$\begin{aligned} I_n^c &:= \Omega_R^{[n]} \left(\Delta^{(0)}, S_{01}(\Delta^{(1)}), \ldots, S_{0(n-1)}(\Delta^{(n-1)}) \right) = \mathrm{Re}(\det(\psi^{(0)}, \ldots, \psi^{(n-1)})), \\ I_n^s &:= \Omega_I^{[n]} \left(\Delta^{(0)}, S_{01}(\Delta^{(1)}), \ldots, S_{0(n-1)}(\Delta^{(n-1)}) \right) = \mathrm{Im}(\det(\psi^{(0)}, \ldots, \psi^{(n-1)})), \end{aligned}$$

are constants of motion for the diagonal prolongation $\mathcal{X}^{H[n]}$ of the Lie-Kähler system $\mathcal{X}^H$ on M_Q defined by a traceless quantum Lie system $H(t)$. These functions satisfy the relations

$$J^{[m]}(\mathrm{d}I_j^c) = \mathrm{d}I_j^s, \quad j = 1, 2, \ldots, n; \qquad \det \begin{pmatrix} \frac{\partial I_1^c}{\partial q_1^{(0)}} & \frac{\partial I_1^s}{\partial q_1^{(0)}} & \cdots & \frac{\partial I_n^c}{\partial q_1^{(0)}} & \frac{\partial I_n^s}{\partial q_1^{(0)}} \\ \frac{\partial I_1^c}{\partial p_1^{(0)}} & \frac{\partial I_1^s}{\partial p_1^{(0)}} & \cdots & \frac{\partial I_n^c}{\partial p_1^{(0)}} & \frac{\partial I_n^s}{\partial p_1^{(0)}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\partial I_1^c}{\partial p_n^{(0)}} & \frac{\partial I_1^s}{\partial p_n^{(0)}} & \cdots & \frac{\partial I_n^c}{\partial p_n^{(0)}} & \frac{\partial I_n^s}{\partial p_n^{(0)}} \end{pmatrix} \neq 0. \tag{2.57}$$

Proof. The Lie-Kähler system is decomposed as in (2.51). The vector fields $X_1, \ldots, X_r$ are Kähler vector fields relative to the Kähler structure (g, ω, J) on M_Q. Therefore, their diagonal prolongations $X_\alpha^{[n]}$ are Kähler relative to the diagonal prolongation $(g^{[n]}, \omega^{[n]}, J^{[n]})$ to $(M_Q)^n$ of the Kähler structure (g, ω, J), namely

$$\begin{aligned} \omega^{[n]} &= \sum_{j=1}^n \sum_{a=0}^{n-1} \mathrm{d}q_j^{(a)} \wedge \mathrm{d}p_j^{(a)}, \quad g^{[n]} = \sum_{j=1}^n \sum_{a=0}^{n-1} (\mathrm{d}q_j^{(a)} \otimes \mathrm{d}q_j^{(a)} + \mathrm{d}p_j^{(a)} \otimes \mathrm{d}p_j^{(a)}), \\ J^{[n]} &= \sum_{j=1}^n \sum_{a=0}^{n-1} \left(\frac{\partial}{\partial p_j^{(a)}} \otimes \mathrm{d}q_j^{(a)} - \frac{\partial}{\partial q_j^{(a)}} \otimes \mathrm{d}p_j^{(a)} \right). \end{aligned} \tag{2.58}$$

Similarly, if X is a Hamiltonian vector field relative to ω with Hamiltonian function h_X, then $X^{[n]}$ is a Hamiltonian vector field with Hamiltonian function $h_X^{[n]}$. As the vector fields $X_1^{[n]}, \ldots, X_m^{[n]}$ are Killing vector fields with respect to $g^{[n]}$ and symmetries of the tensor fields S_{rs} for $r, s = 0, 1, 2, \ldots, n-1$ and $r \neq s$, presented in (2.7), the following common first-integrals for all such vector fields are obtained:

$$\begin{aligned} I_j^c &:= g^{[n]}(\Delta^{(0)}, S_{0j}(\Delta^{(j)})) = \sum_{k=1}^{n}(q_k^{(0)} q_k^{(j)} + p_k^{(0)} p_k^{(j)}), \\ I_j^s &:= g^{[n]}(\Gamma^{(0)}, S_{0j}(\Delta^{(j)})) = \sum_{k=1}^{n}(q_k^{(0)} p_k^{(j)} - p_k^{(0)} q_k^{(j)}), \end{aligned} \qquad j = 1, \ldots, n-1.$$

As $(g^{[n]}, \omega^{[n]}, J^{[n]})$ conform a Kähler structure, the functions satisfy by definition the relation $J^{[n]}(\mathrm{d}I_k^c) = \mathrm{d}I_k^s$, for $k = 1, \ldots, n-1$. Observe that these functions are first-integrals not only for $X_\alpha^{[n]}$, but also for $\Gamma^{[n]}$. Thus, the last two functions I_n^c, I_n^s are not first-integrals of $\Gamma^{[n]}$. They can be constructed with help of the n-forms Ω_R and Ω_I. Let I_n^c, I_n^s be the function defined as

$$\begin{aligned} I_n^c &:= \Omega_R^{[n]}\left(\Delta^{(0)}, S_{01}(\Delta^{(1)}), \ldots, S_{0(n-1)}(\Delta^{(n-1)})\right), \\ I_n^s &:= \Omega_I^{[n]}\left(\Delta^{(0)}, S_{01}(\Delta^{(1)}), \ldots, S_{0(n-1)}(\Delta^{(n-1)})\right). \end{aligned}$$

These functions satisfy also that $J^{[m]}(\mathrm{d}I_n^c) = \mathrm{d}I_n^s$.

It remains to be proved that the determinant of the matrix of derivatives with respect to $q_1^{(0)}$, $p_1^{(0)}$, ..., $q_n^{(0)}$, $p_n^{(0)}$ is not zero. Observe that the pairs of functions (I_j^c, I_j^s) and $(I_{j'}^c, I_{j'}^s)$, with $j, j' = 1, 2, \ldots, n$, depend on different variables if $j \neq j'$, so their derivatives are independent functions. Also, the relation $J^{[m]}(\mathrm{d}I_j^c) = \mathrm{d}I_j^s$ proves that I_j^c and I_j^s are independent, for any $j = 1, 2, \ldots, n$. Thus, the determinant does not cancel (at a generic point). □

With the functions defined in (2.56), consider the following system of equations:

$$I_j^c(\psi^{(0)}, \psi^{(1)}, \ldots \psi^{(n-1)}) = k_{2j-1}, \quad I_j^s(\psi^{(0)}, \psi^{(1)}, \ldots \psi^{(n-1)}) = k_{2j}, \quad j = 1, 2, \ldots, n, \tag{2.59}$$

The solution $\psi^{(0)}$ to the system can be obtained, at least locally, in terms of the coordinates of $\psi^{(1)}$, ..., $\psi^{(n-1)}$ and $2n$ real constants k_1, ..., k_{2n}. In other words, Lemma 2.37, in particular equation (2.57), guarantees that the functions are functionally independent and the system (2.59) can be solved locally for $\psi^{(0)}$. The solution for the system is computed next.

Theorem 2.38. *There exists a superposition rule $\Phi : (M_Q)^{n+1} \times \mathbb{R}^n \to M_Q$ for the Lie-Kähler system $\mathcal{X}^H$ on M_Q associated to a traceless quantum Lie system $H(t)$. Locally, the superposition rule takes the form*

$$\begin{pmatrix} q_1^{(0)} \\ p_1^{(0)} \\ \vdots \\ q_n^{(0)} \\ p_n^{(0)} \end{pmatrix} = \begin{pmatrix} \frac{q_1^{(1)}}{||\psi^{(1)}||^2} & \frac{p_1^{(1)}}{||\psi^{(1)}||^2} & \cdots & \frac{q_1^{(n-1)}}{||\psi^{(n-1)}||^2} & \frac{p_1^{(n-1)}}{||\psi^{(n-1)}||^2} & \frac{1}{\Theta}\frac{\partial I_n^c}{\partial q_1^{(0)}} & \frac{1}{\Theta}\frac{\partial I_n^s}{\partial q_1^{(0)}} \\ \frac{p_1^{(1)}}{||\psi^{(1)}||^2} & -\frac{q_1^{(1)}}{||\psi^{(1)}||^2} & \cdots & \frac{p_1^{(n-1)}}{||\psi^{(n-1)}||^2} & -\frac{q_1^{(n-1)}}{||\psi^{(n-1)}||^2} & \frac{1}{\Theta}\frac{\partial I_n^c}{\partial p_1^{(0)}} & \frac{1}{\Theta}\frac{\partial I_n^s}{\partial p_1^{(0)}} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ \frac{q_n^{(1)}}{||\psi^{(1)}||^2} & \frac{p_n^{(1)}}{||\psi^{(1)}||^2} & \cdots & \frac{q_n^{(n-1)}}{||\psi^{(n-1)}||^2} & \frac{p_n^{(n-1)}}{||\psi^{(n-1)}||^2} & \frac{1}{\Theta}\frac{\partial I_n^c}{\partial q_n^{(0)}} & \frac{1}{\Theta}\frac{\partial I_n^s}{\partial q_n^{(0)}} \\ \frac{p_n^{(1)}}{||\psi^{(1)}||^2} & -\frac{q_n^{(1)}}{||\psi^{(1)}||^2} & \cdots & \frac{p_n^{(n-1)}}{||\psi^{(n-1)}||^2} & -\frac{q_n^{(n-1)}}{||\psi^{(n-1)}||^2} & \frac{1}{\Theta}\frac{\partial I_n^c}{\partial p_n^{(0)}} & \frac{1}{\Theta}\frac{\partial I_n^s}{\partial p_n^{(0)}} \end{pmatrix} \begin{pmatrix} k_1 \\ \vdots \\ k_{2n} \end{pmatrix}. \tag{2.60}$$

where $k_1, \ldots, k_{2n}$ are real numbers, $\psi^{(1)}, \ldots, \psi^{(n-1)} \in M_Q$ are a set of points which are linearly independent when considered as vectors in $\mathcal{H}$, and $\Theta := \prod_{\alpha=1}^{n-1} \|\psi^{(\alpha)}\|^2$.

Proof. Due to (2.57), the system of equations

$$I_j^c(\psi^{(0)},\psi^{(1)},\dots\psi^{(n-1)})=k_{2j-1},\quad I_j^s(\psi^{(0)},\psi^{(1)},\dots\psi^{(n-1)})=k_{2j},\quad j=1,2,\dots,n, \tag{2.61}$$

can be solved locally for $\psi^{(0)}$. The resulting expressions is the superposition rule for the system. Since all functions are linear in the coordinates of $\psi^{(0)}$, then the system can be written in matrix form as

$$\begin{pmatrix} \frac{\partial I_1^c}{\partial q_1^{(0)}} & \frac{\partial I_1^c}{\partial p_1^{(0)}} & \cdots & \frac{\partial I_1^c}{\partial q_n^{(0)}} & \frac{\partial I_1^c}{\partial p_n^{(0)}} \\ \frac{\partial I_1^s}{\partial q_1^{(0)}} & \frac{\partial I_1^s}{\partial p_1^{(0)}} & \cdots & \frac{\partial I_1^s}{\partial q_n^{(0)}} & \frac{\partial I_1^s}{\partial p_n^{(0)}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{\partial I_n^c}{\partial q_1^{(0)}} & \frac{\partial I_n^c}{\partial p_1^{(0)}} & \cdots & \frac{\partial I_n^c}{\partial q_n^{(0)}} & \frac{\partial I_n^c}{\partial p_n^{(0)}} \\ \frac{\partial I_n^s}{\partial q_1^{(0)}} & \frac{\partial I_n^s}{\partial p_1^{(0)}} & \cdots & \frac{\partial I_n^s}{\partial q_n^{(0)}} & \frac{\partial I_n^s}{\partial p_n^{(0)}} \end{pmatrix} \begin{pmatrix} q_1^{(0)} \\ p_1^{(0)} \\ \vdots \\ q_n^{(0)} \\ p_n^{(0)} \end{pmatrix} = \begin{pmatrix} q_1^{(1)} & p_1^{(1)} & \cdots & q_n^{(1)} & p_n^{(1)} \\ p_1^{(1)} & -q_1^{(1)} & \cdots & p_n^{(1)} & -q_n^{(1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ q_1^{(n-1)} & p_1^{(n-1)} & \cdots & q_n^{(n-1)} & p_n^{(n-1)} \\ p_1^{(n-1)} & -q_1^{(n-1)} & \cdots & p_n^{(n-1)} & -q_n^{(n-1)} \\ \frac{\partial I_n^c}{\partial q_1^{(0)}} & \frac{\partial I_n^c}{\partial p_1^{(0)}} & \cdots & \frac{\partial I_n^c}{\partial q_n^{(0)}} & \frac{\partial I_n^c}{\partial p_n^{(0)}} \\ \frac{\partial I_n^s}{\partial q_1^{(0)}} & \frac{\partial I_n^s}{\partial p_1^{(0)}} & \cdots & \frac{\partial I_n^s}{\partial q_n^{(0)}} & \frac{\partial I_n^s}{\partial p_n^{(0)}} \end{pmatrix} \begin{pmatrix} q_1^{(0)} \\ p_1^{(0)} \\ \vdots \\ q_n^{(0)} \\ p_n^{(0)} \end{pmatrix} = \begin{pmatrix} k_1 \\ \vdots \\ k_{2n} \end{pmatrix}.$$

This expression can be simplified enough so that the coefficient matrix can be inverted. Observe that

$$\begin{aligned} &\sum_{j=1}^n (q_j^{(r)}q_j^{(s)}+p_j^{(r)}p_j^{(s)}) = g^{[n]}(\Delta^{(r)},S_{rs}(\Delta^{(s)})), \\ &\sum_{j=1}^n (q_j^{(r)}p_j^{(s)}-p_j^{(r)}q_j^{(s)}) = g^{[n]}(\Gamma^{(r)},S_{rs}(\Delta^{(s)})), \end{aligned} \qquad r,s,=1,\dots,n-1. \tag{2.62}$$

These values are constants of motion. Given a set of linearly independent vectors $\psi^{(1)},\dots,\psi^{(n-1)}\in M_Q$, one can always find linear combinations of them such that these functions are zero for $r\neq s$. Also, the following relations hold:

$$\begin{aligned} &\sum_{\alpha=1}^n \left[q_\alpha^{(i)}\frac{\partial I_n^c}{\partial q_\alpha^{(0)}}+p_\alpha^{(i)}\frac{\partial I_n^c}{\partial p_\alpha^{(0)}}\right] = -\sum_{\alpha=1}^n \left[p_\alpha^{(i)}\frac{\partial I_n^s}{\partial q_\alpha^{(0)}}-q_\alpha^{(i)}\frac{\partial I_n^s}{\partial p_\alpha^{(0)}}\right] = \mathrm{Re}(\det(\psi^{(i)},\psi^{(1)},\dots,\psi^{(n-1)}))=0, \\ &\sum_{\alpha=1}^n \left[p_\alpha^{(i)}\frac{\partial I_n^c}{\partial q_\alpha^{(0)}}-q_\alpha^{(i)}\frac{\partial I_n^c}{\partial p_\alpha^{(0)}}\right] = \sum_{\alpha=1}^n \left[q_\alpha^{(i)}\frac{\partial I_n^s}{\partial q_\alpha^{(0)}}+p_\alpha^{(i)}\frac{\partial I_n^s}{\partial p_\alpha^{(0)}}\right] = \mathrm{Im}(\det(\psi^{(i)},\psi^{(1)},\dots,\psi^{(n-1)}))=0, \\ &\sum_{\alpha=1}^n \left[\left(\frac{\partial I_n^c}{\partial q_\alpha^{(0)}}\right)^2+\left(\frac{\partial I_n^c}{\partial p_\alpha^{(0)}}\right)^2\right] = \sum_{\alpha=1}^n \left[\left(\frac{\partial I_n^s}{\partial q_\alpha^{(0)}}\right)^2+\left(\frac{\partial I_n^s}{\partial p_\alpha^{(0)}}\right)^2\right] = \prod_{\alpha=1}^{n-1}\|\psi^{(\alpha)}\|^2, \end{aligned}$$

for $i=1,\dots,n-1$. Defining $\Theta:=\prod_{\alpha=1}^{n-1}\|\psi^{(\alpha)}\|^2$ and choosing $\psi^{(1)},\dots,\psi^{(n-1)}$, so that the quantities in (2.62) are zero, the coefficient matrix can be inverted, giving as a result (2.60). This expression gives rise to a superposition rule $\Phi:(M_Q)^{n-1}\times\mathbb{R}^{2n}\to M_Q$ for the Lie-Kähler system $\mathcal{X}^H$. □

Corollary 2.39. *The projection $\mathcal{X}_{\mathcal{Q}}^H$ onto $\mathcal{Q}$ of the Lie-Kähler system $\mathcal{X}^H$ has a superposition rule $\Phi_{\mathcal{Q}}:(\mathcal{Q})^{n-1}\times\mathcal{Q}\to\mathcal{Q}$, whose expression is given by (2.60) together with the constraints*

$$\|\psi_1\|=\ldots=\|\psi_{n-1}\|=1,\qquad \sum_{\alpha=1}^{2n}k_\alpha^2=1. \tag{2.63}$$

Proof. This is a direct consequence of the inclusion $\iota_{\mathcal{Q}}:\mathcal{Q}\to M_Q$ already introduced in previous section. Observe that, with the given constraints, the resulting solution satisfies

$$\frac{1}{2}\sum_{\alpha=1}^n\left((q_\alpha^{(0)})^2+(p_\alpha^{(0)})^2\right)=1. \tag{2.64}$$

This makes possible to restrict the above superposition rule to a new one of the form $\Phi_{\mathcal{Q}} : \mathcal{Q}^{n-1} \times \mathcal{Q} \to \mathcal{Q}$ for $\mathcal{X}^H_{\mathcal{Q}}$. □

A non-linear superposition rule for the Schrödinger equation on M_Q has thus been obtained. It is determined by the constants of motion computed on $(M_Q)^n$ for the diagonal prolongation $\mathcal{X}^{H[n]}$ of the Lie-Kähler system $\mathcal{X}^H$. It is possible to obtain an analytic result because of the easy expressions of the coordinates on M_Q. A similar procedure could be carried out in the projective manifold $\mathcal{P}$, as it also has a Kähler structure. However, a general result as the one presented in (2.60) would be, at least, much more complicated. This is due to $\mathcal{P}$ lacking a global chart. Therefore, it will not be computed for the general case. Nevertheless, it is possible to derive a superposition rule for simple cases. Next sections presents the computations for the 2-level system.

2.5 Superposition rules for 2-level systems

This section illustrates the theory presented in this chapter by describing superposition rules for 2-level systems on M_Q and on the quantum quotient manifolds. Recall the existing commutative diagram presented in Figure 2.1. For the sake of completeness, the diagram is reproduced in Figure 2.2, where under each space appear the smallest number of particular solutions for its corresponding superposition rule.

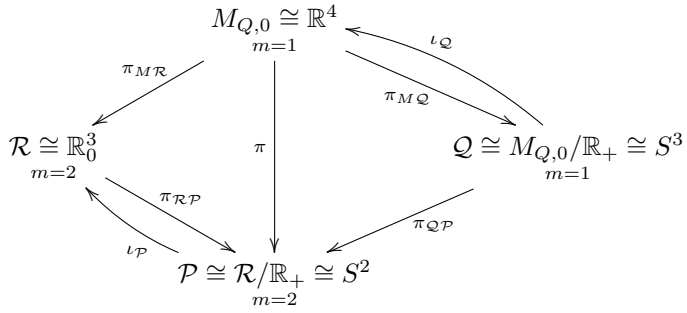


Figure 2.2: Diagram of the differentiable manifold appearing in the study of 2-level quantum systems. The number m under each manifold represents the number of particular solutions of the Schrödinger equation in said manifold that determine the general solution.

On each space, there exists a Lie system admitting Vessiot-Guldberg Lie algebra of Hamiltonian vector fields relative to different compatible geometric structures, which in turn makes possible the obtention of their superposition rules geometrically. The following subsections provide these superposition rules, their relevant geometric properties and their potential applications in Quantum Mechanics.

2.5.1 Superposition rule for a 2-level system on M_Q

Consider a time-dependent vector field $\mathcal{X}^H$ on M_Q of the form

$$\mathcal{X}^H_t = \sum_{j=1}^{3} B_j(t) X_j, \quad t \in \mathbb{R}. \tag{2.65}$$

It is an immediate consequence of Theorem 2.20 that $\mathcal{X}^H$ is a Lie-Kähler system whose Vessiot-Guldberg Lie algebra $V = \langle X_1, X_2, X_3 \rangle$, with X_1, X_2, X_3 given by (2.20), consists of Kähler vector fields relative to the standard Kähler structure (g, ω, J) on M_Q. Also, $\mathcal{X}^H_t$ commutes for any $t \in \mathbb{R}$ with the phase change vector field Γ and with the dilation vector field Δ, namely Γ and Δ are Lie symmetries of $\mathcal{X}^H$.

The superposition rule for $\mathcal{X}^H$ depends on a number m of particular solutions that has to be determine. This is the smallest integer such that the diagonal prolongations to $(M_Q)^m \simeq \left(\mathbb{R}^4\right)^m$ of X_1, X_2, X_3 are linearly independent at a generic point [80]. The coordinate expressions for X_1, X_2, X_3, given in (2.20), show that they are already linearly independent at a generic point of M_Q. Hence $m = 1$, i.e. the superposition rule does depend on a mere particular solution. This is a lower number than in the case of the standard quantum linear superposition rule (2.2), which depends on two particular solutions.

The next step is to obtain the functions that determine the superposition rule. These functions are given by Lemma 2.37, and they are first integrals for the diagonal prolongations $X_1^{[2]}, X_2^{[2]}, X_3^{[2]}$ of X_1, X_2, X_3 to $(M_Q)^2 \simeq (\mathbb{R}^4_0)^2$. Consider the diagonal prolongations $g^{[2]}, \omega^{[2]}, J^{[2]}$ to $(M_Q)^2$ of the Kähler structure on M_Q:

$$\begin{gathered}\omega^{[2]} = \sum_{r=0}^{1}\sum_{j=1}^{2} \mathrm{d}q_j^{(r)} \wedge \mathrm{d}p_j^{(r)}, \qquad g^{[2]} = \sum_{r=0}^{1}\sum_{j=1}^{2} (\mathrm{d}q_j^{(r)} \otimes \mathrm{d}q_j^{(r)} + \mathrm{d}p_j^{(r)} \otimes \mathrm{d}p_j^{(r)}), \\ J^{[2]} = \sum_{r=0}^{1}\sum_{j=1}^{2} \left(\frac{\partial}{\partial p_j^{(r)}} \otimes \mathrm{d}q_j^{(r)} - \frac{\partial}{\partial q_j^{(r)}} \otimes \mathrm{d}p_j^{(r)} \right).\end{gathered} \tag{2.66}$$

The functions presented in Lemma 2.37 are the following:

$$\begin{aligned} I_1^c(\psi^{(0)}, \psi^{(1)}) &:= g^{[2]}(\Delta^{(0)}, S_{01}\Delta^{(1)}) = q_1^{(0)}q_1^{(1)} + p_1^{(0)}p_1^{(1)} + q_2^{(0)}q_2^{(1)} + p_2^{(0)}p_2^{(1)}, \\ I_1^s(\psi^{(0)}, \psi^{(1)}) &:= \omega^{[2]}(\Delta^{(0)}, S_{01}\Delta^{(1)}) = q_1^{(0)}p_1^{(1)} - p_1^{(0)}q_1^{(1)} + q_2^{(0)}p_2^{(1)} - p_2^{(0)}q_2^{(1)}, \\ I_2^c(\psi^{(0)}, \psi^{(1)}) &:= \Omega_R^{[2]}(\Delta^{(0)}, S_{01}\Delta^{(1)}) = q_1^{(0)}q_2^{(1)} - p_1^{(0)}p_2^{(1)} - q_2^{(0)}q_1^{(1)} + p_2^{(0)}p_1^{(1)}, \\ I_2^s(\psi^{(0)}, \psi^{(1)}) &:= \Omega_j^{[2]}(\Delta^{(0)}, S_{01}\Delta^{(1)}) = q_1^{(0)}p_2^{(1)} + p_1^{(0)}q_2^{(1)} - q_2^{(0)}p_1^{(1)} - p_2^{(0)}q_1^{(1)}. \end{aligned} \tag{2.67}$$

With the expression of $J^{[2]}$ given in (2.66), it is immediate to check that these functions satisfy the relations

$$J^{[2]}(\mathrm{d}I_1^c) = \mathrm{d}I_1^s, \quad J^{[2]}(\mathrm{d}I_2^c) = \mathrm{d}I_2^s. \tag{2.68}$$

Thus is seems clear that the four functions are independent, hence the matrix of derivatives presented in (2.57) has to be non-singular in generic points. This matrix can be easily computed in this case, as it has the following expression:

$$\left(\frac{\partial I}{\partial \psi^{(0)}}\right) := \begin{pmatrix} \frac{\partial I_1^c}{\partial q_1^{(0)}} & \frac{\partial I_1^c}{\partial p_1^{(0)}} & \frac{\partial I_1^c}{\partial q_2^{(0)}} & \frac{\partial I_1^c}{\partial p_2^{(0)}} \\ \frac{\partial I_1^s}{\partial q_1^{(0)}} & \frac{\partial I_1^s}{\partial p_1^{(0)}} & \frac{\partial I_1^s}{\partial q_2^{(0)}} & \frac{\partial I_1^s}{\partial p_2^{(0)}} \\ \frac{\partial I_2^c}{\partial q_1^{(0)}} & \frac{\partial I_2^c}{\partial p_1^{(0)}} & \frac{\partial I_2^c}{\partial q_2^{(0)}} & \frac{\partial I_2^c}{\partial p_2^{(0)}} \\ \frac{\partial I_2^s}{\partial q_1^{(0)}} & \frac{\partial I_2^s}{\partial p_1^{(0)}} & \frac{\partial I_2^s}{\partial q_2^{(0)}} & \frac{\partial I_2^s}{\partial p_2^{(0)}} \end{pmatrix} = \begin{pmatrix} q_1^{(1)} & p_1^{(1)} & q_2^{(1)} & p_2^{(1)} \\ p_1^{(1)} & -q_1^{(1)} & p_2^{(1)} & -q_2^{(1)} \\ q_2^{(1)} & -p_2^{(1)} & -q_1^{(1)} & p_1^{(1)} \\ p_2^{(1)} & q_2^{(1)} & -p_1^{(1)} & -q_1^{(1)} \end{pmatrix} \tag{2.69}$$

The determinant of this matrix is

$$\det\left(\frac{\partial I}{\partial \psi^{(0)}}\right) = -\left((q_1^{(0)})^2 + (q_2^{(0)})^2 + (p_1^{(0)})^2 + (p_2^{(0)})^2\right)^2 \tag{2.70}$$

Thus, the matrix is regular everywhere in M_Q except for the point with coordinates $(0, 0, 0, 0)$. It is thus possible to obtain a superposition rule.

Consider the system of equations

$$\begin{cases} I_1^c(\psi^{(0)},\psi^{(1)}) = k_1, \\ I_1^s(\psi^{(0)},\psi^{(1)}) = k_2, \\ I_2^c(\psi^{(0)},\psi^{(1)}) = k_3, \\ I_2^s(\psi^{(0)},\psi^{(1)}) = k_4, \end{cases} \qquad k_1,k_2,k_3,k_4 \in \mathbb{R}. \tag{2.71}$$

As detailed in Theorem 2.38, this system of equations is linear in $\psi^{(0)}$, and thus can be written in matrix form as

$$\begin{pmatrix} q_1^{(1)} & p_1^{(1)} & q_2^{(1)} & p_2^{(1)} \\ p_1^{(1)} & -q_1^{(1)} & -p_2^{(1)} & q_2^{(1)} \\ q_2^{(1)} & p_2^{(1)} & -q_1^{(1)} & -p_1^{(1)} \\ p_2^{(1)} & -q_2^{(1)} & p_1^{(1)} & -q_1^{(1)} \end{pmatrix} \begin{pmatrix} q_1^{(0)} \\ p_1^{(0)} \\ q_2^{(0)} \\ p_2^{(0)} \end{pmatrix} = \begin{pmatrix} k_1 \\ k_2 \\ k_3 \\ k_4 \end{pmatrix}. \tag{2.72}$$

The matrix of coefficients is $\left(\frac{\partial I}{\partial \psi^{(0)}}\right)$, which can be inverted, thus giving the expression of the superposition rule. The inverse of this matrix is

$$\left(\frac{\partial I}{\partial \psi^{(0)}}\right)^{-1} = \frac{1}{(q_1^{(0)})^2+(q_2^{(0)})^2+(p_1^{(0)})^2+(p_2^{(0)})^2} \begin{pmatrix} q_1^{(1)} & p_1^{(1)} & q_2^{(1)} & p_2^{(1)} \\ p_1^{(1)} & -q_1^{(1)} & -p_2^{(1)} & q_2^{(1)} \\ q_2^{(1)} & p_2^{(1)} & -q_1^{(1)} & -p_1^{(1)} \\ p_2^{(1)} & -q_2^{(1)} & p_1^{(1)} & -q_1^{(1)} \end{pmatrix}, \tag{2.73}$$

which is in agreement with the expression given in (2.60). Thus, a non-linear superposition rule in M_Q could be given by

$$\begin{pmatrix} q_1^{(0)} \\ p_1^{(0)} \\ q_2^{(0)} \\ p_2^{(0)} \end{pmatrix} = \left(\frac{\partial I}{\partial \psi^{(0)}}\right)^{-1} \begin{pmatrix} k_1 \\ k_2 \\ k_3 \\ k_4 \end{pmatrix}. \tag{2.74}$$

It is possible to further simplify this expression. Observe that the non-linearity is a consequence of the denominator in (2.73). This denominator is simply the norm of the point in M_Q with coordinates $(q_1^{(1)},p_1^{(1)},q_2^{(1)},p_2^{(1)})$. As proved several times in the preceding sections, the norm is preserved under the evolution due to the unitarity of Schrödinger equations. Thus, the constants k_1,k_2,k_3,k_4 can be replaced by new numbers that incorporate this factor. By defining the numbers

$$c_j = \frac{k_j}{(q_1^{(0)})^2+(q_2^{(0)})^2+(p_1^{(0)})^2+(p_2^{(0)})^2}, \quad j=1,2,3,4, \tag{2.75}$$

expression (2.74) can be rewritten as

$$\begin{pmatrix} q_1^{(0)} \\ p_1^{(0)} \\ q_2^{(0)} \\ p_2^{(0)} \end{pmatrix} = \begin{pmatrix} q_1^{(1)} & p_1^{(1)} & q_2^{(1)} & p_2^{(1)} \\ p_1^{(1)} & -q_1^{(1)} & -p_2^{(1)} & q_2^{(1)} \\ q_2^{(1)} & p_2^{(1)} & -q_1^{(1)} & -p_1^{(1)} \\ p_2^{(1)} & -q_2^{(1)} & p_1^{(1)} & -q_1^{(1)} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix}. \tag{2.76}$$

Lastly, the right-side term can be rewritten as a matrix depending on c_1,c_2,c_3,c_4 acting on a vector of coordinates in M_Q. All these computations are the proof to the following result

Theorem 2.40. *There exists a superposition rule for the Lie-Kähler system $\mathcal{X}^H$ on M_Q of the 2-level system, given on (2.65), depending on a single particular solution. The superposition rule*

$$\begin{array}{rccl} \Phi: & M_Q \times M_Q & \to & M_Q \\ & (\psi^{(1)},c) & \mapsto & \psi^{(0)} = \Phi(\psi^{(1)},c), \end{array} \tag{2.77}$$

can be given the following coordinate expression:

$$\begin{pmatrix} q_1^{(0)} \\ p_1^{(0)} \\ q_2^{(0)} \\ p_2^{(0)} \end{pmatrix} = \begin{pmatrix} c_1 & c_2 & c_3 & c_4 \\ -c_2 & c_1 & c_4 & -c_3 \\ -c_3 & -c_4 & c_1 & c_2 \\ -c_4 & c_3 & -c_2 & c_1 \end{pmatrix} \begin{pmatrix} q_1^{(1)} \\ p_1^{(1)} \\ q_2^{(1)} \\ p_2^{(1)} \end{pmatrix}. \tag{2.78}$$

2.5.2 Superposition rule for the 2-level system on $\mathcal{Q}$

Consider the projection $\pi_{M\mathcal{Q}} : M_{Q,0} \to \mathcal{Q}$ and the natural embedding $\iota_{\mathcal{Q}} : \mathcal{Q} \to M_{Q,0}$ defined in Section 2.3. The Lie-Kähler system $\mathcal{X}^H$ can be projected through $\pi_{M\mathcal{Q}}$ onto a system $\mathcal{X}^H_{\mathcal{Q}}$ on $\mathcal{Q}$, as in Proposition 2.22. This proposition also ensures that the vector fields $X_1|_{\mathcal{Q}}, X_2|_{\mathcal{Q}}$, and $X_3|_{\mathcal{Q}}$ are Hamiltonian with respect to the presymplectic structure $\iota^*_{\mathcal{Q}}\omega$, admitting Hamiltonian functions $\bar{h}_i := \iota^*_{\mathcal{Q}} h_i$. Also, since the vector fields X_1, X_2, and X_3 are Killing vector fields for g on $M_{Q,0}$, then the vector fields $X_1|_{\mathcal{Q}}, X_2|_{\mathcal{Q}}$, and $X_3|_{\mathcal{Q}}$ are also Killing vector fields with respect to $\iota^*_{\mathcal{Q}} g$.

As Proposition 2.22 ensures that the restrictions $X_1|_{\mathcal{Q}}, X_2|_{\mathcal{Q}}, X_3|_{\mathcal{Q}}$ are linearly independent at a generic point of $\mathcal{Q}$, then $X|_{\mathcal{Q}}$ admits a superposition rule depending on a unique particular solution. This superposition rule can be obtained by using a similar approach as in the above section, i.e. obtaining three common first-integrals for the diagonal prolongations $X_1^{[2]}|_{\mathcal{Q}}, X_2^{[2]}|_{\mathcal{Q}}, X_3^{[2]}|_{\mathcal{Q}}$, which are Killing vector fields with respect to $(\iota^*_{\mathcal{Q}} g)^{[2]}$ and Hamiltonian vector fields relative to the presymplectic structure $(\iota^*_{\mathcal{Q}}\omega)^{[2]}$. The latter can be employed to obtain the common first-integrals through invariant functions constructed through $(\iota^*_{\mathcal{Q}} g)^{[2]}$, $(\iota^*_{\mathcal{Q}}\omega)^{[2]}$. Importantly, the vector Δ is not tangent to $\mathcal{Q}$ and it cannot be used to construct invariants. An alternative option is to consider the pull-back via $\iota_{\mathcal{Q}}$ of the first integrals on $(M_{Q,0})^2$ computed in the above section, thus determining the superposition rule.

Instead of the above, the following approach shoes that the superposition rule for $\mathcal{X}^H_{\mathcal{Q}}$ can be obtained from of the superposition for $\mathcal{X}^H$. Observe that $\mathcal{X}^H$ is a Lie system on $M_{Q,0}$ with a superposition rule $\Phi : M_{Q,0} \times M_{Q,0} \to M_{Q,0}$ and that $\mathcal{X}^H_t$ is tangent to the submanifold $\iota_{\mathcal{Q}}(\mathcal{Q}) \subset M_{Q,0}$ for each $t \in \mathbb{R}$. Assume also that there exists $\bar{S} \subset M_{Q,0}$ such that $\Phi(\mathcal{Q} \times \bar{S}) = \mathcal{Q}$. Then, the initial superposition rule can be restricted to elements on $\mathcal{Q}$ giving rise to a new superposition principle.

Indeed, the superposition rule Φ defined in Theorem 2.40 and evaluated on points $\psi^{(1)}_{\mathcal{Q}}, c_{\mathcal{Q}} \in \mathcal{Q}$, i.e. $\|\psi^{(1)}_{\mathcal{Q}}\| = \|c_{\mathcal{Q}}\| = 1$. The resulting point $\Phi(\psi^{(1)}_{\mathcal{Q}}, c_{\mathcal{Q}})$ satisfies that

$$\|\Phi(\psi^{(1)}_{\mathcal{Q}}, c_{\mathcal{Q}})\| = \|c_{\mathcal{Q}}\|^4 \|\psi^{(1)}_{\mathcal{Q}}\| = 1 \Rightarrow \Phi(\psi^{(1)}_{\mathcal{Q}}, c_{\mathcal{Q}}) \in \mathcal{Q}.$$

Conversely, there always exists, for points $\psi^{(0)}_{\mathcal{Q}} \in \mathcal{Q}$ and $c_{\mathcal{Q}} \in \mathcal{Q}$, a point $\psi^{(1)}_{\mathcal{Q}} \in \mathcal{Q}$ such that $\Phi(\psi^{(1)}_{\mathcal{Q}}, c_s) = \psi^{(0)}_{\mathcal{Q}}$. Hence $X_{\mathcal{Q}}$ admits a superposition rule $\Phi_{\mathcal{Q}} : \mathcal{Q} \times \mathcal{Q} \to \mathcal{Q}$ which can be formally written as (2.78).

2.5.3 Superposition rules for the 2-level system on $\mathcal{R}$ and $\mathcal{P}$

The procedure developed for the Lie-Kähler system can be repeated in order to obtain a superposition rule on the quotient manifold $\mathcal{R}$. In particular, the 2-level system is a simple example in which the superposition rule can be written explicitly.

Recall from Lemma 2.25 that there exists a way to obtain coordinate systems in $\mathcal{R}$. In the case of 2-level systems, there exists a global chart with coordinates x, y, z, as given by (2.31). A Lie system $\mathcal{X}^H_{\mathcal{R}}$ on $\mathcal{R}$ determined by a quantum Lie system $H(t)$ can be written as

$$\mathcal{X}^H_{\mathcal{R},t} = \sum_{j=1}^{3} B_j(t) Y_j, \tag{2.79}$$

where Y_1, Y_2, Y_3 are given by (2.36). The superposition rule for $\mathcal{X}^H_{\mathcal{R}}$ depends on m particular solutions, where m is the smallest integer such that the diagonal prolongations $Y_1^{[m]}, Y_2^{[m]}, Y_3^{[m]}$ to $\mathcal{R}^m$ are linearly

independent at a generic point. Observe that Y_1, Y_2, and Y_3 span a two-dimensional distribution on $\mathcal{R}$. As the diagonal prolongations enlarge the dimensions of the distributions, it is enough to consider $\mathcal{R}^2$ to obtain linearly independent vectors at generic points, hence $m = 2$ [80, 82].

The superposition rule is obtained by computing constants of motion of the diagonal prolongation of $\mathcal{X}_{\mathcal{R}}^H$ to $\mathcal{R}^3$. That is to say, it is necessary to compute common first integrals on $\mathcal{R}^3$ for the vector fields

$$\begin{aligned}
Y_1^{[3]} &= z^{(0)}\frac{\partial}{\partial y^{(0)}} - y^{(0)}\frac{\partial}{\partial z^{(0)}} + z^{(1)}\frac{\partial}{\partial y^{(1)}} - y^{(1)}\frac{\partial}{\partial z^{(1)}} + z^{(2)}\frac{\partial}{\partial y^{(2)}} - y^{(2)}\frac{\partial}{\partial z^{(2)}},\\
Y_2^{[3]} &= x^{(0)}\frac{\partial}{\partial z^{(0)}} - z^{(0)}\frac{\partial}{\partial x^{(0)}} + x^{(1)}\frac{\partial}{\partial z^{(1)}} - z^{(1)}\frac{\partial}{\partial x^{(1)}} + x^{(2)}\frac{\partial}{\partial z^{(2)}} - z^{(2)}\frac{\partial}{\partial x^{(2)}},\\
Y_3^{[3]} &= y^{(0)}\frac{\partial}{\partial x^{(0)}} - x^{(0)}\frac{\partial}{\partial y^{(0)}} + y^{(1)}\frac{\partial}{\partial x^{(1)}} - x^{(1)}\frac{\partial}{\partial y^{(1)}} + y^{(2)}\frac{\partial}{\partial x^{(2)}} - x^{(2)}\frac{\partial}{\partial y^{(2)}}.
\end{aligned} \tag{2.80}$$

As proved in Proposition 2.28, vector fields in the Vessiot-Guldberg Lie algebra of $\mathcal{X}_{\mathcal{R}}^H$ are Killing with respect to the metric $g_{\mathcal{R}}$ on $\mathcal{R}$, given in (2.42). As a consequence, the dilation vector field Δ on $\mathcal{R}$, with expression

$$\Delta = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} + z\frac{\partial}{\partial z}, \tag{2.81}$$

is a symmetry of Y_1, Y_2 and Y_3. The same is true with respect to the diagonal prolongations. Thus, from the geometric properties of $\mathcal{X}_{\mathcal{R}}^H$ it is possible to obtain constants of motion $\hat{I}_1, \hat{I}_2, \hat{I}_3 : \mathcal{R}^3 \to \mathbb{R}$ as

$$\begin{aligned}
\hat{I}_1(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) &:= g^{[3]}(\Delta^{(0)}, S_{01}\Delta^{(1)}) = \frac{x^{(0)}x^{(1)} + y^{(0)}y^{(1)} + z^{(0)}z^{(1)}}{\|\mathbf{x}^{(0)}\|},\\
\hat{I}_2(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) &:= g^{[3]}(\Delta^{(0)}, S_{02}\Delta^{(1)}) = \frac{x^{(0)}x^{(2)} + y^{(0)}y^{(2)} + z^{(0)}z^{(2)}}{\|\mathbf{x}^{(0)}\|},\\
\hat{I}_3(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) &:= g^{[3]}(\Delta^{(0)}, \Delta^{(0)}) = \|\mathbf{x}^{(0)}\|,
\end{aligned} \tag{2.82}$$

where $\mathbf{x}^{(j)} \in \mathcal{R}$ denotes a point with coordinates $(x^{(j)}, y^{(j)}, z^{(j)}) \in \mathbb{R}^3$, with $j = 0, 1, 2$, and the norm in $\mathcal{R}$ has the expression $\|\mathbf{x}\| = \sqrt{x^2 + y^2 + z^2}$.

As the considered vector fields are Killing with respect to the metric, norms are preserved. Thus, it is possible to obtain new constants of motion simply by multiplying functions in (2.82) by the norm $\|\mathbf{x}^{(0)}\|$. The new functions are

$$\begin{aligned}
I_1(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) &:= x^{(0)}x^{(1)} + y^{(0)}y^{(1)} + z^{(0)}z^{(1)},\\
I_2(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) &:= x^{(0)}x^{(2)} + y^{(0)}y^{(2)} + z^{(0)}z^{(2)},\\
I_3(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) &:= \|\mathbf{x}^{(0)}\|^2 = (x^{(0)})^2 + (y^{(0)})^2 + (z^{(0)})^2,
\end{aligned} \tag{2.83}$$

The matrix of derivatives of these functions is

$$\left(\frac{\partial I}{\partial \mathbf{x}^{(0)}}\right) := \begin{pmatrix}
\frac{\partial I_1}{\partial x^{(0)}} & \frac{\partial I_1}{\partial y^{(0)}} & \frac{\partial I_1}{\partial z^{(0)}}\\
\frac{\partial I_2}{\partial x^{(0)}} & \frac{\partial I_2}{\partial y^{(0)}} & \frac{\partial I_2}{\partial z^{(0)}}\\
\frac{\partial I_3}{\partial x^{(0)}} & \frac{\partial I_3}{\partial y^{(0)}} & \frac{\partial I_3}{\partial z^{(0)}}
\end{pmatrix} = \begin{pmatrix}
x^{(1)} & y^{(1)} & z^{(1)}\\
x^{(2)} & y^{(2)} & z^{(2)}\\
2x^{(0)} & 2y^{(0)} & 2z^{(0)}
\end{pmatrix}. \tag{2.84}$$

The computation of its determinant,

$$\det\left(\frac{\partial I}{\partial \mathbf{x}^{(0)}}\right) = 2\mathbf{x}^{(0)} \cdot \left(\mathbf{x}^{(1)} \times \mathbf{x}^{(2)}\right), \tag{2.85}$$

shows that the matrix is regular if $\mathbf{x}^{(0)}, \mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ are linearly independent. In this expression and the following, it is useful to use the vector notation that is common in $\mathbb{R}^3$. Thus, $\mathbf{x}\cdot\mathbf{y}$ and $\mathbf{x}\times\mathbf{y}$ denote respectively the scalar and vectorial product of vectors in $\mathbb{R}^3$.

As the matrix of derivatives is regular at a generic point $(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) \in \mathcal{R}^3$, it is possible to solve the following system for $\mathbf{x}^{(0)}$:

$$\begin{cases} I_1(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) = k_1, \\ I_2(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) = k_2, \\ I_3(\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) = k_3, \end{cases} \qquad k_1, k_2, k_3 \in \mathbb{R}, \quad k_3 > 0. \tag{2.86}$$

The solution of these system of equations is precisely the superposition rule for the Lie system $\mathcal{X}^H_{\mathcal{R}}$.

The system of equations can be rewritten as a set of three vector equations in $\mathbb{R}^3$:

$$\mathbf{x}\cdot\mathbf{x}_1 = k_1, \qquad \mathbf{x}\cdot\mathbf{x}_2 = k_2, \qquad \mathbf{x}\cdot\mathbf{x} = k_3, \tag{2.87}$$

with $k_1, k_2, k_3 \in \mathbb{R}$ and $k_3 > 0$. Since $\mathbf{x}_1$ and $\mathbf{x}_2$ are not collinear when the matrix (2.84) is regular, this system is easily solved in $\mathbf{x}$ by defining an orthonormal system relative to the standard scalar product on $\mathbb{R}^3$:

$$\mathbf{x}'_1 := \frac{\mathbf{x}_1}{\|\mathbf{x}_1\|}, \qquad \mathbf{x}'_2 := \frac{\|\mathbf{x}_1\|^2\mathbf{x}_2 - (\mathbf{x}_1\cdot\mathbf{x}_2)\mathbf{x}_1}{\|\mathbf{x}_1\|\sqrt{\|\mathbf{x}_1\|^2\|\mathbf{x}_2\|^2 - (\mathbf{x}_1\cdot\mathbf{x}_2)^2}}.$$

These two new vectors together with their cross product, $\mathbf{x}'_1\times\mathbf{x}'_2$, conform an orthonormal basis for $\mathbb{R}^3$. From (2.87), the general expression for $\mathbf{x}$ is

$$\mathbf{x} = k'_1\mathbf{x}'_1 + k'_2\mathbf{x}'_2 \pm \sqrt{k_3 - (k'_1)^2 - (k'_2)^2}\ \mathbf{x}'_1\times\mathbf{x}'_2, \tag{2.88}$$

where the coefficients k'_1 and k'_2 are

$$k'_1 = \mathbf{x}\cdot\mathbf{x}'_1 = \frac{k_1}{\|\mathbf{x}_1\|}, \qquad k'_2 = \mathbf{x}\cdot\mathbf{x}'_2 = \frac{k_2\|\mathbf{x}_1\|^2 - k_1(\mathbf{x}_1\cdot\mathbf{x}_2)}{\|\mathbf{x}_1\|\sqrt{\|\mathbf{x}_1\|^2\|\mathbf{x}_2\|^2 - (\mathbf{x}_1\cdot\mathbf{x}_2)^2}}.$$

Replacing k'_1 and k'_2 in (2.88), the solution to the system of equations (2.87) is

$$\mathbf{x} = \frac{\delta_{12}\mathbf{x}_1 + \delta_{21}\mathbf{x}_2 \pm \sqrt{k_3[\|\mathbf{x}_1\|^2\|\mathbf{x}_2\|^2 - (\mathbf{x}_1\cdot\mathbf{x}_2)^2] - (k_1\mathbf{x}_1 - k_2\mathbf{x}_2)^2}\ \mathbf{x}_1\times\mathbf{x}_2}{\|\mathbf{x}_1\|^2\|\mathbf{x}_2\|^2 - (\mathbf{x}_1\cdot\mathbf{x}_2)^2},$$

where $\delta_{lj} := k_l\|\mathbf{x}_j\|^2 - k_j(\mathbf{x}_l\cdot\mathbf{x}_j)$. As the Lie system $\mathcal{X}^H_{\mathcal{R}}$ is linear in the chosen coordinate system and the Riemannian metric related to the standard scalar product on $\mathcal{R}$ is invariant under the elements of $V_{\mathcal{R}}$, it follows that $\|\mathbf{x}_1\|^2$, $\|\mathbf{x}_2\|^2$ and $\mathbf{x}_1\cdot\mathbf{x}_2$ are constant along particular solutions of $\mathcal{X}^H_{\mathcal{R}}$. It is thus possible to simplify the expression, leading to the following results.

Theorem 2.41. *The superposition rule for the Lie system $\mathcal{X}^H_{\mathcal{R}}$ on $\mathcal{R}$ is a function*

$$\begin{array}{rccc} \Phi_{\mathcal{R}}: & \mathcal{R}^2\times\mathcal{A} & \to & \mathcal{R} \\ & (\mathbf{x}_1, \mathbf{x}_2, (k_1, k_2, k_3)) & \mapsto & \mathbf{x} = \Phi_{\mathcal{R}}(\mathbf{x}_1, \mathbf{x}_2, (k_1, k_2, k_3)), \end{array} \tag{2.89}$$

with $A := \{(k_1, k_2, k_3) \in \mathbb{R}^3 : k_3 > 0\}$, which can be written as

$$\mathbf{x} = \delta_{12}\mathbf{x}_1 + \delta_{21}\mathbf{x}_2 + \sqrt{k_3 k_{12} - (k_1\mathbf{x}_1 - k_2\mathbf{x}_2)^2}\ \mathbf{x}_1\times\mathbf{x}_2, \tag{2.90}$$

where $k_{12} := \|\mathbf{x}_1\|^2\|\mathbf{x}_2\|^2 - (\mathbf{x}_1\cdot\mathbf{x}_2)^2$.

Regarding the projective manifold $\mathcal{P}$, deriving a superposition rule for $\mathcal{X}^H_{\mathcal{P}}$ amounts to obtain a superposition rule for the solutions to $\mathcal{X}^H_{\mathcal{R}}$ on $\iota_{\mathcal{P}}(\mathcal{P})$, namely those equivalence classes of $\mathcal{R}$ coming from elements of $M_{Q,0}$ with the same module.

To obtain the superposition rule for the system $\mathcal{X}^H_{\mathcal{P}}$ on $\mathcal{P}$, consider the natural embedding of $\mathcal{P}$ into $\mathcal{R}$ whose image is the set of elements $(x, y, z) \in \mathcal{R}$ such that $x^2 + y^2 + z^2 = 1$. Therefore, $\mathcal{P}$ is diffeomorphic to a sphere $S^2 \subset \mathcal{R}^2 \simeq \mathbb{R}^3_0$. Consider the superposition rule defined for $\mathcal{X}^H_{\mathcal{R}}$ when restricted to points in S^2, i.e. with $\|\mathbf{x}_1\| = \|\mathbf{x}_2\| = 1$. The set of constants has to be constrained in order to obtain solutions in $\mathcal{Q}^2$. From (2.87), the constraints are

$$|k_1|, |k_2| \leq 1, \quad k_3 = 1. \tag{2.91}$$

In consequence, the superposition rule for $\mathcal{P}$ can be written in terms of its embedding into $\mathcal{R}$ as

$$\mathbf{x} = \delta_{12}\mathbf{x}_1 + \delta_{21}\mathbf{x}_2 + \sqrt{k_{12} - (k_1\mathbf{x}_1 - k_2\mathbf{x}_2)^2}\, \mathbf{x}_1 \times \mathbf{x}_2, \quad \mathbf{x}_1, \mathbf{x}_2 \in \mathcal{P}, \quad |k_1|, |k_2| \leq 1. \tag{2.92}$$

where $k_{12} := 1 - (\mathbf{x}_1 \cdot \mathbf{x}_2)^2$ and $\delta_{lj} := k_l - k_j(\mathbf{x}_l \cdot \mathbf{x}_j)$, for $j, l = 1, 2$.

2.6 The relevance of Lie systems in Quantum Mechanics

Systems of differential equations appear in every description of Quantum Mechanics. Thus, it is indubitable that any method of resolution has great importance in Physics. Lie systems offer a new perspective in this topic. As proved along this chapter, the geometric formalism offers a suitable framework for the application of this tool. Thus, it is possible to solve the Schrödinger equation for finite-dimensional systems by means of a superposition rule. Even more, the geometric description is not restricted to the Hilbert space, as the projective manifold of pure states can also be characterised in geometric terms. Thus, Lie systems and superposition rules are a powerful tool to describe dynamics on this manifold. This is very relevant, as the common algebraic description of Quantum Mechanics usually ignores the projective manifold.

It is remarkable that the superposition rule obtained in this chapter is non linear. Schrödinger equation, as a linear differentiable equation on a Hilbert space, naturally carries a linear superposition rule, as indicated in (2.2):

$$|\psi(t)\rangle = \sum_{j=1}^{n} k_j |\psi_j(t)\rangle, \quad k_1, \ldots, k_n \in \mathbb{C}, \quad t \in \mathbb{R}, \tag{2.93}$$

where $|\psi_1(t)\rangle$, ..., $|\psi_n(t)\rangle$ are n functionally-independent particular solutions for the Schrödinger system. The existence of this equation is a property of linear spaces, and gives no information on the structure of quantum systems. The approach presented here, however, yields a different result. As seen in Theorem 2.38, Schrödinger equations with traceless Hamiltonians can be solved by means of a non linear superposition rule. This is related to the quantum nature of the problem. The true set of states for a quantum system is the projective manifold $\mathcal{P}$, which is non linear. Thus, it is natural to expect that a Lie system on M_Q, that in some way reproduces the true behaviour of quantum systems, enjoys non linear properties.

Many further studies can be done starting from the results presented here. It is possible to apply numerical methods in conjunction with superposition rules in order to obtain solutions for particular dynamics of quantum systems. This may have innumerable applications in Molecular Dynamics, Solid State Physics and other fields. On the other hand, the theory of Lie systems can be applied to other formulations of Quantum Mechanics. As seen in the following chapters, a joint description of pure and mixed states of quantum systems can also be described in geometrical terms. Therefore, Lie systems may also offer interesting results in field of Molecular Dynamics.

Chapter 3

Geometric formulation: the set of pure and mixed states

In Chapters 1 and 2 of this dissertation, the geometrical description of pure states of quantum systems has been studied. Schrödinger picture plays a key role, as it gives an appropriate framework for the study of quantum systems. A different approach, however, is necessary in order to describe mixed states, i.e. situations appearing in statistical systems in which there is no complete information on the actual state of the system. Due to Gleason's theorem [136], mixed states are usually characterised by density matrices (see below). Density matrices are Hermitian, positive, trace-class operators on the Hilbert space that fully characterise the possible statistical ensembles of a quantum system. For the purpose of developing a geometric formalism, however, it is useful to consider an alternative, although equivalent, approach offered by the Heisenberg picture. According to it, dynamics of quantum systems can be described as evolution of observables. This description allows for a characterisation of the set of pure and mixed states. It is a simple task to perform this analysis in a geometric language, thus appropriately describing the structures present in these sets. The aim of this chapter is thus to describe the set of pure and mixed states of quantum systems by means of a geometric formalism.

In its modern formulation, the Heisenberg picture of Quantum Mechanics associates a complex C*-algebra to each quantum system. Quantum observables are represented by self-adjoint elements in this algebra, i.e. by invariant elements with respect to the existing involution. In the Heisenberg picture, observables are taken as the fundamental objects, instead of states, which are simply identified as functionals on the C*-algebra. Dynamics, therefore is characterised in terms of a trajectory on the C*-algebra of the system. For a careful description of this approach, see the works by Jordan, von Neumann and Wigner [166], Gelfand and Neimark [133], Segal [239], Emch [120] and Strocchi [252].

The foundation of the algebraic approach to physical systems relies on an empirical interpretation of Physics. Accordingly, a system is defined by its physical properties, called observables. A proper mathematical description of the properties of observables is thus enough to completely characterise the system. This interpretation was first proposed in relation with quantum systems; in this context, it is commonly known as the Copenhagen interpretation of Quantum Mechanics.

Before dealing with the proper description of the Heisenberg picture, several properties of the algebraic structures presented here will be discussed. In particular, Jordan algebras and their relation with associative and Lie algebras will be presented.

The chapter is organised as follows. Section 3.1 presents the Heisenberg picture of Quantum Mechanics and describes the Lie-Jordan algebra of observables and the set of states that are associated to quantum systems in this approach. In order to offer a better characterisation of observables, Section 3.2 offers a description of Lie-Jordan algebras. Geometric formalism is introduced in Section 3.3, both on the dual space of the Lie-Jordan algebra of observables and on the set of states of the quantum system. This is illustrated in Section 3.4 by the description of the set of states of a 2-level system.

3.1 The Heisenberg picture of Quantum Mechanics

This section presents a brief description of Heisenberg picture. In its modern formulation, the Heisenberg picture of Quantum Mechanics associates a complex C*-algebra to each quantum system. Quantum observables are represented by self-adjoint elements in this algebra, i.e. by invariant elements with respect to the existing involution. In the Heisenberg picture, observables are taken as the fundamental objects, instead of states, which are simply identified as functionals on the C*-algebra. Dynamics, therefore is characterised in terms of a trajectory on the C*-algebra of the system.

A rigorous derivation of Heisenberg picture can be achieved by means of a careful identification of the mathematical objects describing physical objects. This minimalistic approach to Physics was proposed by authors such as Jordan, von Neumann and Wigner [166], Gelfand and Neimark [133], and Segal [239]. In his work, Segal details the postulates that observables have to satisfy, which are based on physical properties shared by all systems. From them, it is possible to prove that observables are necessarily elements of a complex C*-algebra that encodes their properties. It should be stressed that this mathematical description can be particularised to any physical system, either classical or quantum, as it is based on the physical properties that any observable has to satisfy.

Since its first proposal several works have dealt with this algebraic description of physical systems, such as those by Emch [120] and Strocchi [252]. This last reference presents a pedagogical approach to the algebraic description, which will be summarised in the first part of the section. When particularising to the case of quantum systems, the Heisenberg picture of Quantum Mechanics is obtained. The main features of this picture are presented in the remaining of the section.

3.1.1 An algebraic description of physical systems

From an empirical point of view, physical systems are described by the values of the measurements of physical magnitudes on them. In other words, systems are characterised by the observables that can be measured on them and by the possible values of such measures. Thus, the properties of the set $\mathcal{O}$ of observables of a physical system have to be determined.

An observable $A \in \mathcal{O}$ is characterised by the values of its measurements in different states of the system. These values are always real numbers, hence it is a simple matter to consider additions and sums of observables. Following the book by Strocchi [252], the set $\mathcal{O}$ of observables of a mathematical system can be given the structure of a real linear space. In the same way, it is possible to consider powers A^n, whose measurements will give the corresponding powers of the values of the measurements of A. In particular, the 0-power of an observable is $A^0 = I$, the 'identity observable' whose value is 1 for any measurement.

The linear structure and the existence of powers in $\mathcal{O}$ make possible to define the following symmetric product:

$$A \odot B = (A + B)^2 - A^2 - B^2, \quad A, B \in \mathcal{O}. \tag{3.1}$$

With this definition, the square of an observable $A \in \mathcal{O}$ is obtained as $A \odot A = 2A^2$. If linearity is assumed on its arguments, it satisfies the properties of a Jordan product [165, 166]. Thus, $\mathcal{O}$ has naturally the structure of a linear Jordan algebra, presented in Definition 1.11 and reproduced here.

Definition 3.1. *A linear Jordan algebra over a field K is a pair $(J, \odot)$ where J is a linear space over K and $\odot$ is a symmetric K-bilinear composition law in J, called the Jordan product of the algebra, satisfying the Jordan identity*

$$(x \odot y) \odot x^2 = x \odot (y \odot x^2), \quad x, y \in J, \tag{3.2}$$

where $x^2 := x \odot x$. A linear Jordan algebra is called unital if there exists an element $1 \in J$ such that $x \odot 1 = x$ for any $x \in J$.

As shown by Segal [239], the description of observables as elements in linear Jordan algebras is enough in order to represent most of the desired properties of physical system. It is possible, however, to obtain a simpler characterisation by considering the complex extension of the set of observables $\mathcal{O}$. Its description requires the following definitions.

Definition 3.2. *A Banach algebra $\mathcal{B}$ over a field K is an associative algebra over K which is also a normed and complete space. The norm $\|\cdot\|$ and the associative composition law of a Banach algebra satisfy the condition*

$$\|xy\| \leq \|x\|\|y\|, \quad \forall x, y \in \mathcal{B}. \tag{3.3}$$

Definition 3.3. *A C*-algebra $\mathcal{A}$ is an involutive Banach algebra over the field $\mathbb{C}$ of complex numbers, satisfying the condition*

$$\|x^*x\| = \|x\|^2, \quad \forall x \in \mathcal{A}, \tag{3.4}$$

where $*$ is an involution in $\mathcal{A}$ which is also an antiautomorphism

$$(x^*)^* = x, \quad (xy)^* = y^*x^*, \quad \forall x, y \in A. \tag{3.5}$$

An element $x \in \mathcal{A}$ is said to be self-adjoint if $x^* = x$.

Since its conception, it is known that linear Jordan algebras are divided in two kinds: special and exceptional [4, 165, 166, 201]. Special Jordan algebras can always be embedded in a larger C*-algebra; exceptional Jordan algebras, which are few, do not have this property. Furthermore, exceptional Jordan algebra do not appear in the study of physical systems [201]. Thus, the algebraic description of the Heisenberg picture assumes that, for any physical system, there always exists a complex C*-algebra $\mathcal{A}$ whose self-adjoint elements constitute the set $\mathcal{O}$ of observables.

States of the system are represented in this interpretation by functions on $\mathcal{O}$ that associate to each observable the possible results of its measurements. These functions are assumed to be linear. Thus, the set $\mathcal{S}$ of states of the system is a subset of the dual space $\mathcal{O}^*$, or equivalently a subset of $\mathcal{A}^*$. Given a state $\rho \in \mathcal{S}$ and an observable $A \in \mathcal{O}$, the quantity $\rho(A)$ is known as the expectation value of A for the state ρ. This number represents the average value of A when evaluated on a system in the state ρ, which in general represents a probability distribution on the phase space of the system. Because of the properties of observables and averages of measurements, the states are normalised positive functions:

$$\rho(I) = 1, \quad \rho(A^2) \geq 0, \quad \forall \rho \in \mathcal{S}, \quad \forall A \in \mathcal{O}. \tag{3.6}$$

By linearity, states can be extended to act on the whole C*-algebra. Thus, a state ρ on the C*-algebra $\mathcal{A}$ is a linear map $\rho : \mathcal{A} \to \mathbb{C}$ satisfying

$$\rho(I) = 1, \quad \rho(A^*A) \geq 0, \quad \overline{\rho(A)} = \rho(A^*), \quad \forall \rho \in \mathcal{S}, \quad \forall A \in \mathcal{A}. \tag{3.7}$$

This extension of states to the whole C*-algebra is useful in an algebraic formulation of the theory, as it allows for a matrix characterisation of states. However, a geometric formalism can deal directly with the algebra $\mathcal{O}$ of observables. Thus, (3.6) will be enough in order to characterise the geometric properties of the set $\mathcal{S}$ of states.

As proved in the aforementioned references, it is enough to determine the C*-algebra associated with a physical system and the corresponding set of states in order to fully characterise it. Different theories are represent by different properties of the observables and states. Classical Mechanics is described by a commutative C*-algebra of observables. Quantum systems, on the other hand, require a non-commutative algebra of observables. This is the most important difference between both theories.

3.1.2 The C*-algebra of the Heisenberg picture

Classical Mechanics is a trivial case of the mathematical structure defined above. It is simple to prove that Classical Mechanics is described by an Abelian algebra of observables, and that this algebraic approach recovers the canonical description of classical systems.

In the case of Quantum Mechanics, the situation is different, as shown by experiments carried out in the first years of the 20th century. Realistic measurements on physical systems are always subject to some indetermination, i.e. some dispersion on the values of the measurement. In order to obtain this dispersion, recall that states ρ allow to compute expectation value of observables. Thus, the standard

derivation $\Delta_\rho A$ of an observable A for a system on a state ρ is given in the algebraic setting by the following quantity [252]:

$$\Delta_\rho A = \sqrt{\rho(A^2) - (\rho(A))^2}. \tag{3.8}$$

Classical Mechanics assumes that there exists no lower bound to the values of these dispersions. As proved experimentally, however, this is not always the case when two observables are measured simultaneously. In particular, if the position X_j of a quantum particle along a certain direction and momentum P_j in the same direction are measured, the Heisenberg uncertainty principle holds for any state of the system:

$$(\Delta_\rho X_j)(\Delta_\rho P_j) \geq \frac{1}{2}, \tag{3.9}$$

in natural units, i.e. with $\hbar = 1$. Observe that the Heisenberg uncertainty principle was already deduced in (1.27) in the context of the Schrödinger picture. As in that case, there exists a generalisation of this relation for any pair of observables.

Theorem 3.4. *The following relation between standard derivations of observables holds:*

$$(\Delta_\rho A)(\Delta_\rho B) \geq \frac{1}{2}\big|\rho([A,B])\big|, \quad \forall A, B \in \mathcal{O}, \quad \forall \rho \in \mathcal{S}, \tag{3.10}$$

with $[A,B] = AB - BA$.

Proof. See the book by Strocchi [252] for a derivation of this relation, which is a consequence of the positivity of states. □

This relation is the extention to pure and mixed states of the Robertson uncertainty relation, presented in Corollary 1.16. A non-zero lower bound to the product $(\Delta_\rho A)(\Delta_\rho B)$ exists for any pair $A, B \in \mathcal{O}$ if and only if $\mathcal{O}$ is a non-Abelian algebra. The non-commutativity of observables is a basic notion in Quantum Mechanics, and it represents the most fundamental difference with classical theories.

The characterisation of non-commutative C*-algebras is a relevant topic, necessary in order to understand the equivalence of Schrödinger and Heisenberg pictures. Elements in a C*-algebra can always be represented as operators acting on a Hilbert space, described by the Gelfand-Naimark-Segal (GNS) representation. The result establishes an isomorphism between C*-algebras and bounded operators on Hilbert spaces, as proved by the Gelfand-Naimark theorem. The results are presented next; proofs can be found in [81, 122, 252] and refereces therein.

Theorem 3.5 (GNS representation)**.** *Let $\mathcal{A}$ be a C*-algebra and ρ a state on $\mathcal{A}$. There exists a Hilbert space $(\mathcal{H}_\rho, \langle\cdot|\cdot\rangle_\rho)$ and a representation $\pi_\rho : \mathcal{A} \to \mathcal{B}(\mathcal{H}_\rho)$, with $\mathcal{B}(\mathcal{H}_\rho)$ the algebra of bounded operators on $\mathcal{H}_\rho$, satisfying the following statements:*

1. *There exists a cyclic vector $|\psi_\rho\rangle \in \mathcal{H}_\rho$, i.e. the set $\{\pi_\rho(A)|\psi_\rho\rangle,\ A \in A\}$ is norm dense in $\mathcal{H}_\rho$.*
2. *Expectation values of observables are given by $\rho(A) = \langle\psi_\rho|\pi_\rho(A)|\psi_\rho\rangle_\rho$.*
3. *Any other representation π on a Hilbert space $(\mathcal{H}, \langle\cdot,\cdot\rangle)$ satisfying $\rho(A) = \langle\psi, \pi(A)\psi\rangle$, with $\psi \in \mathcal{H}$ a cyclic vector, is unitarily equivalent to π_ρ, i.e. there exists a unitary operator $U : \mathcal{H} \to \mathcal{H}\rho$ such that*

$$U\pi(A)U^{-1} = \pi_\rho(A), \quad U|\psi\rangle = |\psi_\rho\rangle. \tag{3.11}$$

Theorem 3.6 (Gelfand-Naimark)**.** *A C*-algebra is isomorphic to an algebra $\mathcal{B}(\mathcal{H})$ of bounded operators on a certain Hilbert space $\mathcal{H}$.*

As a consequence of these results, Hilbert spaces arise naturally from an algebraic description of quantum systems. It is in fact possible to relate the Hilbert spaces obtained via the GNS representation with the Schrödinger picture. This proves that the algebraic approach describes all the properties of quantum systems.

The last ingredient that remains to be identified in the Heisenberg picture is the evolution of quantum systems. Consider a family of maps $\Phi_t : \mathcal{A} \to \mathcal{A}$, with $t \in \mathbb{R}$ describing the evolution of an isolated system. If the state of the system is ρ, then $\rho(\Phi_t(A))$ is continuous in t. As argued in [252], this implies that π_ρ and $\pi_\rho \circ \Phi_t$ are unitarily equivalent representations of $\mathcal{A}$ onto $\mathcal{H}_\rho$. Going a step further with the Gelfand-Naimark theorem, because of the isomorphism $\mathcal{A} \cong \mathcal{B}(\mathcal{H}_\rho)$, the evolution map Φ_t can be written as

$$\Phi_t(A) = U_t^{-1} A U_t, \quad A \in \mathcal{A}, \tag{3.12}$$

with $\{U_t\}$ a family of unitary operators on $\mathcal{H}_\rho$. As computed in Section 1.1.5, the expression for U_t in natural units is

$$U_t = \exp(-\mathrm{i}tH), \tag{3.13}$$

where H is a self-adjoint operator on $\mathcal{H}_\rho$. Thus, the differential equation of the family $\{\Phi_t\}$ is the following:

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi_t(A)\bigg|_0 = \mathrm{i}[H, A] = -[\![H, A]\!]. \tag{3.14}$$

This is known as the Heisenberg equation. When restricted to the set of observables $O \subset \mathcal{A}$, it describes the evolution of isolated systems in algebraic terms.

3.1.3 The set of quantum states

As explained in (3.6), the set $\mathcal{S}$ of quantum states is a subset of the dual space $\mathcal{O}^*$. Its defining properties are rewritten here:

$$\rho(I) = 1, \quad \rho(A^2) \geq 0, \quad \forall \rho \in \mathcal{S}, \quad \forall A \in \mathcal{O}. \tag{3.15}$$

This section will provide a complete characterisation of this set. It has a very rich structure with has great relevance in its geometric description.

Proposition 3.7. *The set $\mathcal{S}$ is a convex set.*

Proof. Given two states ρ_1, ρ_2, let us consider the linear combination $\rho = \lambda_1\rho_1 + \lambda_2\rho_2$. For ρ to be a state, relations (3.15) have to be satisfied. The normalization condition requires that $\lambda_1 + \lambda_2 = 1$. Regarding positivity, ρ is a positive function only if both $\lambda_1\rho_1$ and $\lambda_2\rho_2$ are positive, which is guaranteed by imposing $\lambda_1, \lambda_2 \geq 0$. These two conditions imply that any convex combination of states is also a state, and thus $\mathcal{S}$ is a convex set in $\mathcal{O}^*$. □

Definition 3.8. *A state in $\mathcal{S}$ is called pure if it cannot be obtained as a non-trivial convex combination of states. Otherwise, the state is said to be mixed. The set of pure states will be denoted as $\mathcal{S}_1$.*

As a convex set, $\mathcal{S}$ has a boundary, which is determined by the positivity condition. In order to give a proper description of $\mathcal{S}$, consider the set of normalised functions

$$\widehat{\mathcal{S}} = \{\bar{\xi} \in \mathcal{O}^* : \bar{\xi}(I) = 1\}. \tag{3.16}$$

Proposition 3.9. *The set of states $\mathcal{S}$ is a closed set in $\widehat{\mathcal{S}}$, and $\dim \mathcal{S} = \dim \widehat{\mathcal{S}}$. Pure states belong to the boundary of $\mathcal{S}$.*

Proof. Normalization condition implies that $\dim \mathcal{S} = \dim \widehat{\mathcal{S}} = \dim \mathcal{O} - 1$. Any state in the interior of $\mathcal{S}$ is a convex combination of at least two points at the boundary, i.e. it is mixed. Thus, pure states belong necessarily to the boundary of $\mathcal{S}$. □

The boundary of the set of states is a hyper-surface that includes both pure and mixed states. A proper description of this boundary for arbitrarily large quantum systems is a challenging problem. The simplest case corresponds to the 2-level system. As presented below, the set of states of this system can be described by a 3-dimensional sphere, called the Bloch sphere [41]. The boundary is the surface of the sphere, and comprehends only pure states. The 3-level system has been completely described by Goyal *et al.* [140]. Some properties of this system are presented in Appendix A. For larger systems, the description of the boundary of $\mathcal{S}$ is a challenging and greatly difficult problem.

3.1.4 The momentum map

The GNS representation describes how Hilbert spaces can be associated to C*-algebras. Thus, the Schrödinger picture of Quantum Mechanics can be derived from the Heisenberg picture. Obviously, this is not enough to assure that both approaches are equivalent. The missing element is the momentum map. When considered in the quantum setting, the momentum map allows to describe pure states quantum systems in terms of rank-one projectors. From this point, it is a simple task to relate both descriptions of Quantum Mechanics.

Definition 3.10. *Consider a symplectic manifold (M,ω), a Lie group G with Lie algebra $\mathfrak{g}$ and an action $\phi : G \times M \to M$ preserving the symplectic structure ω. For any element $g \in \mathfrak{g}$, there exists an infinitesimal generator of the Lie group action $\bar{\phi}(g) \in \mathfrak{X}(M)$. A momentum map for the action ϕ is a map $\mu : M \to \mathfrak{g}^*$ satisfying*

$$\mathrm{d}\mu_g = \iota_{\bar{\phi}(g)}\omega, \quad \forall g \in \mathfrak{g}, \tag{3.17}$$

with the function μ_g on M being defined as $\mu_g(x) := \mu(x)(g)$.

The momentum map can be considered in the analysis of quantum systems by the Schrödinger picture, presented in Chapter 1. Consider a complex Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle)$. For simplicity, assume in the following that the Hilbert space is finite-dimensional. A linear map $U : \mathcal{H} \to \mathcal{H}$ is said to be unitary if it preserves the Hermitian product:

$$\langle U\psi|U\psi'\rangle = \langle\psi|\psi'\rangle, \quad \forall|\psi\rangle, |\psi'\rangle \in \mathcal{H}. \tag{3.18}$$

The set $U(\mathcal{H})$ of unitary transformation of $\mathcal{H}$ is in fact a real Lie group. Its Lie algebra $\mathfrak{u}(\mathcal{H})$ is the real algebra of linear skew-Hermitian operators on $\mathcal{H}$:

$$\mathfrak{u}(\mathcal{H}) = \{a : \mathcal{H} \to \mathcal{H},\ a = -a^\dagger\}. \tag{3.19}$$

Clearly, there exists an isomorphism $a \in \mathfrak{u}(Hil) \mapsto \mathrm{i}a \in \mathrm{Herm}(\mathcal{H})$ between the unitary Lie algebra and the algebra $\mathrm{Herm}(\mathcal{H})$ of Hermitian operators on $\mathcal{H}$. Furthermore, there exists an inner product $\langle\cdot,\cdot\rangle : \mathfrak{u}(\mathcal{H}) \times \mathfrak{u}(\mathcal{H}) \to \mathbb{R}$ defined by the trace of operators:

$$\langle a, b\rangle = \mathrm{Tr}(a^\dagger b), \tag{3.20}$$

which defines a canonical isomorphism with its dual algebra. Summing up, the canonical isomorphisms $\mathfrak{u}(\mathcal{H}) \cong \mathfrak{u}^*(\mathcal{H}) \cong \mathrm{Herm}(\mathcal{H})$ hold.

Consider now the geometric formulation of the Schrödinger picture, presented in Chapter 1. The Hilbert space $(\mathcal{H}, \langle\cdot|\cdot\rangle)$ of a quantum system can be replaced by a real Kähler manifold (M_Q, ω, g, J). There exists a bijection $\nu : \mathcal{H} \to M_Q$ that relates both approaches, with the Kähler structure being related with the Hermitian product on $\mathcal{H}$. By composition with ν, it is immediate to define an action $\phi_M : U(\mathcal{H}) \times M_Q \to M_Q$ of the unitary group on M_Q which preserves the Kähler structure, and in particular the symplectic form ω. Thus, it is possible to define a momentum map to this action.

Proposition 3.11. *Consider the map $\mu_M : M_Q \to \mathrm{Herm}(\mathcal{H})$ defined by*

$$\mathrm{Tr}\left(\mu_M(\psi)A\right) := f_A(\psi) = \langle\psi|A|\psi\rangle, \quad \psi \in M_Q, \quad A \in \mathrm{Herm}(\mathcal{H}). \tag{3.21}$$

This is a momentum map for the Lie group action ϕ_M of the unitary group on M_Q.

Proof. The infinitesimal generators of the action $\phi_M : U(\mathcal{H}) \times M_Q \to M_Q$ are the Hamiltonian vector fields with respect to functions associated to observables (see Section 1.2.4). For an observable $A \in \mathrm{Herm}(\mathcal{H})$ and the corresponding element $-\mathrm{i}A \in \mathfrak{u}^*(\mathcal{H})$, relation (3.21) implies the following:

$$(\mu_M)_{-\mathrm{i}A} = f_A, \quad \bar{\phi}_M(-\mathrm{i}A) = X_A, \tag{3.22}$$

with the notation of Definition 3.10. Relation (3.17) is satisfied by definition of Hamiltonian vector fields, hence μ_M is a momentum map for the Lie group action ϕ_M. □

Consider now the projection $\pi : M_{Q,0} \to \mathcal{P}$. As detailed in Section 1.3, this projection can be described in terms of an action of the group $\mathbb{C}_0 = \mathbb{R}_+ \times U(1)$ on M_Q, which commutes with the action of the unitary group. Therefore, it is possible to define an action $\phi_{\mathcal{P}} : U(\mathcal{H}) \times \mathcal{P} \to \mathcal{P}$ as $\phi_{\mathcal{P}}(U, [\psi]) := [\phi_M(U, \psi)]$. It is immediate to see that this action preserves the Kähler structure on $\mathcal{P}$. Similarly to the case above, it is possible to define a momentum map for this action.

Proposition 3.12. *Consider a map $\mu_{\mathcal{P}}$ from the projective manifold P to $\mathrm{Herm}(\mathcal{H})$ defined by*

$$\mu_{\mathcal{P}} : \begin{array}{ccc} \mathcal{P} & \to & \mathrm{Herm}(\mathcal{H}) \\ [\psi] & \mapsto & \widehat{\rho}_\psi := \mu_{\mathcal{P}}([\psi]) \end{array}, \qquad \mathrm{Tr}(\widehat{\rho}_\psi A) = \epsilon_A([\psi]) = \frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle}, \quad \forall A \in \mathrm{Herm}(\mathcal{H}). \tag{3.23}$$

The map $\mu_{\mathcal{P}}$ is a momentum map for the Lie group action $\phi_{\mathcal{P}} : U(\mathcal{H}) \times \mathcal{P} \to \mathcal{P}$.

Proof. As in the previous case, the map thus defined associates Hermitian operators with expectation value functions on $\mathcal{P}$. As the action of the unitary group on $\mathcal{P}$ is generated by Hamiltonian vector fields, it is immediate to prove that $\mu_{\mathcal{P}}$ is indeed a momentum map for the Lie group action. □

Corollary 3.13. *The image set $\mu_{\mathcal{P}}(\mathcal{P})$ is the set of rank-one orthogonal projectors on $\mathcal{H}$, satisfying the relations*

$$\widehat{\rho}^2 = \widehat{\rho}, \quad \mathrm{Tr}(\widehat{\rho}) = 1, \quad \forall \widehat{\rho} \in \mu_{\mathcal{P}}(\mathcal{P}). \tag{3.24}$$

Regarding the identification between Schrödinger and Heisenberg picture, recall that the Lie-Jordan algebra $\mathcal{O}$ of observables of the quantum system is precisely the algebra $\mathrm{Herm}(\mathcal{H})$ of Hermitian operators on $\mathcal{H}$. Due to the existing isomorphism, the image set $\mu_{\mathcal{P}}(\mathcal{P})$ can be embedded into the dual space $\mathcal{O}^*$, thus obtaining the following straightforward result.

Proposition 3.14. *There exists a bijection between the set $\mathcal{S} \subset \mathcal{O}^*$ of states of a quantum system and the set $\mathcal{D}(\mathcal{H})$ of density matrices on $\mathcal{H}$, defined as*

$$\mathcal{D}(\mathcal{H}) = \{\widehat{\rho} \in \mathrm{Herm}(\mathcal{H}) \mid \mathrm{Tr}(\widehat{\rho}) = 1,\ \widehat{\rho} \geq 0\}. \tag{3.25}$$

The description of observables and states of a quantum system in terms of Hermitian operators on a Hilbert space $\mathcal{H}$ is useful for their characterisation. In particular, the concepts of rank and eigenvalues are easily defined in this way.

Definition 3.15. *The rank of an element $\bar{\xi} \in \mathcal{O}^*$ is defined to be the rank of the corresponding operator $\widehat{\xi} \in \mathrm{Herm}(\mathcal{H})$ by the isomorphism above described.*

Proposition 3.16. *Let $\rho \in \mathcal{S} \to \widehat{\rho} \in \mathcal{D}(\mathcal{H})$ denote the bijection described in Proposition 3.14. Eigenvalues of $\widehat{\rho}$ satisfy the relations:*

$$\sum_{\lambda \in \mathrm{spec}(\widehat{\rho})} \lambda = 1; \quad \lambda \geq 0,\ \forall \lambda \in \mathrm{spec}(\widehat{\rho}). \tag{3.26}$$

Let $\mathcal{D}_1(\mathcal{H})$ denote the image by this bijection of the set $\mathcal{S}_1$ of pure states. Then, $\widehat{\rho} \in \mathcal{D}_1(\mathcal{H})$ if and only if $\mathrm{spec}(\widehat{\rho}) = \{1, 0, 0, \ldots\}$. In the finite-dimensional case, a state $\rho \in \mathcal{S}$ is said completely mixed if it belongs to the interior of $\mathcal{S}$, in which case all the eigenvalues of $\widehat{\rho}$ are positive, $\lambda > 0$ for any $\lambda \in \mathrm{spec}(\widehat{\rho})$.

Proof. Relations 3.26 are deduced from the definition of the set $\mathcal{D}(\mathcal{H})$ in (3.25). The spectrum for pure states is a consequence of the momentum map. Completely mixed states are positive-definite, which requires the positivity of its eigenvalues. □

The momentum map offers an alternative description in terms of rank-one projectors for pure states of quantum systems. The study of statistical quantum ensembles proves that it is necessary to consider also convex combinations of these operators. Thus, the whole set of density matrices is necessary in order to fully describe pure and mixed states of quantum systems. Next section presents in detail these features.

3.1.5 Statistical quantum ensembles

The treatment of statistical systems of both classical and quantum systems presents similarities, but also important differences. In the classical setting, the symplectic structure of the phase-space plays an important role in the description of the evolution of statistical ensemble. The same is true for quantum systems. However, differences appear in the independence of events. While classical states are independent, quantum ones are not. This feature has a huge relevance in the description of quantum statistical systems.

In general, statistical ensembles are represented by probability densities on the phase-space of the corresponding systems. This is also true in the quantum setting. For simplicity, in the following quantum systems are considered to be finite-dimensional, thus being possible to describe them in geometric terms. The set of pure states of a quantum system is identified a differentiable manifold $\mathcal{P}$, the projective space associated to the usual Hilbert space of the quantum system. Therefore, a quantum statistical ensemble is described by a probability density function $F_{\mathcal{P}}$ on $\mathcal{P}$, i.e. a function on the manifold satisfying a normalisation condition:

$$\int_{\mathcal{P}} F_{\mathcal{P}}([\psi])\ \mathrm{d}\mu_{\mathcal{P}} = 1, \tag{3.27}$$

being $\mathrm{d}\mu_{\mathcal{P}}$ the symplectic volume element on $\mathcal{P}$. The probability density function encodes all the information on the statistical ensemble. In particular, it determines the outcome of measurements on the ensemble.

Definition 3.17. *The expectation value of an observable $A \in \mathcal{O}$ on the statistical ensemble described by the probability distribution F is*

$$\langle A \rangle_F = \int_{\mathcal{P}} F([\psi])\epsilon_A([\psi])\ \mathrm{d}\mu_{\mathcal{P}}, \tag{3.28}$$

with ϵ_A the corresponding expectation value function on $\mathcal{P}$.

The value of $\langle A \rangle_F$ is obtained by weighting the values of ϵ_A on $\mathcal{P}$ with the corresponding probabilities determined by F, analogously to the classical case. However, quantum systems have additional structures that have to be considered. Gleason's theorem [136] shows that expectation values of observables on $\mathcal{P}$ can be written in terms of density matrices. First proved by Gleason in 1957, it is a central result in mathematical physics and quantum information.

Theorem 3.18 (Gleason's theorem)**.** *Let $\mathcal{H}$ be a separable Hilbert space of complex dimension at least 3. For any probability measure $\mathfrak{P}$ on the set Q of self-adjoint projectors on $\mathcal{H}$ there exists a unique trace class operator w such that*

$$\mathfrak{P}(E) = \mathrm{Tr}(wE), \quad \forall E \in Q. \tag{3.29}$$

For a Hilbert space of complex dimension 2, it is not possible to prove the result for generic probability measures. An analogue to the Gleason theorem can be obtained, extending it to the 2-dimensional case [64]. This is obtained by means of the momentum map $\mu_{\mathcal{P}} : \mathcal{P} \to \mathfrak{u}^*(\mathcal{H}) \cong \mathrm{Herm}(\mathcal{H})$ defined in Proposition 3.12.

Theorem 3.19. *Consider a statistical ensemble described by a probability density function F on $\mathcal{P}$. Let $\widehat{\rho}_S(F)$ be the density matrix defined as*

$$\widehat{\rho}_S(F) = \int_{\mathcal{P}} F([\psi])\widehat{\rho}_\psi \mathrm{d}\mu_{\mathcal{P}}, \tag{3.30}$$

with $\widehat{\rho}_\psi = \mu_{\mathcal{P}}([\psi])$ the density matrix associated with $[\psi]$ by the momentum map $\mu_{\mathcal{P}} : \mathcal{P} \to \mathfrak{u}^*(\mathcal{H}) \cong \mathrm{Herm}(\mathcal{H})$. The expectation value of an observable $A \in \mathcal{O}$ for this probability density is

$$\langle A \rangle_F = \mathrm{Tr}(A\,\widehat{\rho}_S(F)). \tag{3.31}$$

Proof. As a consequence of Proposition 3.12, the momentum map defines a unique $\widehat{\rho}_\psi = \mu_{\mathcal{P}}([\psi])$ such that $\epsilon_A([\psi]) = \mathrm{Tr}(A\,\widehat{\rho}_\psi)$. Linearity of the trace makes possible to rewrite (3.28) in terms of density matrices, thus substituting (3.30) and obtaining the result. □

An interesting result can be extracted from Theorem 3.19. The set of density matrices is convex, which means that any $\widehat{\rho}$ can be decomposed as a sum of rank-one projectors

$$\widehat{\rho} = \sum_{j=1}^{r} \lambda_j \widehat{\rho}_j, \tag{3.32}$$

with $r \leq \dim \mathcal{H}$. Recall that this decomposition is not unique. Observe that mixed density matrices no longer satisfy the first condition in (3.24). A measurement of the grade of mixture represented by a density matrix is obtained by the purity P, defined as

$$P(\widehat{\rho}) = \mathrm{Tr}(\widehat{\rho}^2). \tag{3.33}$$

Clearly, pure states have purity 1, as $\widehat{\rho}^2 = \widehat{\rho}$. The minimum purity is $\frac{1}{n}$, with n the complex dimension of the Hilbert space of the system. It corresponds to the maximally mixed state of the system, with density matrix $\frac{1}{n} I$.

There exists a certain freedom in the choice of the probability density function determining a quantum ensemble. It is possible to modify F in such a way that the expectation value (3.28) of any observable is invariant. In other words, there exist infinitely many probability density functions that define the same density matrix for the quantum ensemble. Among them, the following proposition gives a preferred choice for the characterisation of the ensemble.

Proposition 3.20. *Let F be a probability density function on $\mathcal{P}$, and $\widehat{\rho}_S(F)$ its associated density matrix by (3.30). Consider a particular decomposition of $\widehat{\rho}_S(F)$ in terms of rank-one projectors as*

$$\widehat{\rho}_S(F) = \sum_{j=1}^{r} \lambda_j \widehat{\rho}_j. \tag{3.34}$$

Then, there exists a discrete probability density function F_D on $\mathcal{P}$ defined by

$$F_D([\psi]) = \sum_{j=1}^{r} \lambda_j \delta\left([\psi] - [\psi_j]\right), \quad [\psi] \in \mathcal{P}, \tag{3.35}$$

with $[\psi_j]$ the pre-image of $\widehat{\rho}_j$ by the momentum map for $j = 1, 2, \ldots, r$, which satisfies that

$$\widehat{\rho}_S(F) = \widehat{\rho}_S(F_D). \tag{3.36}$$

Proof. By relation (3.30) and decomposition (3.34), it is immediate to check that probability density functions F and F_D are pre-images of the same density matrix. □

As a consequence of Proposition (3.20), any statistical ensemble on $\mathcal{P}$ can be redefined as an ensemble of mutually exclusive pure states. This description is particularly useful in the comparison of properties of classical and quantum statistical ensembles. In particular, it is possible to relate the concept of von Neuman entropy for density matrices [267] with the entropy of a classical statistical ensemble. In general, the entropy is a measurement of the information that a statistical ensemble gives on the actual state of the system. The Gibbs formula gives the entropy S_G for a classical statistical ensemble with a discrete set of microstates. If the probability of the microstate j is p_j, then the Gibbs entropy is

$$S_G = -k_B \sum_j p_j \ln p_j, \tag{3.37}$$

with k_B the Boltzmann constant.

Consider now a quantum system described by a density matrix $\widehat{\rho}$. The von Neumann entropy S_N for $\widehat{\rho}$ is defined as [41, 267]

$$S_N(\widehat{\rho}) := -\sum_{\lambda\in \mathrm{spec}(\widehat{\rho}} \lambda \ln(\lambda) = -\widehat{\rho}\ln\widehat{\rho}, \tag{3.38}$$

Proposition (3.20) shows that the density matrix $\widehat{\rho}$ can decomposed as in (3.32). Thus, it is always possible to obtain a discrete probability density function F_D as in (3.35) such that $\widehat{\rho} = \widehat{\rho}_S(F_D)$. In this way, classical entropy S_G and von Neumann entropy S_N are obtained by similar formulas. Observe that quantum pure states are characterised by having zero von Neumann entropy, while the maximally mixed state of an n-level system has entropy equal to $\ln n$. Thus, the von Neumann entropy measures the grade of mixture of quantum system, in a similar way to the purity introduced in (3.33).

Regarding dynamics, consider a time-dependent probability density function F_t on $\mathcal{P}$. Becaus of (3.30), it induces a trajectory $\widehat{\rho}_S(F_t)$ on the set of density matrices. In the case of isolated systems, the evolution of density matrices is determined by the Liouville-von Neumann equation [59],

$$\frac{\mathrm{d}}{\mathrm{d}t}F_t = \{F_t, \epsilon_H\}, \tag{3.39}$$

with $\epsilon_H \in \mathcal{E}_{\mathcal{O}}(\mathcal{P})$ the expectation value function on $\mathcal{P}$ of the Hamiltonian operator $H \in \mathcal{O}$ of the quantum system. The corresponding trajectory $\widehat{\rho}_S(F_t)$ on the set of density matrices evolves accordingly to the Liouville-von Neumann equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\rho}_S(F_t) = -\mathrm{i}[H, \widehat{\rho}_S(F_t)]. \tag{3.40}$$

Because of the expression of the Liouville-von Neumann equation, any two equivalent Markovian probability density functions on $\mathcal{P}$ determine the same evolution for the density matrix defined by them. In other words, expectation values and the evolution of density matrices are identical for equivalent probability density functions. This supports the statement that the objects that truly represents quantum statistical ensembles are density matrices.

The computation of the density matrix associated to a given statistical ensemble may be a difficult problem. Some particular ensembles are however easy to describe. It is possible to apply this description to the microcanonical and canonical ensembles of quantum systems. An extension to the description of hybrid classical-quantum systems is also possible. These aspects will be presented in Chapter 5.

3.2 Characterisation of Lie-Jordan algebras

Before describing the geometrical formalism of the Heisenberg picture, thi section presents a deeper analysis of the observables of quantum systems. According to the Heisenberg picture, observables are self-adjoint elements in a C*-algebra. However, recall from Section 3.1.1 that this was proposed as a simplification of the actual structure of observables, namely the existence of a Jordan product. Thus, it is advisable to take a look to linear Jordan algebras, its relation with Lie brackets and the possible extensions to these structures [169].

The discovery of Jordan algebras is closely related to the first formulations of Quantum Mechanics. When Heisenberg first proposed his theory of 'matrix mechanics' [152], it was clear that the properties of the set of observables led to its identification as a Lie algebra. A short time later, Jordan realised that an additional structure was needed in order to properly describe the theory in algebraic terms. Jordan first presented and described a new algebraic structure that was defined in terms of the anticommutator of observables [165, 166]. This operation is now called a Jordan product in his honour.

Since its conception by Jordan, there have been many works devoted to the study of Jordan algebras. Reviews on the history and properties of Jordan algebras can be found in the works by Jacobson [162], McCrimmon [201, 202] and Springer [248]. An alternative conception of that proposed by Jordan can be achieved in terms of quadratic operators, as presented by Jacobson [161] and McCrimmon [200]. There have also been attempts to generalise the Jordan structure, which led to the definition of Jordan triple systems and Jordan pairs [160, 192].

Definition 3.1 of linear Jordan algebras is the one originally presented by Jordan [165,166]. In particular, given an associative algebra $\mathcal{A}$, a Jordan product can be obtained by symmetrising the associative product:

$$x \odot y = xy + yx, \quad x, y \in \mathcal{A}. \tag{3.41}$$

Associative algebras are therefore a particular case of linear Jordan algebras. They are also Lie algebras, as a Lie bracket can be obtained by the antisymmetrisation of the associative product:

$$[\![x, y]\!] = xy - yx, \quad x, y \in \mathcal{A}. \tag{3.42}$$

Thus, $\mathcal{A}$ can be given different algebraic structures satisfying some compatibility relations among them. It is possible to generalise this characterisation and define Lie-Jordan algebras, algebraic structures consisting of two different products over a linear space such that they satisfy certain properties [121,185].

Definition 3.21. *A Lie-Jordan algebra over a field K (either $\mathbb{R}$ or $\mathbb{C}$) is a triple $(J, [\![\cdot,\cdot]\!], \odot)$ where $(J, [\![\cdot,\cdot]\!])$ is a Lie algebra over K, $(J, \odot)$ is a linear Jordan algebra over K and the Lie bracket and Jordan product satisfy the relations:*

$$[\![x, y \odot z]\!] = [\![x, y]\!] \odot z + y \odot [\![x, z]\!], \quad (x \odot y) \odot z - x \odot (y \odot z) = \lambda [\![[\![x, z]\!], y]\!], \quad \forall x, y, z \in J, \tag{3.43}$$

where λ is some real positive scalar.

Due to its relevance in the study of quantum systems, the present section intends to properly characterise Lie-Jordan algebras. The relations in (3.43) indicate some interesting properties. The Lie bracket defines derivations of the Jordan product by fixing one of its arguments. Therefore, in order to determine the conditions under which a Jordan algebra can be provided with a Lie structure, derivations of the Jordan product have to be carefully examined. The second relation also plays an important role in determining which are these derivations.

Lie-Jordan algebras appear naturally in the realm of quantum observables. In fact, the structure given to them is obtained when self-adjoint elements of a C*-algebra are considered.

Proposition 3.22. *Let $\mathcal{A}$ be a C*-algebra, and $\mathcal{O}$ the set of real elements in $\mathcal{A}$. The triple $(\mathcal{O}, \odot, [\![\cdot,\cdot]\!])$, is a Lie-Jordan algebra over the field of real numbers $\mathbb{R}$, where the Lie product and the Jordan product are defined in terms of the associative product in $\mathcal{A}$ by*

$$[\![x, y]\!] = -\mathrm{i}(xy - yx), \quad x \odot y = xy + yx, \quad x, y \in \mathcal{O}. \tag{3.44}$$

Proof. The set $\mathcal{O}$ inherits the $\mathbb{R}$-linear structure of $\mathcal{A}$. Direct computations show that $(\mathcal{O}, \odot, [\![\cdot,\cdot]\!])$ fulfils the requirements to be a Lie-Jordan algebra. □

Observe that the relation between complex C*-algebras and real Lie-Jordan algebras can be inverted. The associative product in the C*-algebra is recovered in the complexification of $\mathcal{O}$ as

$$xy = \frac{1}{2} x \odot y + \frac{\mathrm{i}}{2} [\![x, y]\!]. \tag{3.45}$$

In particular, $x^2 = \frac{1}{2} x \odot x$.

3.2.1 Inner derivations of Jordan algebras

Modern theory of Jordan algebras put aside the binary product and consider a different approach based on the definition of an appropriate set of operators [202]. Some of the properties of Jordan algebras are thus obtained in terms of these operators. In the particular case of unital algebras, both approaches are equivalent. In fact, linear Jordan algebras can also be described in terms of operators, as seen next.

Definition 3.23. *Consider a linear Jordan algebra $(J, \odot)$. For every $x \in J$, let the linear operator $L_x : J \to J$ be the Jordan multiplication operator defined as*

$$L_x(y) := x \odot y = y \odot x. \tag{3.46}$$

The set of Jordan multiplication operators will be denoted as $L(J)$.

Proposition 3.24. *The Jordan multiplication operators of a linear Jordan algebra $(J, \odot)$ satisfy the following relation:*

$$[L_x, L_{x^2}] = 0, \quad \forall x \in J, \tag{3.47}$$

where $[\cdot, \cdot]$ denotes the usual commutator of operators.

Proof. This is a direct consequence is immediate from definition (3.46) of Jordan multiplication operators L_x and expression (3.2) for Jordan identity. □

This approach allows for a generalisation of the properties of linear Jordan algebras. Different sets of operators can be defined, leading to equivalent Jordan structures. This is the case of the so-called quadratic Jordan algebras.

Definition 3.25. *A quadratic Jordan algebra over a field K is a pair (J, U_J), where J a linear space over K and the family $U_J := \{U_x : x \in J\}$ consists of K-linear operators on J satisfying the fundamental formula*

$$U_{U_x(y)} = U_x U_y U_x, \quad x, y \in J. \tag{3.48}$$

A quadratic Jordan algebra is called unital if there exists an element $1 \in J$ such that U_1 is the identity operator on J.

The formula (3.48) plays the role of the Jordan identity in the case of quadratic Jordan algebras, as will be shown below. A new family of operators can be defined in this algebra as

$$V_{x,y}(z) := (U_{x+z} - U_x - U_z)(y), \quad x, y, z \in J. \tag{3.49}$$

Proposition 3.26. *The set $V_{J,J}$ of linear combinations of operators of the form $V_{x,y}$, with $x, y \in J$, has a Lie algebra structure with respect to the following commutation relation:*

$$[V_{x,y}, V_{z,w}] = V_{V_{x,y}(z),w} - V_{z,V_{y,x}(w)}. \tag{3.50}$$

Proof. As seen in [201], this formula is a direct consequence of (3.48). □

The relation (3.50) is the starting point of the so-called Jordan triple systems, linear spaces together with a family of operators satisfying this relation. This and other generalisations of Jordan algebras, such as Jordan pairs, lay beyond the scope of the present work; see [202] for a description of these structures.

Consider again the case of an associative algebra $\mathcal{A}$. Families of operators U_x and $V_{x,y}$ can be obtained by the simple expressions

$$U_x(y) = xyx, \quad V_{x,y}(z) = xyz + zyx, \quad x, y, z \in \mathcal{A}. \tag{3.51}$$

The quadratic dependence in x of the operator U_x is the reason that led to the name of quadratic Jordan algebras.

The linear and quadratic approaches to Jordan algebras are equivalent when a unit element is present in the Jordan algebra [202].

Proposition 3.27. *A pair $(J, \odot)$ is a unital linear Jordan algebra if and only if (J, U_J) is a unital quadratic Jordan algebra with the following relations between operators $U_x, V_{x,y}$ and L_x:*

$$U_x = 2L_x^2 - L_{x^2}, \quad V_{x,y} = 2(L_{x \odot y} + [L_x, L_y]), \quad L_x(y) = \frac{1}{2} V_{x,y}(1), \quad \forall x, y, z \in J. \tag{3.52}$$

From now onwards, when the context is clear, a unital linear and unital quadratic Jordan algebra will be simply referred to as a unital Jordan algebra and denoted as J.

The operators defined here are enough to deal with the relation between Lie and Jordan algebras, in the compatibility sense of (3.43). It is possible to construct a Lie algebra associated with a given Jordan algebra in terms of the so-called Tits-Kantor-Koecher (TKK) construction [172,178,179,258,259]. In its more general form, Jordan pairs are the main ingredient in this construction, which can be particularised to the case of Jordan algebras as follows.

Theorem 3.28 (Tits-Kantor-Koecher contruction). *Given a unital Jordan algebra J, there always exists a graded Lie algebra $TKK(J) := L_{-1} \oplus L_0 \oplus L_{+1}$, where $L_{-1} = L_{+1} = J$ and $L_0 = V_{J,J}$, while the graded Lie brackets of elements are*

$$\begin{aligned} &[T, x_+] = (T(x))_+, \quad [T, x_-] = -(T^*(x))_-, \quad [T, T'] = TT' - T'T, \\ &[x_+, y_-] = V_{x,y}, \quad [x_-, y_+] = -V_{y,x}, \quad [x_+, y_+] = [x_-, y_-] = 0, \end{aligned} \tag{3.53}$$

where $T, T' \in L_0$, $x, y \in J$, and the subindices indicate the component of $TKK(J)$ to which each element belongs, i.e. $x_+, y_+ \in L_{+1}$, $x_-, y_- \in L_{-1}$ and so on. The conjugation in $L_0 = V_{J,J}$ is defined by $V^*_{x,y} = V_{y,x}$.

The TKK construction establishes a relation between elements in the Jordan algebra and operators. Its connection with Lie-Jordan algebras is not, however, immediate, as the operators $V_{x,y}$ are not derivations of the Jordan algebra. Instead, a new type of operators have to be defined.

Lemma 3.29. *Given a unital Jordan algebra J and arbitrary elements $x, y \in J$, let $D_{x,y}$ denote the linear operator on J defined as*

$$D_{x,y} := \frac{1}{4}(V_{x,y} - V_{y,x}) = [L_x, L_y]. \tag{3.54}$$

Such an operator is a derivation of the Jordan product. Let $\mathfrak{d}$ denote the set of these operators and their linear combinations. Such a set is a Lie algebra with respect to the commutator of operators. Elements in $\mathfrak{d}$ are called inner derivations of J.

Proof. The operator $D_{x,y} = [L_x, L_y]$ satisfies the relations

$$D_{x,y}(z) = x \odot (z \odot y) - (x \odot z) \odot y, \quad D_{x,y}(z \odot z') = D_{x,y}(z) \odot z' + z \odot D_{x,y}(z'), \quad \forall x, y, z, z' \in J. \tag{3.55}$$

The second relation proves that $D_{x,y}$ is a derivation of the Jordan product. This derivation relation can be rewritten as $[D_{x,y}, L_z] = L_{D_{x,y}(z)}$, from which follows that

$$[D_{x,y}, D_{z,w}] = D_{D_{x,y}(z),w} + D_{z,D_{x,y}(w)}. \tag{3.56}$$

The commutator of operators is thus an inner operation in the set of inner derivations $\mathfrak{d}$, which proves that $\mathfrak{d}$ is a Lie algebra. □

By comparison of (3.43) and (3.55), it can be deduced that inner derivations of a Jordan algebra are related to a compatible Lie bracket, in the sense of (3.43). A more formal description can be obtained in terms of the TKK construction. Let J be a Jordan algebra and $TKK(J)$ its associated Lie algebra as in Theorem 3.28. The map

$$\omega : J \times J \to \mathfrak{d}, \quad \omega(x, y) := \frac{1}{4}([x_+, y_-] - [y_+, x_-]) = D_{x,y}, \tag{3.57}$$

where $[\cdot, \cdot]$ denotes the Lie bracket in $TKK(J)$, makes possible to obtain the inner derivations in terms of this construction. Recall that $\mathfrak{d}$ contains also linear combinations of operators of the form $D_{x,y}$; therefore, in general $\omega(J, J) \subsetneq \mathfrak{d}$. In the particular case of Lie-Jordan algebras, the algebra of inner derivations satisfies a series of properties.

Theorem 3.30. *Let $(J, [\![\cdot,\cdot]\!], \odot)$ be a Lie-Jordan algebra. The following statements are satisfied*

1. *Inner derivations of the Jordan product are the adjoint representation (with respect to the Lie product) of elements in $[\![J, J]\!]$, i.e.*

$$\mathfrak{d} = \omega(J, J) = \mathrm{ad}([\![J, J]\!]) \cong [\![J, J]\!]/Z, \tag{3.58}$$

   where Z is the centre of the Lie algebra $(J, [\![\cdot,\cdot]\!])$.

2. *If the algebra is unital, i.e. there exists an element $1 \in J$ that acts as the unit element for the Jordan product, then $1 \in Z$.*

3. *The action of the inner derivations on J is such that $\mathfrak{d}(J) = [\![[\![J, J]\!], J]\!]$.*

4. *The centre Z of the Lie structure satisfies $Z \subset \ker \mathfrak{d}$.*

5. *Elements in the derived series of the algebra of inner derivations $\mathfrak{d}$ are the adjoint representations (with respect to the Lie bracket) of elements in the derived series of J:*

$$\mathfrak{d}^{(n)} = \mathrm{ad}(J^{(n+1)}), \quad n = 0, 1, 2, \ldots, \tag{3.59}$$

   with $\mathfrak{d}^{(n+1)} = [\mathfrak{d}^{(n)}, \mathfrak{d}^{(n)}]$, $\mathfrak{d}^{(0)} = \mathfrak{d}$, $J^{(n+1)} = [\![J^{(n)}, J^{(n)}]\!]$ and $J^{(0)} = J$. In particular, J is solvable if and only if $\mathfrak{d}$ is solvable.

6. *Elements in the central series of J satisfy the following properties:*

$$\mathfrak{d}_{(n)} = \mathrm{ad}(J_{(2n+1)}), \quad \mathfrak{d}_{(n)}(J) = J_{(2n+2)}, \quad n = 0, 1, 2, \ldots, \tag{3.60}$$

   with $\mathfrak{d}_{(n+1)} = \omega(\mathfrak{d}_{(n)}(J), (J))$, $\mathfrak{d}_{(0)} = \mathfrak{d}$, $J_{(n+1)} = [\![J_{(n)}, J]\!]$ and $J_{(0)} = J$. In particular, J is nilpotent if and only if $\mathfrak{d}_{(n)} = \{0\}$ for some n.

Proof. Statement *1.* is proved by considering equations (3.43), (3.54) and (3.57). It can be deduced from them that $\omega(x, y) = -\lambda \,\mathrm{ad}_{[\![x,y]\!]}$. Furthermore, as $\mathrm{ad}(z) + \mathrm{ad}(z') = \mathrm{ad}(z + z')$ and $[\![J, J]\!]$ is a linear space, then ω is an exhaustive function and $\mathfrak{d} = \omega(J, J)$. Statement *2.* is directly proved by taking $y = z = 1$ in the derivation relation (3.43). It follows that $[\![x, 1]\!] = 0$ for any $x \in J$, and therefore $1 \in Z$. Statements *3.-6.* are a direct consequence of *1.*, as they are standard properties of adjoint representations of Lie algebras. □

These results characterise the Lie structure of a Lie-Jordan algebra in terms of only the inner derivations of the Jordan product. Therefore, they are useful in order to solve the inverse problem: to determine when a certain Jordan algebra is compatible with a Lie product in the sense of (3.43). The study of the algebra of inner derivations and its properties, together with a classification of Lie algebras, may give information on which Lie products, if any, are compatible with the initial Jordan algebra. Such an analysis has relevance in the study of the contractions of algebras presented in Chapter 4.

From a physical point of view, the connection between Lie and Jordan algebras is fundamental in order to undertand the properties of quantum systems. Both structures are physically relevant. The Lie bracket determines the dynamics of isolated systems. Either in the Heisenberg picture, via the Heisenberg equation, or in the case of density matrices, by the von Neumann equation, the differential equation governing the evolution of an isolated system is defined by means of this Lie bracket. On the other side, the Jordan product plays an important role in the description of the probabilistic nature of Quantum Mechanics. Together, they are needed in order to fully characterise quantum systems. And as a result of the above results, they are not fully independent. The Lie and Jordan structures, hence the dynamics and the probabilistic nature, are interconnected. Thus, the analysis of Lie-Jordan algebras as a whole [72, 169, 202], either algebraically or geometrically, is necessary for a correct description of Quantum Mechanics.

3.2.2 Four-dimensional Lie-Jordan algebras

Simple cases can be studied in order to illustrate Theorem 3.30. Four-dimensional examples are relevant from a physical perspective, as they model the algebra of observables of a 2-level quantum system. Thus, consider a 4-dimensional unital Jordan algebra J over $\mathbb{R}$, and let $\{1, a, b, c\}$ be a basis of J. The element 1 is the unit element of the product $\odot$; the product of the remaining elements are

$$a \odot a = b \odot b = c \odot c = 1, \quad a \odot b = b \odot c = c \odot a = 0. \tag{3.61}$$

In terms of the given basis, linear operators on J are represented by 4×4 matrices. In particular, the coordinate expression of the left-multiplication operators are the following (where dots represents 0 elements):

$$L_1 = \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix}, \quad L_a = \begin{pmatrix} \cdot & 1 & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}, \quad L_b = \begin{pmatrix} \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}, \quad L_c = \begin{pmatrix} \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot \end{pmatrix}.$$

The algebra of inner derivations of the Jordan algebra is generated by the commutators of these operators:

$$D_1 := [L_c, L_b] = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & -1 \\ \cdot & \cdot & 1 & \cdot \end{pmatrix}, \qquad D_2 := [L_a, L_c] = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & -1 & \cdot & \cdot \end{pmatrix},$$

$$D_3 := [L_b, L_a] = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & -1 & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix},$$

and $[L_1, \cdot] = 0$. These generators satisfy the commutation relations

$$[D_1, D_2] = D_3, \quad [D_2, D_3] = D_1, \quad [D_3, D_1] = D_2. \tag{3.62}$$

Therefore, in this example $\mathfrak{d} = \omega(J, J) \cong \mathfrak{su}(2)$, the Lie algebra of the special unitary group on $\mathbb{C}^2$.

Assume now that J is in fact a Lie-Jordan algebra with a certain Lie bracket $[\![\cdot, \cdot]\!]$. Theorem 3.30 can be applied to this hypothesis, with the aim of checking its compatibility with the obtained algebra of inner derivation. As a first consequence, observe that the centre of is the 1-dimensional space spanned by the unity element. Because of (3.43), the unity element in a Lie-Jordan algebra is always in the centre. Hence it can be concluded that $Z = \ker \mathfrak{d} = \{t1 : t \in \mathbb{R}\}$. If this is the case, then $Z \cap [\![J, J]\!] = \{0\}$ and, because of (3.58), it can be concluded that $[\![J, J]\!] \cong \mathfrak{d} \cong \mathfrak{su}(2)$. As J is 4-dimensional, the only possibility is

$$J \cong \mathfrak{su}(2) \oplus Z. \tag{3.63}$$

A direct computation shows that the triple $(J, [\![\cdot, \cdot]\!], \odot)$ with Lie bracket

$$[\![a, b]\!] = c, \quad [\![b, c]\!] = a, \quad [\![c, a]\!] = b, \tag{3.64}$$

and Jordan product given by (3.61) is in fact a Lie-Jordan algebra.

Another example of a 4-dimensional unital Jordan algebra can be given by the following product between elements in the basis:

$$a \odot a = 0, \quad b \odot b = c \odot c = 1, \quad a \odot b = b \odot c = c \odot a = 0. \tag{3.65}$$

The coordinate expressions of the left-multiplication operators of this Jordan algebra read:

$$L_1 = \begin{pmatrix} 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 \end{pmatrix}, \quad L_a = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}, \quad L_b = \begin{pmatrix} \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}, \quad L_c = \begin{pmatrix} \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot \end{pmatrix},$$

while the inner derivations of the Jordan algebra are generated by

$$D_1 := [L_c, L_b] = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & -1 \\ \cdot & \cdot & 1 & \cdot \end{pmatrix}, \qquad D_2 := [L_a, L_c] = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix},$$

$$D_3 := [L_b, L_a] = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix},$$

and $[L_1, \cdot] = 0$. These generators satisfy the commutation relations

$$[D_1, D_2] = D_3, \quad [D_2, D_3] = 0, \quad [D_3, D_1] = D_2. \tag{3.66}$$

The algebra of inner derivations $\mathfrak{d}$ is isomorphic to the Lie algebra of the Euclidean group on the plane, $\mathfrak{e}(2)$. In this case, the centre of $\mathfrak{d}$ has dimension 2, and it is generated by elements $\{1, a\}$.

Let us assume that a Lie bracket exists on J. As $\mathfrak{d}$ is 3-dimensional, then the centre of the corresponding Lie algebra has to be at most 1-dimensional, which would give as in the previous example $Z = \{t1 : t \in \mathbb{R}\}$. This leads to the only possibility that J is isomorphic, as a Lie algebra, to $A_3 \oplus Z$, where A_3 is a 3-dimensional Lie algebra such that $[\![A_3, A_3]\!] \cong \mathfrak{e}(2)$. Such an algebra does not exist; therefore, the given Jordan algebra is not compatible with any Lie structure.

There are cases in which a Jordan algebra is compatible with more than one Lie structure. Consider once again a 4-dimensional unital Jordan algebra J, with basis $\{1, a, b, c\}$ and a Jordan product such that the product of any two non-unit elements in the basis is zero:

$$a \odot a = b \odot b = c \odot c = a \odot b = b \odot c = c \odot a = 0, \qquad x \odot 1 = x, \quad \forall x \in J. \tag{3.67}$$

A computation identical to those of the previous examples shows that the algebra of inner derivations is $\mathfrak{d} = \{0\}$. This indicates that any Lie bracket on J such that $[\![J, J]\!] \subset Z$ is compatible with the given Jordan product. In particular, the Jordan algebra is compatible with an Abelian algebra in which any two elements commute. However, this is not the only possibility. The Heisenberg algebra $\mathfrak{h}(1)$ is a nilpotent algebra determined by the product

$$[\![a, b]\!] = c, \quad [\![a, c]\!] = [\![b, c]\!] = 0. \tag{3.68}$$

Thus, it is possible to find several different Lie structures compatible with a given Jordan algebra.

It can be concluded from this analysis that the relation between Lie and Jordan algebras can be characterised by Theorem 3.30. In the following, both structures will be represented by tensor fields on differentiable manifolds. Their compatibility can be described in similar terms. In Chapter 4, changes in these tensor fields will be considered, thus being necessary to check the compatibility of the new structures.

3.3 The geometry of the set of states

Once that the set of states $\mathcal{S}$ is fully characterised in algebraic terms, a geometric formulation of its properties can be addressed. Recall that $\mathcal{S}$ is a subset of the dual space $\mathcal{O}^*$ of the Lie-Jordan algebra of observables $\mathcal{O}$. Thus, it is natural to consider first the geometric properties of $\mathcal{O}^*$, and from them derive the properties of $\mathcal{S}$. This is the aim of the present section.

A comment should be made regarding the dimensionality of quantum systems. Heisenberg picture can be modelled on Hilbert spaces of infinite dimensions, such as atomic systems (which in fact was the aim of its original formulation). However, as mentioned previously, the reason why the geometric formulation presented along this dissertation is restricted to the case of finite-dimensional quantum systems, which nevertheless is useful to describe a huge number of physical problems, either exactly (such as spin systems and problems of quantum information) or by approximations (by considering a finite number of energy levels, restricting the wave functions to a grid with a finite number of points, etc.).

3.3.1 The dual space of the algebra of observables

Given an algebra, there exists a natural tensorial description of its algebraic properties on its dual space [81, 122, 141, 142]. In the case of the Lie-Jordan algebra $\mathcal{O}$ of observables of a finite-dimensional quantum system, consider the dual space $\mathcal{O}^*$ of real $\mathbb{R}$-linear functionals on $\mathcal{O}$. Because of the linear structure, tangent and cotangent bundles of $\mathcal{O}^*$ satisfy the following canonical isomorphisms:

$$T\mathcal{O}^* \cong \mathcal{O}^* \times \mathcal{O}^*, \quad T^*\mathcal{O}^* \cong \mathcal{O}^* \times (\mathcal{O}^*)^* \cong \mathcal{O}^* \times \mathcal{O}. \tag{3.69}$$

In particular, at each point on $\mathcal{O}^*$, the tangent and cotangent spaces to the manifold are canonically isomorphic to $\mathcal{O}^*$ and $\mathcal{O}$, respectively. Consider furthermore the inner product in $\mathcal{O}$ given by the trace:

$$\langle A, B\rangle = \mathrm{Tr}(AB), \quad A, B \in \mathcal{O}. \tag{3.70}$$

As usual, the inner product defines an isomorphism between the algebra $\mathcal{O}$ and its dual space. Regarding notation, elements in $\mathcal{O}^*$ are denoted with a bar, as follows:

$$\bar{A}(B) := \langle A, B\rangle, \quad \forall A, B \in \mathcal{O}, \tag{3.71}$$

where $\bar{A}$ is an element in $\mathcal{O}^*$. The existing isomorphisms are summarised in the diagram in Figure 3.1.

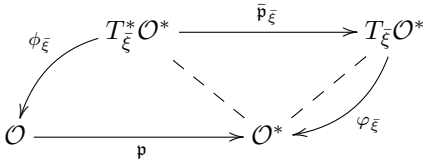


Figure 3.1: The diagram represents the canonical isomorphism $\phi_{\bar{\xi}} : T^*_{\bar{\xi}}\mathcal{O}^* \to \mathcal{O}$ and $\varphi_{\bar{\xi}} : T_{\bar{\xi}}\mathcal{O}^* \to \mathcal{O}^*$ for the tangent and cotangent spaces to $\mathcal{O}^*$ at any point $\bar{\xi}$. The inner product in $\mathcal{O}$ determines by (3.71) an isomorphism $\mathfrak{p} : \mathcal{O} \to \mathcal{O}^*$, with $\mathfrak{p}(A) = \bar{A}$. By composition, an isomorphism $\bar{\mathfrak{p}}_{\bar{\xi}} = \varphi^{-1}_{\bar{\xi}} \circ \mathfrak{p} \circ \phi_{\bar{\xi}} : T^*_{\bar{\xi}}\mathcal{O}^* \to T_{\bar{\xi}}\mathcal{O}^*$ is obtained.

In order to simplify the notation, isomorphisms $T_{\bar{\xi}}\mathcal{O}^* \cong \mathcal{O}^*$ and $T^*_{\bar{\xi}}\mathcal{O}^* \cong \mathcal{O}$ will be implicitly assumed. Thus, it will be clear for the context if the elements are either tangent and cotangent vectors to $\mathcal{O}^*$, or elements in $\mathcal{O}$ and $\mathcal{O}^*$, respectively.

Several geometric objects on $\mathcal{O}$ are related with relevant structures in the description of Quantum Mechanics. In particular, quantum observables are identified with linear functions on $\mathcal{O}^*$.

Definition 3.31. *Given an observable $A \in \mathcal{O}$, the $\mathbb{R}$-linear function $f_A : \mathcal{O}^* \to \mathbb{R}$ is defined by*

$$f_A(\bar{\xi}) = \bar{\xi}(A), \quad \forall \xi \in \mathcal{O}^*. \tag{3.72}$$

The set of such functions will be denoted as $\mathcal{F}_{\mathcal{O}}(\mathcal{O}^*)$.

This is an injective $\mathbb{R}$-linear homomorphism of linear spaces, $A \in \mathcal{O} \mapsto f_A \in (O^*)^*$, which is an isomorphism for the finite-dimensional case that is being considered here.

Proposition 3.32. *At any point $\bar{\xi} \in \mathcal{O}^*$, the differential of a function $f_A \in \mathcal{F}_{\mathcal{O}}(\mathcal{O}^*)$ associated to an observable $A \in \mathcal{O}$ takes the value*

$$(\mathrm{d}f_A)_{\bar{\xi}} = A \in T^*_{\bar{\xi}}\mathcal{O}^* \cong \mathcal{O}. \tag{3.73}$$

Thus, the cotangent space $T^*_{\bar{\xi}}\mathcal{O}^*$ to the dual space at any point $\bar{\xi} \in \mathcal{O}^*$ is generated by the differentials of functions in $\mathcal{F}_{\mathcal{O}}(\mathcal{O}^*)$.

As a consequence of this property, it is immediate to describe the Lie bracket and the Jordan product on $\mathcal{O}$ in terms of $(2,0)$-tensor fields on $\mathcal{O}^*$.

Theorem 3.33. *There exist two contravariant $(2,0)$-tensor fields Λ and R, respectively skew-symmetric and symmetric, defined by their actions on functions in $\mathcal{F}_{\mathcal{O}}(\mathcal{O}^*)$ by*

$$\Lambda(\mathrm{d}f_A, \mathrm{d}f_B)(\bar{\xi}) = \bar{\xi}([\![A, B]\!]) = f_{[\![A,B]\!]}(\bar{\xi}), \quad R(\mathrm{d}f_A, \mathrm{d}f_B)(\bar{\xi}) = \bar{\xi}(A \odot B) = f_{A\odot B}(\bar{\xi}), \tag{3.74}$$

for any $A, B \in \mathcal{O}$, any $\bar{\xi} \in \mathcal{O}^*$.

Proof. Proposition 3.32 shows that it is enough to consider functions in $\mathcal{F}_{\mathcal{O}}(\mathcal{O}^*)$ in order to fully determine geometrical objects. The requirements of $C^\infty(\mathcal{O}^*)$-linearity on the arguments are satisfied by the $\mathbb{R}$-linearity of the Lie bracket and the Jordan product. □

The tensor field Λ is the canonical Kirillov-Kostant-Souriau Poisson tensor field, while R is a symmetric tensor field [141]. Their coordinate expressions will be computed next. Assume that $\mathcal{O}$ carries an inner product, and consider an orthonormal basis $\{\sigma_j\}_{j=1}^n$ for $\mathcal{O}$. An observable $A \in \mathcal{O}$ takes the form $A = a^j\sigma_j$, with $a^1, \ldots, a^n \in \mathbb{R}$ and where summation over repeated indices is understood. The composition laws in $\mathcal{O}$ are determined by their structure constants c^l_{jk} and d^l_{jk}:

$$[\![\sigma_j, \sigma_k]\!] = c^l_{jk}\sigma_l, \quad \sigma_j \odot \sigma_k = d^l_{jk}\ \sigma_l, \quad j,k = 1,2,\ldots,n, \tag{3.75}$$

where $c^l_{jk} = -c^l_{kj}$ and $d^l_{jk} = d^l_{kj}$. Let $\{\sigma^j\}_{j=1}^n$ be the dual basis on $\mathcal{O}^*$, i.e. the set of linear functions on $\mathcal{O}$ satisfying

$$\sigma^j(\sigma_k) = \delta^j_k, \quad j,k = 1,2,\ldots,n. \tag{3.76}$$

Any element $\bar{\xi} \in \mathcal{O}^*$ can be decomposed in this basis as $\bar{\xi} = \xi_j\sigma^j$. Coordinate functions on $\mathcal{O}^*$ with respect to the given basis are functions associated to the elements in the basis of $\mathcal{O}^*$:

$$\xi_j = \bar{\xi}(\sigma_j) = f_{\sigma_j}(\bar{\xi}), \quad \bar{\xi} \in \mathcal{O}^*. \tag{3.77}$$

Coordinate functions on $\mathcal{O}^*$ will be denoted as $x_j = f_{\sigma_j}$. The function associated to an observable $A = a^j\sigma_j$ is thus $f_A = a^j x_j$. With this notation, and in view of (3.74) and (3.75), the coordinate expressions of the tensor fields Λ and R are the following:

$$\Lambda = \frac{1}{2}\ c^l_{jk}x_l \frac{\partial}{\partial x_j} \wedge \frac{\partial}{\partial x_k}, \quad R = d^l_{jk}x_l \frac{\partial}{\partial x_j} \otimes \frac{\partial}{\partial x_k}. \tag{3.78}$$

where $v \wedge w = v \otimes w - w \otimes v$, as in the notation introduced in Section 1.2.1 and following the definition for the exterior product by Crampin and Pirani [104].

The properties of Λ and R as tensor fields makes possible to associate a Hamiltonian and a gradient vector fields to any smooth function on $\mathcal{O}^*$ [142]. These vector fields act, as usual, as derivations on the algebra of smooth functions with respect to the usual point-wise product.

Definition 3.34. *Let X_f and Y_f denote the Hamiltonian and gradient vector fields, respectively, on $\mathcal{O}^*$ associated with a smooth function $f \in C^\infty(\mathcal{O}^*)$ by means of Λ and R:*

$$X_f = -\iota_{\mathrm{d}f}\Lambda, \quad Y_f = \iota_{\mathrm{d}f}R, \quad f \in C^\infty(\mathcal{O}^*). \tag{3.79}$$

Proposition 3.35. *Hamiltonian and gradient vector fields of functions in $\mathcal{F}_{\mathcal{O}}(\mathcal{O}^*)$ take the following values at each point:*

$$(X_{f_A})_{\bar{\xi}} = \overline{[\![A, \xi]\!]}, \quad (Y_{f_B})_{\bar{\xi}} = \overline{B \odot \xi}, \quad \forall A, B \in \mathcal{O}, \quad \forall \xi \in \mathcal{O}^*. \tag{3.80}$$

Proof. By definitions (3.79) and (3.74), it is immediate that

$$(X_{f_A})_{\bar{\xi}}(f_C) = -\bar{\xi}([\![A, C]\!]) = -\mathrm{Tr}(\xi[\![A, C]\!]) = -\mathrm{Tr}([\![\xi, A]\!]C) = \overline{[\![A, \xi]\!]}(C), \quad \forall A, C \in \mathcal{O}, \quad \forall \bar{\xi} \in \mathcal{O}^*,$$

and where $\xi = \mathfrak{p}^{-1}(\bar{\xi})$. The desired results follows from the identification $(\mathrm{d}f_C)_{\bar{\xi}} = C$ by (3.73). The value of Y_{f_B} at each point is found in a similar way. □

Proposition 3.36. *Tensor fields Λ and R define respectively a Poisson bracket and a symmetric product of functions as*

$$\{f,g\} = \Lambda(\mathrm{d}f,\mathrm{d}g), \quad (f,g) = R(\mathrm{d}f,\mathrm{d}g), \quad \forall f,g \in C^\infty(\mathcal{O}^*). \tag{3.81}$$

Furthermore, their restriction to the set $(\mathcal{O}^*)^*$ of $\mathbb{R}$-linear functions defines a Lie-Jordan structure with products

$$(f_A, f_B) = f_{A\odot B}, \quad \{f_A, f_B\} = f_{[\![A,B]\!]}, \quad A,B \in \mathcal{O}. \tag{3.82}$$

Proof. The composition laws can be rewritten in terms of Hamiltonian and gradient vector fields as $\{f,g\} = X_f(g)$ and $(f,g) = Y_f(g)$. These relations and the defining properties of the composition laws of Lie-Jordan algebras, presented in Definition 3.21, prove the asserted statements. □

Observe that Hamiltonian vector fields of $\mathbb{R}$-linear functions are also derivations of the algebras $(\mathcal{F}_{\mathcal{O}}(\mathcal{O}^*), \{\cdot,\cdot\})$ and $(\mathcal{F}_{\mathcal{O}}(\mathcal{O}^*), (\cdot,\cdot))$ of $\mathbb{R}$-linear functions. In the language of Dirac [112], Hamiltonian vector fields are both c-derivations and q-derivations.

Proposition 3.37. *The commutator of two Hamiltonian vector fields is a Hamiltonian vector field. More specifically,*

$$[X_f, X_g] = -X_{\{f,g\}}, \quad \forall f,g \in C^\infty(\mathcal{O}^*). \tag{3.83}$$

Moreover, Hamiltonian and gradient vector fields corresponding to functions in $\mathcal{F}_{\mathcal{O}}(\mathcal{O}^*)$ satisfy the following commutation relations:

$$[Y_{f_A}, Y_{f_B}] = X_{\{f_A,f_B\}} = X_{f_{[\![A,B]\!]}}, \quad [X_{f_A}, Y_{f_B}] = -Y_{\{f_A,f_B\}} = -Y_{f_{[\![A,B]\!]}}, \quad \forall A,B \in \mathcal{O}. \tag{3.84}$$

Proof. If X_f and X_g are Hamiltonian vector fields, then, for each $h \in C^\infty(\mathcal{O}^*)$, the following relation holds:

$$[X_f, X_g](h) = \{f,\{g,h\}\} - \{g,\{f,h\}\} = \{\{f,g\},h\} = -X_{\{f,g\}}(h).$$

Similar expressions are found for the other identities when properly restricted to $\mathbb{R}$-linear functions. □

3.3.2 Geometric characterisation of the set of quantum states

As states of a quantum system can always be identified with density matrices, the results by Grabowski, Kuś and Marmo [141,142] can be applied to the description of states. These works deal with the properties of the sets of positive operators and of density matrices. Both sets can be described as stratified manifolds, with each stratum being determined by the rank of its elements. Due to the existing isomorphism between $\mathcal{S}$ and $\mathcal{D}(\mathcal{H})$, it is possible to obtain similar results on the set $\mathcal{S}$ of quantum states of a quantum. The first step is the identification of distributions of gradient and Hamiltonian vector fields.

Definition 3.38. *Let D_Λ and D_R denote respectively the generalised distribution on $\mathcal{O}^*$ of Hamiltonian and gradient vector fields. That is, D_Λ and D_R are maps that associate to each point $\bar\xi \in \mathcal{O}^*$ the subspace of $T_{\bar\xi}\mathcal{O}^*$ generated respectively by Hamiltonian and gradient vector field:*

$$\begin{aligned} D_\Lambda &: \bar\xi \in \mathcal{O}^* \mapsto D_\Lambda(\bar\xi) = \mathrm{span}\{(X_f)_{\bar\xi} \mid f \in C^\infty(\mathcal{O}^*)\} \subset T_{\bar\xi}\mathcal{O}^*, \\ D_R &: \bar\xi \in \mathcal{O}^* \mapsto D_R(\bar\xi) = \mathrm{span}\{(Y_f)_{\bar\xi} \mid f \in C^\infty(\mathcal{O}^*)\} \subset T_{\bar\xi}\mathcal{O}^*. \end{aligned} \tag{3.85}$$

Let $D_1 : \bar\xi \in \mathcal{O}^* \mapsto D(\bar\xi) \subset T_{\bar\xi}\mathcal{O}^*$ denote the generalised distribution defined by

$$D_1(\bar\xi) = D_\Lambda(\bar\xi) \oplus D_R(\bar\xi), \quad \bar\xi \in \mathcal{O}^*. \tag{3.86}$$

As proved in [142], the distributions D_Λ and D_1 on $\mathcal{O}^*$ are involutive. By Frobenius theorem, they can be integrated to generalised foliations $\mathcal{F}_\Lambda$ and $\mathcal{F}_1$, respectively. Their leaves are characterised in the finite-dimensional case by the GNS representation. For physical systems, there exists an isomorphism $\pi_\rho : \mathcal{A} \to \mathcal{B}(\mathcal{H}_\rho)$, with $\rho \in S$ and $\mathcal{H}_\rho$ being a finite-dimensional complex Hilbert space $\mathcal{H}_\rho$. With this identification, and due to the canonical isomorphism between $\mathcal{O}$ and $\mathcal{O}^*$ induced by the inner product, the relation $O^* \cong \mathcal{O} = \mathrm{Herm}(\mathcal{H}_\rho)$ follows. It is thus possible to state the following results, proved in [142]

Proposition 3.39. *The distribution D_Λ on $\mathcal{O}^*$ is involutive and can be integrated to a generalised foliation $\mathcal{F}_\Lambda$. The leaves correspond to the orbits of the action of the unitary group $U(\mathcal{H}_\rho)$ on $\mathcal{A}$ via its isomorphism with $\mathcal{B}(\mathcal{H}_\rho)$, defined by $(U, \bar{\xi}) \mapsto U\pi_\rho(\bar{\xi})U^*$.*

Distribution D_R is not involutive, as seen clearly from (3.84). The commutator of two gradient vector fields is a Hamiltonian vector field. Thus, distribution D_1, spanned by both Hamiltonian and gradient vector fields, is involutive.

Proposition 3.40. *The distribution D_1 on $\mathcal{O}^*$ is involutive and can be integrated to a generalised foliation $\mathcal{F}_1$. The leaves correspond to the orbits of the action of the general linear group $GL(\mathcal{H}_\rho)$ on $\mathcal{A}$ via its isomorphism with $\mathcal{B}(\mathcal{H}_\rho)$, defined by $(T, \bar{\xi}) \mapsto T\pi_\rho(\bar{\xi})T^*$. Leaves are classified by the rank of their elements.*

This result has a direct application to the description of the set of states $\mathcal{S}$. From Proposition 3.16, states can be classified according to their rank as points in $\mathcal{O}^*$, or equivalently, according to the leave of the foliation $\mathcal{F}_1$ on which they lay. It can be proved [141] that states of constant rank conform submanifolds of $\mathcal{O}^*$, and therefore $\mathcal{S}$ has the structure of a stratified manifold. The following statements clarify these concepts.

Proposition 3.41. *Let $\Pi \subset O^*$ denote the set of real positive linear functionals $\zeta : \mathcal{O} \to \mathbb{R}$. It is a stratified manifold,*

$$\Pi = \bigcup_{k=0}^{n} \Pi_k, \tag{3.87}$$

where the stratum Π_k is the set of rank k elements in Π.

Proof. By definition, each stratum Π_k is a leaf of the foliation $\mathcal{F}_1$ corresponding to the distribution D_1 of Hamiltonian and gradient vector fields, hence a submanifold of $\mathcal{O}^*$. □

Proposition 3.42. *The set of states $\mathcal{S}$ is a stratified manifold,*

$$\mathcal{S} = \bigcup_{k=1}^{n} \mathcal{S}_k, \quad \textit{where} \quad \mathcal{S}_k = \Pi_k \bigcap \widehat{\mathcal{S}}. \tag{3.88}$$

Proof. It is clear from (3.15) that $S = \Pi \cap \widehat{S}$, from which the result follows. □

Strata of $\mathcal{S}$ are determined by the rank of their elements. Special attention has to be paid to the stratum $\mathcal{S}_1$. This is precisely the image by the momentum map of the projective manifold $\mathcal{P}$ of pure states of the system. Thus, the momentum map embeds in a natural way the pure states in the whole set of states of the system. This has important consequences, as seen later, in order to relate the geometric structures on $\mathcal{S}$ and the ones previously introduced in Chapter 1.

Observe that, as a result of Propositions 3.41 and 3.42, both Π and $\mathcal{S}$ have a boundary. Then cannot therefore be described as differentiable manifolds. It is however possible to use differentiable calculus if adequate definitions and properties are established.

Definition 3.43. *A manifold with boundary N of dimension n is a topological space together with an atlas $\{(U_i, \phi_i)\}$, where U_i are open sets in N and $\phi_i : U_i \to \mathbb{R}^{n-1} \times \mathbb{R}_{\geq 0}$, with $\mathbb{R}_{\geq 0} = \{x \in \mathbb{R} : x \geq 0\}$, and such that no atlas defines a differentiable structure on N.*

Observe that any differentiable manifold satisfies the first condition in this definition. The second condition is added so that manifolds with boundary are explicitly assumed not to be differentiable manifolds.

Proposition 3.44. *Both Π and $\mathcal{S}$ are manifolds with boundary, with a natural embedding into $\mathcal{O}^*$. There also exists a natural embedding of $\mathcal{S}$ into $\widehat{\mathcal{S}}$.*

Proof. By definition, Π and $\mathcal{S}$ are closed. The embeddings are also clear from the definitions. □

The embedding of a manifold with boundary into a differentiable manifold with same dimension is the key to carry out differential calculus on them. In practice, computations will be carried out on the larger manifold. At each particular situation, the results obtained have to be compatible with the boundary, even though if they are obtained by differential operations that could not be naturally carried out in the manifold with boundary. Thus, the boundary is seen simply as a constraint for the possible results of the problems.

Because of Definition 3.43 and Proposition 3.44, in the following $\mathcal{S}$ will usually be understood as a closed subset of $\widehat{\mathcal{S}}$. This presents many advantages from a computational perspective. Also, for physical systems, the set of space $\mathcal{S}$ inherits an affine structure. Consider the usual identification of observables as Hermitian operators on a complex Hilbert space $\mathcal{H}$, i.e. $\mathcal{O} = \mathrm{Herm}(\mathcal{H})$. Thus, there exists an inner product on the Lie-Jordan algebra of observables $\mathcal{O}$, defined by the trace as in (3.70). This, in turn, defines a metric on the dual space $\mathcal{O}^*$. The subspace $\widehat{\mathcal{S}}$ is an affine subspace of $\mathcal{O}^*$ with respect to this metric. The appropriate restriction of this metric to $\widehat{\mathcal{S}}$ allows to define distances on the subspace, and by extension on the set of states $\mathcal{S}$.

3.3.3 Reduction of tensor fields

The next step in the description of quantum systems is the characterisation of geometric objects on the set of states $\mathcal{S}$. This can be achieved in an analogous way to the method presented for the Schrödinger picture. It is possible to relate $\mathcal{S}$ with the action of a Lie group on the manifold, thus allowing for a reduction of the tensorial structures. See Section 1.3.1 for a description of the reduction procedure.

Consider the dilation vector field $\Delta_{\mathcal{O}}$ on $\mathcal{O}^*$

$$\Delta_{\mathcal{O}} = Y_{f_I} \;\Rightarrow\; (\Delta_{\mathcal{O}})_{\bar{\xi}} = \bar{\xi}, \quad \forall\, \bar{\xi} \in \mathcal{O}^*. \tag{3.89}$$

As in any linear space, such a vector field defines an integrable distribution on $\mathcal{O}_0^* := \mathcal{O}^* - \{0\}$. Equivalently, $\Delta_{\mathcal{O}}$ is the infinitesimal generator of the group action $r_{\mathcal{O}} : \mathbb{R}_+ \times \mathcal{O}_0^* \to \mathcal{O}_0^*$ defined as

$$r_{\mathcal{O}}(a, \bar{\xi}) = a\bar{\xi}, \quad \forall a \in \mathbb{R}_+,\ \forall\, \bar{\xi} \in \mathcal{O}_0^*. \tag{3.90}$$

This is free and transitive, hence the quotient $\mathcal{O}_0^*/\mathbb{R}_+$ is a differentiable manifold. The reduction of the algebra of functions on the manifold, described in Proposition 3.36, is carried out by considering invariant functions under $r_{\mathcal{O}}$.

It is immediate to check that the Lie-Jordan algebra $\mathcal{F}_{\mathcal{O}}(\mathcal{O}^*)$ of functions associated to observables is not invariant under the group action:

$$\Delta_{\mathcal{O}}(f_A) = (f_I, f_A) = f_A, \quad \forall f_A \in \mathcal{F}_{\mathcal{O}}(\mathcal{O}^*). \tag{3.91}$$

As in the case of the Schrödinger picture, it is necessary to obtain a new set of functions which are invariant under the described group action.

Definition 3.45. *The expectation value function e_A on $\mathcal{O}_0^*$ of an observable $A \in \mathcal{O}$ is defined as*

$$e_A(\bar{\xi}) = \frac{f_A(\bar{\xi})}{f_I(\bar{\xi})} = \frac{\mathrm{Tr}(A\xi)}{\mathrm{Tr}(\xi)}, \quad \forall \bar{\xi} \in \mathcal{O}_0^*. \tag{3.92}$$

The set of expectation value functions on $\mathcal{O}^*$ is denoted as $\mathcal{E}_{\mathcal{O}}(\mathcal{O}_0^*)$.

Proposition 3.46. *Expectation value functions on $\mathcal{O}^*$ are invariant under the group action $r_{\mathcal{O}} : \mathbb{R}_+ \times \mathcal{O}_0^* \to \mathcal{O}_0^*$.*

Proof. The vector field $\Delta_{\mathcal{O}}$, which is the infinitesimal generator of the action, acts on a differential way on the definition (3.92):

$$\Delta_{\mathcal{O}}(e_A) = \frac{1}{f_I}\Delta_{\mathcal{O}}(f_A) - \frac{f_A}{f_I^2}\Delta_{\mathcal{O}}(f_I) = \frac{1}{f_I}f_A - \frac{f_A}{f_I^2}f_I = 0, \quad \forall e_A \in \mathcal{E}_{\mathcal{O}}(\mathcal{O}_0^*).$$

Thus, expectation value functions are invariant under the group action. □

The next step is the characterisation of the algebraic structure of $\mathcal{E}_{\mathcal{O}}(\mathcal{O}_0^*)$. Recall that the Poisson bracket and the symmetric product on $\mathcal{O}^*$, as presented in Proposition 3.36, act on a differential way on their arguments. Thus, it is immediate to compute the following expressions:

$$\{e_A, e_B\} = \frac{1}{f_I}e_{[\![A,B]\!]}, \quad (e_A, e_B) = \frac{1}{f_I}(e_{A\odot B} - 2e_A e_B), \quad \forall e_A, e_B \in \mathcal{E}_{\mathcal{O}}(\mathcal{O}_0^*). \tag{3.93}$$

From these expressions, the following result is deduced.

Proposition 3.47. *The set of expectation value functions $\mathcal{E}_{\mathcal{O}}(\mathcal{O}_0^*)$ is closed under the following composition rules:*

$$\{e_A, e_B\}' := f_I\{e_A, e_B\}, \quad (e_A, e_B)' := f_I(e_A, e_B) + 2e_A e_B, \quad \forall e_A, e_B \in \mathcal{E}_{\mathcal{O}}(\mathcal{O}_0^*). \tag{3.94}$$

The composition laws thus defined can be extended to the whole set of smooth functions on $\mathcal{O}_0^*$. They can be given a tensorial description, in terms of the contravariant $(2,0)$-tensor fields Λ' and R' defined as

$$\Lambda' := f_I\Lambda, \quad R' := f_I R. \tag{3.95}$$

By definition, these tensor fields are invariant along the orbits of the group action $r_{\mathcal{O}}$.

A last step has to be taken in order to properly describe the set of states of quantum systems. Recall that this set is characterised in (3.15) by positivity and normalisation conditions. The connection between these conditions and the projection onto the quotient manifold described above is represented in Figure 3.2. The quotient manifold $\mathcal{O}_0^*/\mathbb{R}_+$ can be embedded into $\mathcal{O}_0^*$ as the unit sphere. However, only the intersection of this sphere with the cone $\Pi - 0$ of positive elements in $\mathcal{O}_0^*$ represent states of the quantum system. It is thus immediate to map this intersection onto the hyperplane $\widehat{\mathcal{S}}$ of trace-one elements. The result is the set $\mathcal{S}$ of states of the quantum system. The map $\varpi : (\mathcal{O}_0^*/\mathbb{R}_+) \cap \Pi_0 \to \mathcal{S}$ is in fact a bijection. Observe in Figure 3.2 that orbits of the described group action are rays steaming from the origin. Thus, the only difference between both sets is the choice of representative of these orbits.

All these tools are enough to describe the geometric properties of the set of states $\mathcal{S}$. By Proposition 3.46, the Lie-Jordan algebra $\mathcal{E}_{\mathcal{O}}(\mathcal{O}^*)$ of expectation value functions on $\mathcal{O}^*$ is invariant under the group action. Thus, its restriction $\mathcal{E}_{\mathcal{O}}(\mathcal{S})$ to $\mathcal{S}$ is also a Lie-Jordan algebra, with identical composition laws. In fact, as these can be given a tensorial description, they can be obtained as the projection onto $\mathcal{O}_0^*/\mathbb{R}_+$, and then the mapping onto $\mathcal{S}$, of the tensor fields Λ' and R'. The results are summarised as follows.

Theorem 3.48. *There exists a pair of tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ on the manifold with boundary $\mathcal{S}$ which are $(\varpi \circ \pi_{\mathcal{O}})$-related with the restrictions of Λ' and R' to the cone Π_0:*

$$\Lambda_{\mathcal{S}} = (\varpi \circ \pi_{\mathcal{O}})_*(\Lambda'), \quad R_{\mathcal{S}} = (\varpi \circ \pi_{\mathcal{O}})_*(R'). \tag{3.96}$$

Consider the composition laws on $C^\infty(\mathcal{S})$ defined as

$$\{f, f'\}_{\mathcal{S}} := \Lambda_{\mathcal{S}}(\mathrm{d}f, \mathrm{d}f'), \quad (f, f')_{\mathcal{S}} := R_{\mathcal{S}}(\mathrm{d}f, \mathrm{d}f') + 2ff', \quad \forall f, f' \in C^\infty(\mathcal{S}). \tag{3.97}$$

The set $\mathcal{E}_{\mathcal{O}}(\mathcal{S})$ is a Lie-Jordan algebra with respect to these composition laws:

$$\{\epsilon_A, \epsilon_B\}_{\mathcal{S}} = \epsilon_{[\![A,B]\!]}, \quad (\epsilon_A, \epsilon_B)_{\mathcal{S}} = \epsilon_{A\odot B}, \quad \forall A, B \in \mathcal{O}. \tag{3.98}$$

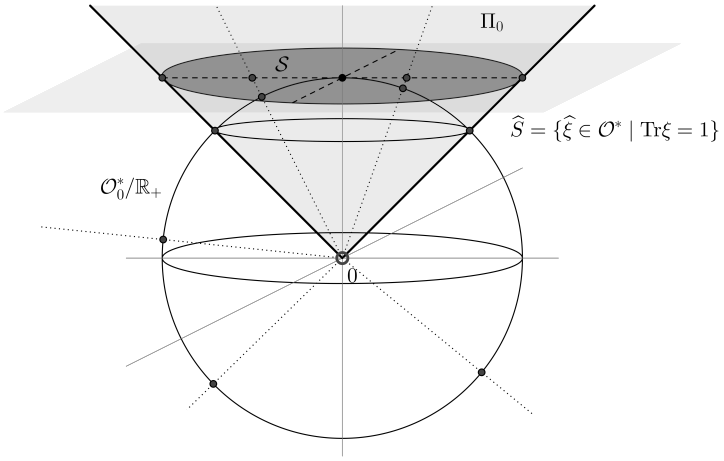


Figure 3.2: Orbits of the group action $r_{\mathcal{O}} : \mathbb{R}_+ \times \mathcal{O}_0^* \to \mathcal{O}_0^*$ are rays steaming from the point $0 \in \mathcal{O}^*$. By taking out this point, it is possible to describe the projection $\pi_{\mathcal{O}} : \mathcal{O}_0^* \to \mathcal{O}_0^*/\mathbb{R}_+$. The resulting quotient manifold can be embedded as the unit sphere in $\mathcal{O}_0^*$. On the other side, the set $\mathcal{S}$ of states of the system, defined in (3.15), is defined as the intersection of the hyperplane $\widehat{\mathcal{S}}$ of trace-one elements and the cone Π_0 of positive elements. It is thus possible to define a bijection $\varpi : (\mathcal{O}_0^*/\mathbb{R}_+) \cap \Pi_0 \to \mathcal{S}$ by relating points in the same orbits of the described group action. Regarding dimensions, recall that $\mathcal{O}^*$ is a n^2-dimensional real space, with $n \geq 2$, hence $\widehat{S}$ is a (n^2-1)-dimensional affine space. The axis are only meant to reflect the linear nature of the manifold, and are not in relation with its dimensionality.

Proof. The action of tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ on the differentials of expectation value functions on $\mathcal{S}$ are

$$\Lambda_{\mathcal{S}}(\mathrm{d}\epsilon_A, \mathrm{d}\epsilon_B) = \epsilon_{[\![A,B]\!]}, \quad R_{\mathcal{S}}(\mathrm{d}\epsilon_A, \mathrm{d}\epsilon_B) = \epsilon_{A\odot B} - 2\epsilon_A\epsilon_B, \quad \forall \epsilon_A, \epsilon_B \in \mathcal{E}_{\mathcal{O}}(\mathcal{S}). \tag{3.99}$$

From these, the composition laws of $\mathcal{E}_{\mathcal{O}}(\mathcal{S})$ follow. □

Corollary 3.49. *The algebra of expectation value functions $\mathcal{E}_{\mathcal{O}}(\mathcal{S})$ gives rise to an associative complex algebra by defining the following product:*

$$\epsilon_A * \epsilon_B = \frac{1}{2}(\epsilon_A, \epsilon_B)_{\mathcal{S}} + \frac{\mathrm{i}}{2}\{\epsilon_A, \epsilon_B\}_{\mathcal{S}} = \epsilon_{AB}, \quad A, B \in \mathcal{O}. \tag{3.100}$$

Some comments could be added with respect to these structures. The bracket $(\cdot,\cdot)_{\mathcal{S}}$ in (3.98) can be rewritten as

$$R_{\mathcal{S}}(\mathrm{d}\epsilon_A, \mathrm{d}\epsilon_B)(\rho) = (\epsilon_A, \epsilon_B)_{\mathcal{S}}(\rho) - 2\epsilon_A(\rho)\epsilon_B(\rho), \quad A, B \in \mathcal{O}, \quad \rho \in \mathcal{S}. \tag{3.101}$$

The action of $R_{\mathcal{S}}$ on expectation value function gives the deviation of the Jordan product from the pointwise product, i.e. of the non-local product with respect to the local product. In this sense, this tensor field captures non-locality of Quantum Mechanics.

In connection with the probabilistic nature of Quantum Mechanics, the tensor field $R_{\mathcal{S}}$ is related with the definitions of variance $\mathrm{Var}(A)$ and covariance $\mathrm{Cov}(A,B)$ of observables:

$$\begin{aligned} \mathrm{Var}(A)(\rho) &= R_{\mathcal{S}}(\mathrm{d}\epsilon_A, \mathrm{d}\epsilon_A)(\rho) = 2\epsilon_{A^2}(\rho) - 2(\epsilon_A(\rho))^2, \\ \mathrm{Cov}(A,B)(\rho) &= R_{\mathcal{S}}(\mathrm{d}\epsilon_A, \mathrm{d}\epsilon_B)(\rho) = \epsilon_{A\odot B}(\rho) - 2\epsilon_A(\rho)\epsilon_B(\rho), \end{aligned} \tag{3.102}$$

i.e. the variance and covariance in terms of expectation values of observables. The relation between Jordan algebras and statistics was already present in the original works by Jordan [165, 166]. Future works will further develop the importance of this tensor field; for now, it is enough to consider that it represents the Jordan product of observables and is therefore necessary to properly describe their algebraic properties.

Definition 3.50. *Let $\widetilde{X}_g$ and $\widetilde{Y}_g$ denote, respectively, the Hamiltonian and gradient vector fields on $\mathcal{S}$, that is, the evaluations of $R_{\mathcal{S}}$ and $\Lambda_{\mathcal{S}}$ on the exact 1-form $\mathrm{d}g$, i.e.*

$$\widetilde{X}_g = -\iota_{\mathrm{d}g}\Lambda_{\mathcal{S}}, \quad \widetilde{Y}_g = \iota_{\mathrm{d}g}R_{\mathcal{S}}. \tag{3.103}$$

for any $g \in C^\infty(\mathcal{S})$. In particular, for expectation value functions, the notation will be simplified as

$$\widetilde{X}_A = \widetilde{X}_{\epsilon_A}, \quad \widetilde{Y}_A = \widetilde{Y}_{\epsilon_A} \quad A \in \mathcal{O}. \tag{3.104}$$

Proposition 3.51. *The commutators of Hamiltonian and gradient vector fields are*

$$[\widetilde{X}_A, \widetilde{X}_B] = -\widetilde{X}_{[\![A,B]\!]}, \quad [\widetilde{Y}_A, \widetilde{Y}_B] = \widetilde{X}_{[\![A,B]\!]}, \quad [\widetilde{X}_A, \widetilde{Y}_B] = widetildeY_{[\![A,B]\!]}, \tag{3.105}$$

for any $A, B \in \mathcal{O}$.

Proof. The result follows by use of Jacobi identity, Jordan identity and relations (3.43). □

Corollary 3.52. *For a quantum n-level system, the Hamiltonian and gradient vector fields of expectation value functions span the complexification $\mathfrak{sl}(n,\mathbb{C})$ of the Lie algebra of the special unitary group $\mathfrak{su}(n)$.*

Thus, a geometric characterisation of the set of states $\mathcal{S}$ is obtained. Due to it being a manifold with a non-smooth boundary, the differentiable structure of the set $\mathcal{S}$ is described in terms of a larger differentiable manifold of which $\mathcal{S}$ is a subset. Thus, it is possible to obtain a pair of tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ that reproduce the algebraic properties of observables. These tensor fields have additionally physical relevance. The Poisson tensor field $\Lambda_{\mathcal{S}}$ characterises the unitary evolution of quantum systems, represented by the von Neumann equation in the language of density operators. On the other hand, the symmetric tensor field $R_{\mathcal{S}}$ is related to the variance and covariance of observables, a characteristic of quantum systems that had not been described geometrically before. Finally, functions associated to observables are also in connection with physical systems, as they give precisely the expectation values that are measured on the system. The geometric characterisation thus described represents satisfactorily the physical properties of quantum systems.

3.3.4 Relation with the geometric description of the Schrödinger picture

The results obtained above can be compared with those computed in Chapter 1 concerning the manifold $\mathcal{P}$ of pure states. Similarities, and also differences, exist between both descriptions. The reduction procedure that defines the new set of contravariant tensor fields are analogous in both cases. This is not a simple coincidence. In fact, it is possible to relate both approaches by means of the momentum maps $\mu_M : M \to \mathcal{O}^*$ and $\mu_{\mathcal{P}} : \mathcal{P} \to \mathcal{O}^*$ defined in Section 3.1.4. Recall that the projection $\pi_{:}M_{Q,0} \to \mathcal{P}$ is defined by the orbits of the Lie group action $r : (\mathbb{R}_+ \times U(1)) \times M_{Q,0} \to M_{Q,0}$. The orbits by $U(1)$ are mapped into a single point by μ_M. Thus, the diagram in Figure 3.3 is obtained.

$$\begin{array}{ccc} M_{Q,0} & \xrightarrow{\mu_M} & \mu_M(M_{Q,0}) = \Pi_1 \\ \pi \downarrow & & \downarrow \pi_{\mathcal{O}}|_{\Pi_1} \\ \mathcal{P} & \xrightarrow{\mu_{\mathcal{P}}} & \mu_{\mathcal{P}}(\mathcal{P}) = \mathcal{S}_1 \end{array}$$

Figure 3.3: Relation between the reduction procedures on the Schrödinger pictures and on the space $\mathcal{O}^*$. The description of pure states by means of the differentiable manifold $\mathcal{P}$ is a part of the total description of states by the state $\mathcal{S}$. Results for both approaches can thus be related in an appropriate way.

Not only the projections, but also the geometric structure of both approaches is related. Observe that, unlike in the case of the manifold $\mathcal{P}$, the structure present in $\mathcal{S}$ is not that of an almost Kähler manifold. The reason is the lack of an almost complex structure on $\mathcal{S}$ relating contravariant tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$. Nevertheless, such a structure can be defined for some submanifolds of $\mathcal{S}$ [142]. For the purpose at hand, it is enough to consider the stratum $\mathcal{S}_1$ of rank-one elements.

Theorem 3.53. *The contravariant tensor fields $\Omega_{\mathcal{P}}$ and $G_{\mathcal{P}}$ on $\mathcal{P}$ are related with the tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ on $\mathcal{S}$ by means of the push-forward of the momentum map $\mu_{\mathcal{P}} : \mathcal{P} \to \mathcal{O}^*$:*

$$(\mu_{\mathcal{P}})^*_{[\psi]}((\Omega_{\mathcal{P}})_{[\psi]}) = (\Lambda_{\mathcal{S}})_{\mu_P([\psi])}, \quad (\mu_{\mathcal{P}})^*_{[\psi]}((G_{\mathcal{P}})_{[\psi]}) = (R_{\mathcal{S}})_{\mu_P([\psi])}, \quad \forall [\psi] \in \mathcal{P}. \tag{3.106}$$

The stratum $\mathcal{S}_1$ is an almost Kähler manifold.

Proof. As in previous proofs, it is enough to consider the action of these tensor fields on the differential of expectation value functions. Thus, consider a function $\epsilon_A \in \mathcal{E}_{\mathcal{O}}(\mathcal{S})$. Its action on points in $\mathcal{S}_1 = \mu_{\mathcal{P}}(\mathcal{P})$ is

$$\epsilon_A(\mu_P([\psi])) = \mathrm{Tr}\,(A\mu_P([\psi])) = \frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle}, \quad \forall [\psi] \in \mathcal{P}.$$

Hence $(\mu_P)_*(\epsilon_A|_{\mathcal{S}_1}) \in \mathcal{E}_{\mathcal{O}}(P)$. As any function in $\mathcal{E}_{\mathcal{O}}(P)$ can be obtained in this way, it is concluded that the pull-back by $\mu_{\mathcal{P}}$ of the restriction to $\mathcal{S}_1$ of expectation value functions is precisely $(\mu_P)_*(\mathcal{E}_{\mathcal{O}}(\mathcal{S})|_{\mathcal{S}_1}) = \mathcal{E}_{\mathcal{O}}(\mathcal{P})$. It is thus immediate, by the similarity of definitions of the contravariant tensor fields, that relation (3.106) holds. As a corollary, the restrictions to $\mathcal{S}_1$ of $\Lambda_{\mathcal{S}}$ and $\mathcal{R}_{\mathcal{S}}$ satisfy the same relations that their preimages $\Omega_{\mathcal{P}}$ and $G_{\mathcal{P}}$, hence the stratum is a Kähler manifold with respect to an appropriate almost complex structure, which shall be $\mu_{\mathcal{P}}$-related with the one existing on $\mathcal{P}$. □

It is immediate to conclude from this theorem that Hamiltonian and gradient vector fields on $\mathcal{S}$, when restricted to $\mathcal{S}_1$, are in one-to-one correspondence with Hamiltonian and gradient vector fields on $\mathcal{P}$. This restriction can always be done, as these vector fields are always tangents to the strata of $\mathcal{S}$, as proved by Graboswki, Kuś and Marmo [141, 142]. This identification between both approaches explains the similarity of commutations relations obtained in (1.64) and in (3.51), both being related with the Lie and Jordan products of observables.

As a last comment, unitary dynamics in both descriptions is represented by means of Hamiltonian vector fields. When restricted to $\mathcal{S}_1$, the unitary evolution of pure states is related by the momentum map with the representation of the Schrödinger equation on the manifold $\mathcal{P}$. Thus, pure states are completely described by the properties of the set $\mathcal{S}$, as expected.

3.3.5 Vector fields as transformations on the set of states

Among the many properties of the geometric formalism, it is important for later chapters to consider the objects on $\mathcal{S}$ representing $\mathbb{R}$-linear operators on $\mathcal{O}^*$. As fully explained in [81, p. 108], the 'easy' tensorialisation principle gives a clear relation between operators and vector fields on linear spaces. A direct application of this principle is the following result

Proposition 3.54. *For any $\mathbb{R}$-linear transformation $T : \mathcal{O}^* \to \mathcal{O}^*$, there exists a vector field $\widehat{Z}_T \in \mathfrak{X}(\mathcal{O}^*)$, whose value at each point is*

$$(\widehat{Z}_T)_{\bar{\xi}} = T(\bar{\xi}) \tag{3.107}$$

Proof. For any $\bar{\xi} \in \mathcal{O}^*$, consider the isomorphism $\mathcal{O}^* \cong T_{\bar{\xi}}\mathcal{O}^*$. Following the 'easy' tensorialisation principle, the transformation T can be interpreted as associating to every point $\bar{\xi}$ a tangent vector $T(\bar{\xi})$. This defines a vector field $\widehat{Z}_T \in \mathfrak{X}(\mathcal{O}^*)$ with value $T(\bar{\xi})$ at each point $\bar{\xi} \in \mathcal{O}^*$. □

In particular, the action of $\widehat{Z}_T$ on linear functions is

$$\widehat{Z}_T(f_A)(\bar{\xi}) = f_A(T(\bar{\xi})) = f_{T^\sharp(A)}(\bar{\xi}) = \bar{\xi}(T^\sharp(A)), \quad \bar{\xi} \in \mathcal{O}^*,\ A \in \mathcal{O}. \tag{3.108}$$

where $T^\sharp : \mathcal{O} \to \mathcal{O}$ denotes the dual map of T, defined as

$$T(\bar{\xi})(A) = \bar{\xi}(T^\sharp(A)), \quad \forall \bar{\xi} \in \mathcal{O}^*,\ \forall A \in \mathcal{O} \tag{3.109}$$

Lemma 3.55. *Let $T, T' : \mathcal{O}^* \to \mathcal{O}^*$ be two linear transformations. Their associated vector fields by Proposition 3.54 satisfy*

$$[\widehat{Z}_T, \widehat{Z}_{T'}] = -\widehat{Z}_{[T,T']}. \tag{3.110}$$

Proof. Due to the linear structure of $\mathcal{O}^*$, the flow Φ_t^T associated to the vector field $\widehat{Z}_T$ can be written as

$$\Phi_t^T(\bar{\xi}) = \bar{\xi} + tT(\bar{\xi}) + \frac{1}{2}t^2T^2(\bar{\xi}) + O(t^3), \quad \bar{\xi} \in \mathcal{O}^*,\ t \in \mathbb{R}. \tag{3.111}$$

It is possible thus to compute the commutator $[\widehat{Z}_T, \widehat{Z}_{T'}]$ by applying the following relation [104]:

$$[\widehat{Z}_T, \widehat{Z}_{T'}]_{\bar{\xi}} = \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\,(\Phi_{-t}^{T'} \circ \Phi_{-t}^{T} \circ \Phi_t^{T'} \circ \Phi_t^T)(\bar{\xi})\Big|_{t=0} = \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\,(\bar{\xi} - t^2[T,T'](\bar{\xi}) + O(t^3))\Big|_{t=0} = -[T,T'](\bar{\xi}).$$

at each point $\bar{\xi} \in \mathcal{O}^*$, thus proving the proposition. □

Particular cases of vector fields presented in Proposition 3.54. are Hamiltonian and gradient vector fields on $\mathcal{O}^*$. Lie and Jordan products on $\mathcal{O}$ define respectively adjoint and L_A operators (see Definition 3.23):

$$\mathrm{ad}_A(B) = [\![A, B]\!], \quad L_A(B) = A \odot B, \quad A, B \in \mathcal{O}. \tag{3.112}$$

Let coad_A and $\mathrm{co}L_A$ be the respective dual operators on $\mathcal{O}^*$, related with the respective operators on $\mathcal{O}$ by in (3.109):

$$(\mathrm{coad}_A)^\sharp = \mathrm{ad}_A,\ (\mathrm{co}L_A)^\sharp = L_A, \quad A \in \mathcal{O}. \tag{3.113}$$

If the identification $\mathcal{O}^* \cong \mathcal{O} \cong \mathrm{Herm}(\mathcal{H})$ for some Hilbert space $\mathcal{H}$, then these operators take the form

$$\mathrm{coad}_A(\bar{\xi}) = -[\![A, \bar{\xi}]\!], \quad \mathrm{co}L_A = A \odot \bar{\xi}, \quad \forall A \in \mathcal{O},\ \forall \bar{\xi} \in \mathcal{O}^*. \tag{3.114}$$

These operators are in direct relation with the Hamiltonian and gradient vector fields, as proved in [141] and presented next.

Proposition 3.56. *The Hamiltonian and gradient vector fields on $\mathcal{O}^*$ satisfy the relations*

$$X_A = -\widehat{Z}_{\mathrm{coad}_A}, \quad Y_A = \widehat{Z}_{\mathrm{co}L_A}, \quad A \in \mathcal{O}. \tag{3.115}$$

Proof. Because of linearity, it is enough to prove these relations for linear functions. By (3.108), the following relation holds:

$$\widehat{Z}_{\mathrm{coad}_A}(f_B)(\bar{\xi}) = \bar{\xi}(\mathrm{ad}_A(B)) = \bar{\xi}([\![A, B]\!]) = X_A(f_B)(\bar{\xi}), \quad \forall A, B \in \mathcal{O},\ \forall \bar{\xi} \in \mathcal{O}^*.$$

A similar relation holds for gradient vector fields, thus completing the proof. □

As in the case of tensor fields, presented in previous sections, these vector field are not in general projectable onto $\mathcal{S}$. It is however possible to define appropriate vector fields on $\mathcal{S}$ by the action of $\widehat{Z}_T$ on expectation value functions.

Theorem 3.57. *An $\mathbb{R}$-linear transformation $T : \mathcal{O}^* \to \mathcal{O}^*$ that preserves positivity defines a vector field $Z_T \in \mathfrak{X}(\mathcal{S})$ whose action on expectation value functions is*

$$Z_T(\epsilon_A)(\rho) = \epsilon_{T^\sharp(A)}(\rho) - \epsilon_{T^\sharp(I)}(\rho)\epsilon_A(\rho), \quad \rho \in \mathcal{S}, \quad A \in \mathcal{O}. \tag{3.116}$$

Proof. The transformation T defines a vector field $\widehat{Z}_T \in \mathfrak{X}(\mathcal{O}^*)$ by Proposition 3.54. Its action on the pull-back of expectation value functions is:

$$\widehat{Z}_T(\epsilon_A)(\bar{\xi}) = \frac{1}{f_I(\bar{\xi})}\,\widehat{Z}_T(f_A)(\bar{\xi}) - \frac{f_A(\bar{\xi})}{f_I(\bar{\xi})^2}\,\widehat{Z}_T(f_I)(\bar{\xi}) = \epsilon_{T^\sharp(A)}(\bar{\xi}) - \epsilon_{T^\sharp(I)}(\bar{\xi})\epsilon_A(\bar{\xi}), \quad \bar{\xi} \in \mathcal{O}^*,\ A \in \mathcal{O}, \tag{3.117}$$

This expression can be restricted to $\widehat{\mathcal{S}}$. The additional requirement regarding preservation of positivity ensures that the vector field can be further restricted to $\mathcal{S}$, thus completing the proof. □

The properties of these vector fields on $\mathcal{S}$ are similar to those obtained for the larger manifold $\mathcal{O}^*$. In particular, by Lemma 3.55 and equation (3.117) it is immediate to conclude that

$$[Z_T, Z_{T'}] = -Z_{[T,T']}. \tag{3.118}$$

It is important to notice the role of linearity in the geometric description of states. A generic linear vector field on the larger manifold $\mathcal{O}^*$ does not preserve the normalisation of states, and thus cannot be restricted to $\mathcal{S}$. It is possible to consider its action on relevant functions, i.e. on the pull-back to $\mathcal{O}^*$ of expectation value functions. Thus, vector fields are obtained on $\mathcal{S}$ which by definition preserve the normalisation. Linearity, however, is lost in (3.116). Observe that, if the defining transformation T preserves the set of states, then $T^\sharp(I) = 0$ and the resulting vector field Z_T is also linear on $\mathcal{S}$, as expected. This is for example the case of Hamiltonian vector fields. Gradient vector fields, on the contrary, are not linear on $\mathcal{S}$, as seen in the example of a 2-level system.

3.4 Example: pure and mixed states of a 2-level system

The geometric formalism presented above will be illustrated by considering the space of states of a 2-level system. The aim of this section is to find the expressions of the tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$, thus determining Hamiltonian and gradient vector fields. These vector fields can be plotted on a 3-dimensional space, giving some insight into the geometric properties of the space of states.

Recall from Section 1.1.7 that the C*-algebra associated to a 2-level system is isomorphic to $\mathrm{End}(\mathbb{C}^2)$. Therefore, both the set of observables $\mathcal{O}$ and its dual space $\mathcal{O}^*$ are isomorphic to the set $\mathrm{Herm}(2)$ of 2×2 Hermitian matrices. A basis $\{\sigma_\mu\}_{\mu=0}^3$ of $\mathcal{O}$ is given by the three Pauli matrices and the identity matrix:

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.119}$$

The Lie and Jordan product of the elements in the basis $\{\sigma_\mu\}$ have been computed in (1.39). They can be written in a compact form as

$$\begin{aligned} &[\![\sigma_j, \sigma_k]\!] = 2\epsilon_{jkl}\sigma_l, \quad \sigma_j \odot \sigma_k = 2\delta_{jk}\sigma_0, && j,k = 1,2,3 \\ &[\![\sigma_0, \sigma_\mu]\!] = [\![\sigma_\mu, \sigma_0]\!] = 0, \quad \sigma_0 \odot \sigma_\mu = \sigma_\mu \odot \sigma_0 = 2\sigma_\mu, && \mu = 0,1,2,3. \end{aligned} \tag{3.120}$$

In the following, indexes denoted by Greek letters will run from 0 to 3, while those represented by Latin letters will take values 1, 2 and 3.

Consider the inner product in $\mathcal{O}$ defined as in (3.70) by the trace:

$$\langle A, B \rangle = \mathrm{tr}(AB). \tag{3.121}$$

As $\mathcal{O}$ is finite-dimensional, the inner product defines an isomorphism between $\mathcal{O}$ and O^*. The dual basis $\{\sigma^\mu\}_{\mu=0}^3$ in $\mathcal{O}^*$ is defined as:

$$\sigma^\mu(\sigma_\nu) = \delta^\mu_\nu, \quad \mu,\nu = 0,1,2,3 \quad \Rightarrow \quad \sigma^\mu = \frac{1}{2}\sigma_\mu, \quad \mu = 0,1,2,3. \tag{3.122}$$

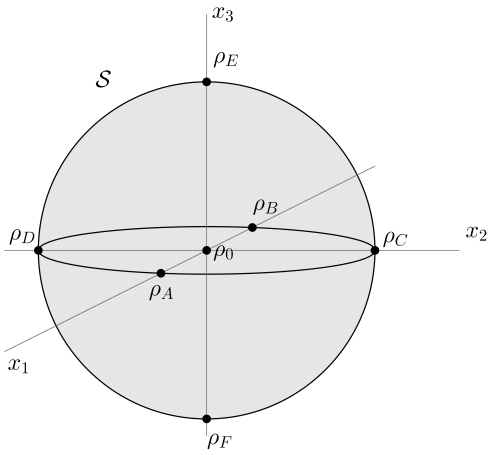
where all the elements are considered as Hermitian matrices on $\mathbb{C}^2$. An element $\bar{\xi} \in \mathcal{O}^*$ takes the form

$$\bar{\xi} = x_\mu \sigma^\mu = \frac{1}{2} x_\mu \sigma_\mu. \tag{3.123}$$

In particular, states $\rho \in \mathcal{S} \subset \mathcal{O}^*$ must be unit-trace positive elements, which gives the following result.

Proposition 3.58. *The coordinate expression of a state of the 2-level system is*

$$\rho = \sigma^0 + x_j \sigma^j = \frac{1}{2}\begin{pmatrix} 1 + x_3 & x_1 - ix_2 \\ x_1 + ix_2 & 1 - x_3 \end{pmatrix}, \quad x_1^2 + x_2^2 + x_3^2 \leq 1. \tag{3.124}$$



$$\rho_A = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \rho_B = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix},$$
$$\rho_C = \frac{1}{2}\begin{pmatrix} 1 & -\mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix}, \quad \rho_D = \frac{1}{2}\begin{pmatrix} 1 & \mathrm{i} \\ -\mathrm{i} & 1 \end{pmatrix},$$
$$\rho_E = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \rho_F = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix},$$
$$\rho_0 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Figure 3.4: Three-dimensional representation of pure and mixed states of a 2-level systems as points in a ball of unit radius, called the Bloch ball. The surface $\mathcal{S}_1$ of the sphere corresponds to pure states, while mixed states are represented by points in the interior $\mathcal{S}_2$. Via the momentum map, it is ismmediate to identify the surface $\mathcal{S}_1$ with the manifold $\mathcal{P}$ of pure states presented in Section 1.4. See in particular Figure 1.5, as this identification allows to associate the pure states there represetned with the corresponding points in $\mathcal{S}$. Observe that, unlike Figure 1.5, in the present case also the interior points of the ball are considered. In particular, the centre of the ball is the maximally mixed state ρ_0.

Proof. Consider a generic element $\bar{\xi} = x_\mu \sigma^\mu \in \mathcal{O}^*$. Then:

$$\mathrm{tr}(\bar{\xi}) = x_0, \quad \mathrm{tr}(\bar{\xi}^2) = \frac{1}{2}(x_0^2 + x_1^2 + x_2^2 + x_3^2).$$

An element in $\mathcal{O}^*$ is a state if it satisfies conditions in (3.15), or in matrix notation, if it is normalised and positive. This leads to the expression presented in the proposition. □

Therefore, the set of states is 3-dimensional, as it can be parametrised by points $(x_1, x_2, x_3) \in \mathbb{R}^3$ such that their norm is not greater than 1. That is to say, the set of states is parametrised by the solid ball of radius 1 in $\mathbb{R}^3$, as presented in Figure 3.4. This representation of the set of states of the 2-level system is called the Bloch ball [41]. Points on the surface of the ball (that is, vectors with radius 1) parametrise states that are rank-1 projectors, as $\rho^2 = \rho$; these are the pure states of the system. The interior of the ball parametrises mixed states. In the language of Proposition 3.42, the set of states is stratified as

$$\mathcal{S} = \mathcal{S}_1 \cup \mathcal{S}_2, \tag{3.125}$$

with $\mathcal{S}_1$ the surface of the Bloch ball and $\mathcal{S}_2$ its interior. It is thus immediate to identify the sphere $\mathcal{S}_1$ with the manifold $\mathcal{P}$ of pure states of the system, as in Section 1.4.

Observables are represented by expectation value functions on $\mathcal{S}$. With the given basis, the association between observables and expectation value functions is

$$A = a^\mu \sigma_\mu \Rightarrow \epsilon_a = a^0 + a^j x_j, \quad a^0, a^1, a^2, a^3 \in \mathbb{R}, \tag{3.126}$$

Proposition 3.59. *The coordinate expressions for the contravariant tensor fields $\Lambda_\mathcal{S}$ and $R_\mathcal{S}$ are*

$$\Lambda_\mathcal{S} = \sum_{j,k,l=1}^{3} \epsilon_{jkl}\, x_l \frac{\partial}{\partial x_j} \wedge \frac{\partial}{\partial x_k}, \qquad R_\mathcal{S} = 2\sum_{j=1}^{3} \frac{\partial}{\partial x_j} \otimes \frac{\partial}{\partial x_j} - \sum_{j,k=1}^{3} 2x_j x_k \frac{\partial}{\partial x_j} \otimes \frac{\partial}{\partial x_k}. \tag{3.127}$$

Proof. Coordinate functions on $\mathcal{S}$ are given by the expectation value functions associated to the Pauli matrices. The values of $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ on these coordinate functions are the following

$$\begin{aligned}\Lambda_{\mathcal{S}}(\mathrm{d}x_j,\mathrm{d}x_k)(\rho) &= \epsilon_{[\![\sigma_j,\sigma_k]\!]}(\rho) = 2\epsilon_{jkl}x_l,\\ R_{\mathcal{S}}(\mathrm{d}x_j,\mathrm{d}x_k)(\rho) &= \epsilon_{\sigma_j\odot\sigma_k}(\rho) - 2\epsilon_j(\rho)\epsilon_k(\rho) = 2\delta_{jk} - 2x_jx_k.\end{aligned} \tag{3.128}$$

From these results follow the coordinate expressions presented in the Proposition. □

Observe that, when restricted to the surface of the ball, it is possible to relate (3.128) with the expression (1.167) for the Poisson and symmetric tensors $\Omega_{\mathcal{P}}$ and $G_{\mathcal{P}}$ on the manifold $\mathcal{P}$. This is in total agreement with the result of Theorem 3.53, thus illustrating the embedding of the manifold of pure states into the set $\mathcal{S}$.

The algebra of observables is recovered on $\mathcal{S}$ as the algebra of expectation value functions $\mathcal{E}_{\mathcal{O}}(\mathcal{S})$ with products

$$\{\epsilon_A,\epsilon_B\}_{\mathcal{S}} = \Lambda_{\mathcal{S}}(\mathrm{d}\epsilon_A,\mathrm{d}\epsilon_B), \quad (\epsilon_A,\epsilon_B)_{\mathcal{S}} = R_{\mathcal{S}}(\mathrm{d}\epsilon_A,\mathrm{d}\epsilon_B) + 2\epsilon_A\epsilon_B, \quad forall A,B\in\mathcal{O}. \tag{3.129}$$

With the decomposition given in (3.126), their explicit expressions are

$$\begin{aligned}\{\epsilon_A,\epsilon_B\}_{\mathcal{S}} =& 2\epsilon_{jkl}\ a^jb^kx_l = \epsilon_{[\![A,B]\!]},\\ (\epsilon_A,\epsilon_B)_{\mathcal{S}} =& 2a^\mu b^\mu + 2(a^jb^0 + a^0b^j)x_j = \epsilon_{A\odot B},\end{aligned} \qquad \forall A,B,\in\mathcal{O}. \tag{3.130}$$

As expected, the algebra $\mathcal{E}_{\mathcal{O}}(\mathcal{S})$ is isomorphic to the algebra of observables.

With the given expressions, it is possible to compute explicitely gradient and Hamiltonian vector fields on the Bloch ball. In order to compare with the results presented in Section 1.4 for the geometric description of the Schrödinger picture and the manifold $\mathcal{P}$, consider a diagonal Hamiltonian H in the given basis:

$$H = \begin{pmatrix} E_0 & 0\\ 0 & E_1\end{pmatrix}, \quad E_0\leq E_1. \tag{3.131}$$

Its associated expectation value function on $\mathcal{S}$ is

$$\epsilon_H(\rho) = \mathrm{Tr}(H\rho) = \frac{E_1+E_0}{2} - \frac{E_1-E_0}{2}x_3, \quad \forall\rho\in\mathcal{S}. \tag{3.132}$$

Observe that the restriction of this function to the surface of the sphere, i.e. to pure states, gives as a result the expectation value function computed in (1.168). Again, this is in agreement with the embedding of the manifold $\mathcal{P}$ of pure states into $\mathcal{S}$, as described in Section 3.3.4.

The Hamiltonian vector field $\widetilde{X}_H$ associated to this function is obtained by the contractoin of the tensor field $\Lambda_{\mathcal{S}}$ by the 1-form $\mathrm{d}\epsilon_H$:

$$\widetilde{X}_H = -\iota_{\mathrm{d}\epsilon_H}\Lambda_{\mathcal{S}} = (E_1-E_0)\left(x_2\frac{\partial}{\partial x_1} - x_1\frac{\partial}{\partial x_2}\right). \tag{3.133}$$

The corresponding system of differential equations determining the integral curves of the Hamiltonian vector field is

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = \frac{E_1-E_0}{2}\,x_2, \quad \frac{\mathrm{d}x_2}{\mathrm{d}t} = -\frac{E_1-E_0}{2}\,x_1, \quad \frac{\mathrm{d}x_3}{\mathrm{d}t} = 0. \tag{3.134}$$

The vector field $\widetilde{X}_H$ is therefore the generator of rotations around the x_3-axis. The plot of this vector field for $E_0 < E_1$ can be found in Figure 3.5. The distance to the center of the Bloch ball is preserved along the integral curves. In fact, as proved in [141,142], the distribution D_Λ of Hamiltonian vector fields define a foliation of the Bloch ball whose leaves are all possible spheres with centre in $(0,0,0)$.

The stratification of the Bloch ball, however, is different for gradient vector fields. In order to understand the difference, consider the gradient vector field $\widetilde{Y}_H$ associated to ϵ_H:

$$\widetilde{Y}_H = \iota_{\mathrm{d}\epsilon_H}R_{\mathcal{S}} = (E_1-E_0)\left(x_1x_3\frac{\partial}{\partial x_1} + x_2x_3\frac{\partial}{\partial x_2} - (1-x_3^2)\frac{\partial}{\partial x_3}\right). \tag{3.135}$$

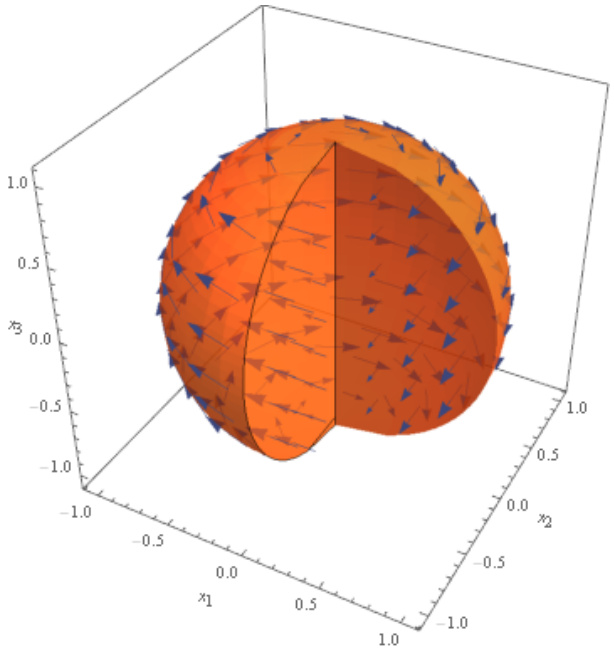


Figure 3.5: 3-dimensional plot of the Hamiltonian vector field $\widetilde{X}_H$, defined in (3.133). The integral curves of the vector field are rotations around the x_3 axis. Therefore, the fixed points are the points on the axis.

The corresponding system of differential equations for its integral curves is

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = (E_1 - E_0)x_1x_3, \quad \frac{\mathrm{d}x_2}{\mathrm{d}t} = (E_1 - E_0)x_1x_3, \quad \frac{\mathrm{d}x_3}{\mathrm{d}t} = -(E_1 - E_0)(1 - x_3^2). \tag{3.136}$$

The values of the vector field at each point of $\mathcal{S}$ are plotted in Figure 3.6. Contrary to the case of the Hamiltonian vector field $\widetilde{X}_H$, the integral curves of $\widetilde{Y}_H$ are not periodic. Instead, there exist two fixed points of the dynamics, with coordinates $(0, 0, 1)$ and $(0, 0, -1)$, which are respectively unstable and stable. This is identical to the case studied in Section 1.4.

Regarding the stratification of the set $\mathcal{S}$ of states, observe that the gradient vector field does not, in general, preserve the distance to the center along its integral curves. Only integral curves on the surface preserve it. Thus, as expected, both gradient and Hamiltonian vector fields are tangent to the surface of the Bloch ball. In the interior, gradient vector fields break the stratification in terms of concentric spheres generated by Hamiltonian vector fields. Thus, a distribution of both gradient and Hamiltonian vector fields requires to consider the interior of the Bloch ball as a single stratum, in agreement with [141, 142].

3.5 Relevance of a geometric description of pure and mixed states

The present chapter offers a new description of the states of quantum systems in geometric terms, which allows for a better characterisation of quantum systems. The developed geometrical formalism can be seen as an extension of the one presented in Chapter 1 for the description of pure states. In both cases, the main geometrical objects are the tensor fields that represent the algebraic properties of observables. As seen in Sections 3.1 and 3.2, two main algebraic structures have to be considered. The Lie bracket of observables describes the dynamics of the system, while the Jordan product is connected with the probabilistic nature of Quantum Mechanics. Both structures are interconnected, and both are necessary in order to understand the mathematical properties of the theory and the differences with Classical Mechanics.

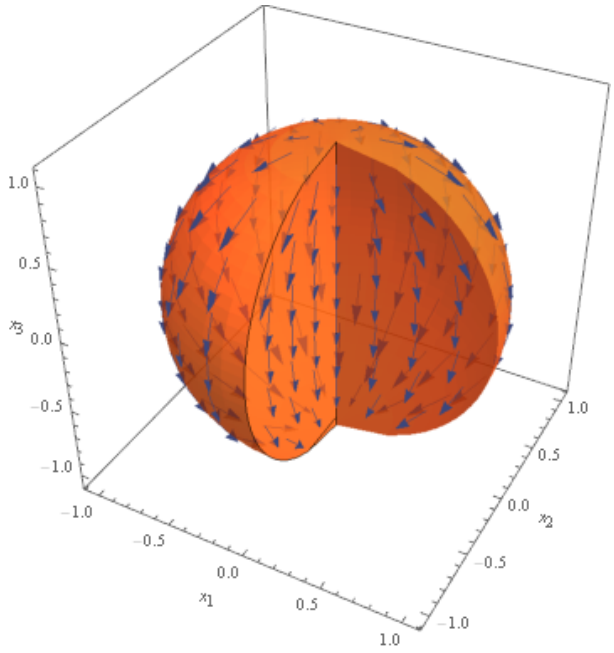


Figure 3.6: Full 3-dimensional plot of the gradient vector field defined in (3.135). The vector field takes value zero nowhere except at points $(0, 0, 1)$ and $(0, 0, -1)$. It is important to notice that the vector field is tangent to the surface of the ball, that is, to the subset of pure states.

It is possible to move from an algebraic description of observables to a geometric one [141, 142]. A further step can be taken by considering, as in Chapter 1, a reduction procedure. In this way, a new geometric description of quantum states is obtained. The set $\mathcal{S}$ of pure and mixed states is thus described by a stratified manifold, each stratum being itself a differentiable manifold. The whole set, however, lacks a differentiable structure. Instead, in order to carry out differential calculus, it is necessary to embed it into a larger manifold $\widehat{S}$, with the properties explained in the text. The set $\mathcal{S}$ thus presents a boundary, a property that has to be taken into account mainly in the analysis of dynamical systems (see Chapter 4).

Regarding tensor fields, most the conclusions reached in Chapter 1 can be restated here. There exist two tensor fields, $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$, representing respectively the Lie bracket and Jordan product of observables. The tensor fields $\Lambda_{\mathcal{S}}$ defines a Poisson bracket on smooth functions, and it determines the unitary evolution of quantum systems. Regarding the symmetric tensor field $R_{\mathcal{S}}$, it represents in a geometrical way the statistical properties of quantum systems. In particular, the standard derivation of an observable $A \in \mathcal{O}$ for a state $\rho \in \mathcal{S}$, given by (3.8), is recovered as

$$R_{\mathcal{S}}(\mathrm{d}\epsilon_A, \mathrm{d}\epsilon_A)(\rho) = 2\epsilon_{A^2}(\rho) - 2(\epsilon_A(\rho]))^2 = 2(\Delta_\rho A)^2, \quad \forall \rho \in \mathcal{S}. \tag{3.137}$$

This is clearly an extension to pure and mixed states of expression (1.173).

The geometric formalism allows for a better characterisation of quantum systems and their dynamics. Thus, Chapter 4 presents some applications of this formalism to the analysis of open quantum systems. It is possible to consider more general dynamics than the unitary evolution determined by the Poisson tensor $\Lambda_{\mathcal{S}}$. In particular, the Markovian evolution of open quantum systems will be presented in geometric terms. Different aspects of the dynamics can thus be considered. For example, the geometric setting is useful in order to describe control problems on open quantum systems. Furthermore, it is possible to analyse from a new light some problems that are hard to describe in a geometric setting. In particular, Chapter 4 describes the behaviour of tensorial structures under Markovian evolution, thus leading to a geometric description of the contraction of algebras of observables. The analysis of these contractions,

presented by Marmo and co-workers [7, 92, 158], can now be given an intrinsic formulation in geometric terms. The behaviour and evolution of tensor fields can be directly analysed in the geometric setting. Thus, it can be concluded that a geometric formalism offers the possibility to study the intrinsic properties of quantum systems and their behaviour in different situations.

Chapter 4

Markovian evolution of open quantum systems

The geometric formalism presented in previous chapters offers a new setting for the study of open quantum system and to the description of their interaction with an environment. This interaction implies an interchange of energy and information, and thus statistical ensembles are to be considered. The geometric description of pure and mixed states can thus be applied to the analysis of open quantum systems. In particular, this chapter focuses on the characterisation of Markovian evolution, for which a rigorous mathematical framework exists [59, 139, 191].

The geometric formalism makes possible to describe also the evolution of algebraic structures that are intrinsic to Quantum Mechanics. In the realm of differential geometry, every geometric object evolves along a given trajectory. Thus, it is a simple issue to compute the change of the tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$, which encode the algebraic structure of the set of quantum observables. Quantum evolution may thus modify the algebraic properties of observables in a non trivial matter. This is in connection with the mathematical construction known as contraction of algebras [78, 268, 270]. Although contractions of algebras of quantum observables can be computed in an algebraic setting [7,92,158], the procedure requires an explicit computation of the evolution of observables before computing the contraction. The geometric formalism is much more suitable for this characterisation, as it provides a setting in which the algebraic structures, represented by tensor fields, can be dealt with directly. These and other considerations motivate a geometric analysis of the dynamics of open quantum systems.

The chapter is organised as follows. Section 4.1 offers a definition and characterisation of open quantum systems and Markovian evolution, both from algebraic and geometric perspectives. The description of the evolution in terms of vector fields makes possible to study the contraction of algebras of observables. Thus, Section 4.2 presents a mathematical introduction to the theory of contractions of algebras. In the sight of that, Section 4.3 presents a geometric approach to the contraction of algebras, particularised to the case of quantum systems with Markovian evolution. Section 4.4 offers a mathematical description of the action of Markovian evolution on the manifold of states, the set of limit points of the evolution and its relation with the contraction of algebras. Finally, Section 4.5 presents an application of geometric control theory to Markovian systems. Examples will be offered in order to illustrate the results.

4.1 Open quantum systems

A quantum system is called open if it is not isolated, i.e. if it interacts with its environment in any way. Assuming that there is no change in the number of particles in the system, interactions take the form of interchanges of energy and information. Consider for example the decay of a quantum system, such as an atom or molecule. If the system is in an excited state, then it has a certain probability of decaying onto the ground state and emitting a photon with the exceeding energy. In this way, energy is interchanged

between the system and the environment. In addition, if the decay is subject to probabilistic rules, there is also a change on the entropy of the system. A characterisation of open quantum systems and their dynamics can be found in many works [5, 59, 123]. Refer also to the book by Rivas and Huelga [226], which is the main source for many of the arguments presented in this introduction.

The study of open quantum systems has to deal with the characterisation of the states of the systems and the description of their evolution. Consider a quantum system with associated Hilbert space $\mathcal{H}$; as described in Chapter 1, pure states of the systems are represented by points in the projective Hilbert space $\mathcal{P}$. By definition, however, the available information on the actual state of an open quantum system may change as a result of the interaction with the environment. In other words, a pure state may evolve into a mixed state, and viceversa. For this reason, the state of the system has to be described by statistical ensembles on $\mathcal{P}$. As it was detailed in Section 3.1.5, these ensembles are represented by density matrices on $\mathcal{H}$. Geometrically, the set $\mathcal{D}(\mathcal{H})$ of density matrices is identified as a manifold with boundary $\mathcal{S}$, which has been fully described in Chapter 3. Thus, the analysis of open quantum systems motivates the characterisation of the manifold with boundary $\mathcal{S}$ of pure and mixed states of the system.

Open quantum systems can be analysed from the perspective of composite systems. This point of view is useful for the characterisation of observables and evolution. Thus, consider an open quantum system A and its environment B. Assuming the universal validity of Quantum Mechanics, the result is a composite quantum system AB with no external interactions, i.e. an isolated composite quantum system. It is thus subject to unitary evolution, and the state and properties of the composite system AB completely characterise the original open quantum system A.

In the Schrödinger picture, composition of quantum systems is carried out by means of tensorial products [102]. Thus, let $\mathcal{H}_A$ and $\mathcal{H}_B$ be the Hilbert spaces associated with the open quantum system A and its environment B, respectively. The Hilbert space of the composite system AB is then $\mathcal{H}_{AB} := \mathcal{H}_A \otimes \mathcal{H}_B$. Observables and states of each system are described as usual; assume in the following for simplicity that all the involved Hilbert spaces are finite-dimensional. It is possible to relate states and observables of an open quantum system with those of its corresponding composite system by means of the properties of tensorial products. See the book by Nielsen and Chuang for a pedagogical description of these relations [214, p. 107], reproduced here. The following proposition mathematically describes observables of the subsytem A on the composite system, as graphically presented in Figure 4.1.

Proposition 4.1. *The representation of an observable $M \in \mathcal{O}_A = \mathrm{Herm}(\mathcal{H}_A)$ on the composite system with Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ is*

$$\overline{M} = M \otimes I_B \in \mathcal{O}_{AB} = \mathrm{Herm}(\mathcal{H}_{AB}), \tag{4.1}$$

with $I_B \in \mathcal{O}_B = \mathrm{Herm}(\mathcal{H}_B)$ the identity observable on $\mathcal{H}_B$.

Proof. Consider the spectral decomposition of M:

$$M = \sum_{m \in \mathrm{spec}(M)} m P_m, \tag{4.2}$$

with P_m the orthogonal projectors onto the corresponding eigenspaces of M. Physically, the eigenvalues $m \in \mathrm{spec}(M)$ represent the possible results of a measurement of M on the system A. Consider now the situation in which the same observable is measured on the composite system AB. It is now represented by $\overline{M} = \mathcal{O}_{AB}$, but the possible results of the measurement do not change, thus $\mathrm{spec}(M) = \mathrm{spec}(\overline{M})$. Regarding projectors, the state of the environment B has no influence on the outcome of the measurement process. Thus, the spectral decomposition of $\overline{M}$ is

$$\overline{M} = \sum_{m \in \mathrm{spec}(M)} m P_m \otimes I_B, \tag{4.3}$$

hence $\overline{M} = M \otimes I_B$. □

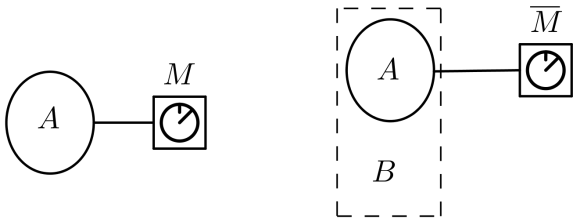


Figure 4.1: Consider a physical quantity being measured on a system A, represented by $M \in \mathcal{O}_A$. If A is seen as a subsystem of a larger composite system AB, then the quantity is now represented by $\overline{M} \in \mathcal{O}_{AB}$. The outcome of the measurement process, however, are independent of these considerations, as the measure is carried only on A. As a consequence of this fact, Proposition 4.1 shows that $\overline{M}$ is indeed unique, given by $\overline{M} = M \otimes I_B$.

The opposite relation, from AB to A, is carried out by means of the partial trace. Let $\mathrm{Tr}_B^{\mathcal{O}} : \mathcal{O}_{AB} \to \mathcal{O}_A$ be the map defined as

$$\mathrm{Tr}_B^{\mathcal{O}}(M \otimes N) := M \,\mathrm{Tr}(N), \quad \forall M \in \mathcal{O}_A, \quad \forall N \in \mathcal{O}_B, \tag{4.4}$$

and extended by linearity to the whole space $\mathcal{O}_{AB} = \mathcal{O}_A \otimes \mathcal{O}_B$. The restriction of $\mathrm{Tr}_B^{\mathcal{O}}$ to density matrices defines a map $\mathrm{Tr}_B : \mathcal{S}_{AB} \to \mathcal{S}_A$, called the partial trace, with the following property.

Theorem 4.2. *The partial trace $\mathrm{Tr}_B : \mathcal{S}_{AB} \to \mathcal{S}_A$ is the unique map satisfying the relation*

$$\epsilon_M(\mathrm{Tr}_B(\rho_{AB})) = \epsilon_{\overline{M}}(\rho_{AB}), \quad \forall \rho_{AB} \in \mathcal{S}_{AB}, \quad \forall M \in \mathcal{O}_A, \tag{4.5}$$

where $\epsilon_M \in \mathcal{E}_{\mathcal{O}_A}(\mathcal{S}_A)$ and $\epsilon_{\overline{M}} \in \mathcal{E}_{\mathcal{O}_{AB}}(\mathcal{S}_{AB})$ are the expectation value functions of M and $\overline{M} = M \otimes I_B$, respectively.

Proof. Consider a map $f : \mathcal{S}_{AB} \to \mathcal{S}_A$ such that the following relation holds:

$$\epsilon_M(f(\rho_{AB})) = \epsilon_{\overline{M}}(\rho_{AB}), \quad \forall \rho_{AB} \in \mathcal{S}_{AB}, \quad \forall M \in \mathcal{O}_A, \tag{4.6}$$

The goal is to prove that this map is unique. Let $\{\sigma_j\}$ be an orthogonal basis for $\mathcal{O}_A$ (with respect to the usual inner product defined by the trace), and $\{\sigma^j\}$ its dual basis on $\mathcal{O}_A^*$. Consider the inclusion $\mathcal{S}_A \subset \mathcal{O}_A^*$; any ρ_A is thus written as

$$\rho_A = \sum_j \epsilon_{\sigma_j}(\rho_A)\sigma^j. \tag{4.7}$$

In particular, for any $\rho_{AB} \in \mathcal{S}_{AB}$, consider the decomposition of $f(\rho_{AB})$ in this basis:

$$f(\rho_{AB}) = \sum_j \epsilon_{\sigma_j}(f(\rho_{AB}))\sigma^j = \sum_j \epsilon_{\overline{\sigma}_j}(\rho_{AB})\sigma^j.$$

Thus, by assuming that f satisfies (4.6), the image $f(\rho_{AB})$ is uniquely determined. In other words, f is unique. Lastly, it is immediate to check that relation (4.5) holds for the partial trace, thus completing the proof. □

The partial trace plays an important role in the description of the dynamics of open quantum systems. The postulates of Quantum Mechanics describe the dynamics of isolated quantum systems in terms of unitary maps. Thus, if the evolution of the composite system starting at t_0 is given by a family of unitary map $\{U(t,t_0) : \mathcal{S}_{AB} \to \mathcal{S}_{AB}, t \geq t_0\}$, its composition with the partial trace defines, for every initial condition $\rho_{AB,0} \in S_{AB}$, a trajectory on S_A by

$$\rho_A(t) = \mathrm{Tr}_B\big(U(t,t_0)(\rho_{AB,0})\big), \quad t \geq t_0. \tag{4.8}$$

The description of these trajectories are the main goal of the study of open quantum systems. Observe that, in general, $\rho_A(t)$ depends on the initial state $\rho_{AB,0}$ of the composite system. In other words, the evolution of an open quantum system depends on the state of the environment with which it is interacting. As this state is in general impossible to determine, the description of the evolution of an open quantum system is a challenging problem. Different strategies have been designed in order to deal with the dynamics of open quantum systems. Refer to the works by Davies, Huelga, Kossakowski, Kraus, Rivas, Stinespring, Sudarshan and many others [32, 35, 59, 93, 105, 123, 137–139, 167, 181, 182, 205, 219, 224, 226, 232, 249, 250].

4.1.1 Completely positive maps

Consider an open quantum system, with $\mathcal{S}$ as its set of pure and mixed states. Its evolution between any two instants t_0, t_1 can always be described by a dynamical map

$$\mathcal{E}_{t_1,t_0} : \mathcal{S} \to \mathcal{S}. \tag{4.9}$$

If this map is derived from (4.8), then it depends strongly on the state of the environment and its interaction with the system. Some assumptions have to be made in order to characterise dynamical maps. The concepts of completely positive maps and Kraus operators are useful in this characterisation

Definition 4.3. *A linear map $K : \mathrm{Herm}(\mathcal{H}) \to \mathrm{Herm}(\mathcal{H})$, with $\mathcal{H}$ a complex Hilbert space, is said to be completely positive if the image of a positive element is a positive element. The map f is said to be completely positive if, for any complex Hilbert space $\mathcal{H}'$, the map $K \otimes Id : \mathrm{Herm}(\mathcal{H} \otimes \mathcal{H}') \to \mathrm{Herm}(\mathcal{H} \otimes \mathcal{H}')$ is positive.*

Lemma 4.4. *[182] Any completely positive map $K : \mathrm{Herm}(\mathcal{H}) \to \mathrm{Herm}(\mathcal{H})$, with $\mathcal{H}$ an n-dimensional complex Hilbert space, can be written as*

$$K(A) = \sum_{j=1}^{r} V_j A V_j^\dagger, \tag{4.10}$$

with $1 \leq r \leq n^2$ and $V_1, \ldots, V_r \in GL(\mathcal{H})$. The map K is called a Kraus operator. The right-hand side decomposition is not unique.

Proposition 4.5. *Let $\mathcal{K}(\mathcal{H})$ denote the set of Kraus operators on $\mathrm{Herm}(\mathcal{H})$. Composition of maps defines a semigroup structure on $\mathcal{K}(\mathcal{H})$. Any $K \in \mathcal{K}(\mathcal{H})$ whose inverse is also a Kraus map, i.e $K^{-1} \in \mathcal{K}(\mathcal{H})$, can be uniquely written as*

$$K(A) = VAV^\dagger, \quad V \in GL(\mathcal{H}). \tag{4.11}$$

Proof. It is immediate from (4.10) that the composition of any two Kraus maps is also a Kraus map. As the composing matrices $V_1, \ldots, V_r$ are not required to be invertible, Kraus maps are not in general invertible. The characterisation of invertible Kraus maps was done by Grabowski, Kuś and Marmo [142]. Consider the spectral decomposition of a Kraus map K given by (4.10), which determines a unique expression in terms of mutually orthogonal operators $C_1, \ldots, C_R \in GL(\mathcal{H})$:

$$K(A) = \sum_{s=1}^{R} C_s A C_s^\dagger, \quad \mathrm{Tr}(C_s C_{s'}) = \delta_{s,s'}, \quad V_j = \sum_{s=1}^{R} \alpha_{js} C_s, \quad j = 1, 2, \ldots, r, \quad s, s' = 1, 2, \ldots, R \leq n^2. \tag{4.12}$$

If $K \in \mathcal{K}(\mathcal{H})$ is invertible as a Kraus map, then there exist operator $W_1, \ldots, W_{r'} \in GL(\mathcal{H})$ such that

$$K^{-1}(A) = \sum_{k=1}^{r'} W_k A W_k^\dagger \;\Rightarrow\; (K \circ K^{-1})(A) = \sum_{j,k} (V_j W_k) A (V_j W_k)^\dagger = A, \quad \forall A \in \mathrm{Herm}(\mathcal{H}).$$

The map $K \circ K^{-1}$ is trivially decomposed by (4.12) as $(K \circ K^{-1})(A) = IAI$, hence $V_j W_k = \alpha_{jk} I$ for some complex numbers α_{jk}. Assuming that none of these operators is zero, the only possibility is that all operators $V_1, \ldots, V_r$ are invertible and proportional among them. Hence $K(A) = VAV^\dagger$ for some $V \in GL(\mathcal{H})$ proportional to each $V_1, \ldots, V_r$. □

When the initial correlations with the environment can be neglected, and the dynamical map $\mathcal{E}_{t_1,t_0}$ is assumed to be linear (with respect to the linear structure in $\mathcal{O}^*$), then $\mathcal{E}_{t_1,t_0}$ is a completely positive map [6, 59, 181]. In this case, it is possible to describe the dynamical map in terms of a trace-preserving Kraus operator [226]:

$$\mathcal{E}(t_1,t_0)(\rho) = \sum_{j=1}^{r} V_j(t_1,t_0)\,\rho\,V_j^\dagger(t_1,t_0), \quad \sum_{j=1}^{r} V_j^\dagger(t_1,t_0)V_j(t_1,t_0) = I. \tag{4.13}$$

Such a map is called a universal dynamical map. Observe that the composition of universal dynamical maps is not well defined. In order to understand the problem, consider three different times t_0, t_1, t_2, such that the system is uncorrelated with the environment at t_0. Maps $\mathcal{E}(t_1,t_0)$ and $\mathcal{E}(t_2,t_0)$ are therefore universal dynamical maps. One could be tempted to decompose the evolution as

$$\overline{\mathcal{E}}_{t_2,t_1} \circ \mathcal{E}_{t_1,t_0} = \mathcal{E}_{t_2,t_0}. \tag{4.14}$$

The map $\overline{\mathcal{E}}_{t_2,t_1}$, however, is not in general an universal dynamical map. The reason is that at t_1 there may exist correlation between the open system and the environment. In fact, if the maps are obtained as in (4.8), then unitary evolution of the composite system naturally produces correlation between its composing parts. The evolution of open quantum systems in correlated states with the environment is carried out by means of non-positive dynamical maps. These maps, however, have to be dealt with care, as non-physical descriptions may occur. See the works by Jordan, Shaji and Sudarshan [167, 241, 242], and other references [227, 233, 260], for a discussion of the relevance of completely positive maps in the description of open quantum systems and the evolution of correlated states by non-positive maps.

4.1.2 Markovian evolution

As seen above, the difficulties in the description of universal dynamical maps comes from the correlation between the open system and its environment. Consider a case in which the environment is much larger than the open system, for example, if it is a thermal bath or a measurement equipement. In such cases, it is safe to neglect correlations and any dynamical map is completely positive. This is a situation in which a more detailed description of the evolution can be offered.

Definition 4.6. *The evolution of an open quantum system is said to be Markovian if the universal dynamical maps $\mathcal{E}_{t',t} : \mathcal{S} \to \mathcal{S}$ for every $t' \geq t$ satisfy the condition*

$$\mathcal{E}_{t_2,t_1} \circ \mathcal{E}_{t_1,t_0} = \mathcal{E}_{t_2,t_0}, \quad \forall t_2 \geq t_1 \geq t_0. \tag{4.15}$$

It is usually said that systems subject to Markovian evolution 'have no memory'. This expression means that the evolution at a given time t depends only on the state of the system at t, and not on any previus state at $t'' < t$. In the context of composite systems, the 'memory' of a system is represented by the state of the interacting environment. If, as in the case at hand, this environment is not affected by the system, then Markovian evolution is achieved. Observe also the similarities between this description of the evolution of open quantum systems and the analysis of unitary evolutions presented in Section 1.1.5, in relation with the description of the Schrödinger picture of Quantum Mechanics.

In the context of Quantum Mechanics, the study of Markovian evolution of open quantum systems was given a formal description by Gorini, Kossakowski and Sudarshan [139] and independently by Lindblad [191]. They were able to determine explicitely the differential equation goverining Markovian dynamics. For simplicity, assume in the following that maps $\mathcal{E}_{t_2,t_1}$ depend only on the difference $t_2 - t_1$. Thus, the evolution of an open quantum system starting at time t_0 is described by a family of linear completely-positive transformations $\{\Phi_t^L : \mathcal{S} \to \mathcal{S}, t \geq 0\}$, with $\mathcal{E}_{t_2,t_1} = \Phi^L_{t_2-t_1}$ for any $t_2 \geq t_1 \geq t_0$ and with Φ_0^L being the identity map. By (4.15), this family has a semigroup structure:

$$\Phi_t^L \circ \Phi_{t'}^L = \Phi_{t+t'}^L, \quad t, t' \geq 0. \tag{4.16}$$

Theorem 4.7 (**The Kossakowski-Lindblad equation** [139,191]). *Let $\mathcal{H}$ be a n-dimensional Hilbert space describing a quantum system and $\mathcal{S} \subset \mathrm{Herm}(\mathcal{H})$ its set of pure and mixed states. Assume that the evolution of the system is given by a semigroup of linear completely-positive maps $\{\Phi_t^L : \mathcal{S} \to \mathcal{S}, t \geq 0\}$. These maps satisfy the differential equation*

$$\frac{d}{dt}\Phi_t^L(\rho) = L(\Phi_t^L(\rho)), \tag{4.17}$$

The linear map $L : \mathrm{Herm}(\mathcal{H}) \to \mathrm{Herm}(\mathcal{H})$ is called the Kossakowski-Lindblad operator. It is given by the expression

$$L(\rho) = -\mathrm{i}[H,\rho] + \frac{1}{2}\sum_{j=1}^{n^2-1}([V_j\rho, V_j^\dagger] + [V_j, \rho V_j^\dagger]) = -\mathrm{i}[H,\rho] - \frac{1}{2}\sum_{j=1}^{n^2-1}[V_j^\dagger V_j, \rho]_+ + \sum_{j=1}^{n^2-1} V_j\rho V_j^\dagger, \tag{4.18}$$

with $\rho \in \mathcal{S}$, $H^\dagger = H$, $\mathrm{tr}(H) = 0$, $\mathrm{tr}(V_j) = 0$ and $\mathrm{tr}(V_j^\dagger V_k) = 0$ if $j \neq k$, for $j,k = 1,2,\ldots,n^2-1$. For a given evolution, H is uniquely determined by the trace restriction.

Kossakowski-Lindblad equation characterises the evolution of states of a quantum system. Due to the natural equivalence between density matrices and points in the manifold with boundary $\mathcal{S}$, fully described in Chapter 3, it is immediate to describe this equation in geometric terms. In this way, it is possible to analyse the change in the properties and structures associated with quantum systems evolving under Markovian dynamics.

It is important to notice that the decomposition in (4.18) is not unique. The observable H is fully determined by imposing $\mathrm{Tr}H =$. However, there exist multiple sets of operators $V_1,\ldots,V_r$ yielding the same Kossakowski-Lindblad operator. This is a consequence of the properties of Kraus maps, introduced in Lemma 4.4. Thus, in the analysis of Markovian dynamics of open quantum systems, it is advisable to consider the Kraus term in (4.18) as a whole. This approach is followed in the next section when vector fields determined by linear maps on $\mathcal{O}^*$ are considered.

A simple generalisation of the Kossakowksi-Lindblad equation can be easily obtained by dropping the description of evolution in terms of a semigroup of maps. If general maps $\mathcal{E}_{t_2,t_1} : \mathcal{S} \to \mathcal{S}$, not necessarily depending only on the difference $t' - t$, then the evolution is determined by a time-dependent generator $L(t)$ [226]:

$$\frac{d}{dt}\mathcal{E}_{t,t_1}(\rho) = L(t)(\mathcal{E}_{t,t_1}((\rho)), \quad t \geq t_1 \geq t_0 \tag{4.19}$$

For each t, the operator $L(t)$ can be expressed as in (4.18). In other words, this evolution is described by a time-dependent Kossakowski-Lindblad equation. Althogh this topic will not be further explored in this dissertation, analogies with the study of time-dependent Schrödinger equations exist. In particular, the geometric formalism offers the possibility to introduce the study of Lie systems in the context of open quantum systems, which as in the cases presented in Chapter 2 would profit from the existing geometric structures on the set of pure and mixe states.

4.1.3 The Kossakowski-Lindblad vector field

According to (4.18), Kossakowski-Lindblad operator L is a linear transformation of matrices acting on $\mathcal{H}$. Within the geometric formalism developed in Chapter 3, it is thus natural to consider it as a map $L : \mathcal{O}^* \to \mathcal{O}^*$. The next result follows.

Proposition 4.8. *There exists a unique vector field $Z_L \in \mathfrak{X}(\mathcal{S})$, whose action on expectation value functions is*

$$Z_L(\epsilon_A)(\rho) = \epsilon_{L^\sharp(A)}(\rho), \quad \rho \in S,\ A \in \mathcal{O}, \tag{4.20}$$

and whose integral curves are solutions to the Kossakowski-Lindblad equation.

Proof. By application of Theorem 3.57, it is immediate to associate a vector field $Z_L \in \mathfrak{X}(\mathcal{S})$ to the Kossakowski-Lindblad operator. Let $L^\sharp : \mathcal{O} \to \mathcal{O}$ be the dual operator. It is immediate from (4.18) that $L^\sharp(I) = 0$, from which the expression given for Z_L follows. □

Clearly, the new vector field Z_L is neither Hamiltonian, gradient nor a combination of them. It is thus expectable that it presents new characteristics, different from those deduced of Hamiltonian and gradient vector fields. In particular, recall the stratification of the set of states in terms of the rank, described in Proposition 3.42. At each point of the manifold, gradient and Hamiltonian vector fields are tangent to the corresponding stratum. This is not so, in general, for Kossakowski-Lindblad vector fields of the form (4.20). Their integral curves may thus intersect different strata of the manifold $\mathcal{S}$. The following result, by Grabwoski, Kuś and Marmo [141], illustrates the properties of this vector field.

Theorem 4.9. [141] *Every smooth curve in $\mathcal{S}$ is tangent to the stratum $\mathcal{S}_k$ to which it actually belongs.*

Corollary 4.10. *Under Markovian evolution, the rank of the state of a quantum system may change either at the initial time or at infinite time. It cannot change under finite time evolution.*

Proof. The rank of a state is uniquely determined by the stratum of $\mathcal{S}$ to which it belongs. Theorem 4.9 rules out almost every possible change in ranks. The only two possibilities are the ones stated. A non-invertible evolution is by definition not differentiable at initial time, which means that the rank may change. It is also possible to define smooth curves on a stratum of $\mathcal{S}$ whose limit belongs to the boundary of the stratum, which is, by definition, a different stratum. □

Corollary 4.10, together with smoothness condition, characterises the geometric properties of vector field Z_L. The vector field has clearly no limitation in the interior of the set $\mathcal{S}$. The boundary has to be taken into consideration. Clearly, as the Kossakowski-Lindblad operator preserves positivity, the vector field Z_L never points outside of the boundary. Because of continuity, this means that, at each point with certain rank, the vector field never points towards another stratum with larger rank. This proves the following result.

Proposition 4.11. *Let $\gamma : [0, \infty) \to \mathcal{S}$ be an integral curve of the Kossakowski-Lindblad vector field. Then,*

$$\operatorname{rank}(\gamma(t)) \geq \operatorname{rank}(\gamma(0)), \quad \forall t > 0. \tag{4.21}$$

Rank of states may only increase in infinite time if the asymptotic limit of an integral curve belongs to a different stratum. These properties of vector fields are graphically represented for the 2-level system in Figure 4.2.

New aspects of the Kossawkoski-Lindblad vector field can be studied by inspection of (4.18). Observe that it can be decomposed in three parts: a commutator, an anti-commutator and a Kraus operator on ρ. Recall from Chapter 3 that the first two summands are respectively related with Hamiltonian and gradient vector fields. In order to understand the relevance of the third summand, consider first a vector field on $\mathcal{S}$ of the form

$$W = \widetilde{X}_H + \widetilde{Y}_F, \quad H, F \in \mathcal{O}. \tag{4.22}$$

This is a generic linear combination of a Hamiltonian vector field $\widetilde{X}_H$ and a gradient vector field $\widetilde{Y}_F$. The action of the vector field W on an expectation value function ϵ_A, with $A \in \mathcal{O}$, is the following:

$$W(\epsilon_A)(\rho) = \epsilon_{[\![H,A]\!]}(\rho) + \epsilon_{F \odot A}(\rho) - \epsilon_F(\rho)\epsilon_A(\rho), \quad \rho \in \mathcal{S}. \tag{4.23}$$

Recall that expectation value functions are linear on $\mathcal{S}$. Thus, because of the last summand, $W(\epsilon_A)$ is in general a non-linear function on the set of states. In short, the vector field W is said to be non-linear. Observe that this non-linearity comes from the gradient part of the vector field W. Linearity is obtained only for $F = 0$.

In contraposition with W, the Kossakowski-Lindblad vector field Z_L is linear, as deduced from its simple expression (4.20). The Kraus operator in (4.18) is responsible for the linear nature of this vector field. In order to understand its relevance, consider a Kraus map K as in (4.10):

$$K(A) = \sum_{j=1}^{r} V_j A V_j^*, \quad A \in \mathrm{Herm}(\mathcal{H}). \tag{4.24}$$

The isomorphism $\mathcal{O} \cong \mathcal{O}^* \cong \mathrm{Herm}(\mathcal{H})$ allows for the identification of the Kraus operator as a map $K : \mathcal{O}^* \to \mathcal{O}^*$. Hence it is possible to apply Theorem 3.57, obtaining a vector field $Z_K \in \mathfrak{X}(\mathcal{S})$.

Proposition 4.12. *The action of the vector field Z_K on an expectation value function ϵ_A is*

$$Z_K(\epsilon_A)(\rho) = \epsilon_{K^\sharp(A)}(\rho) - \epsilon_V(\rho)\epsilon_A(\rho), \quad V = \sum_{j=1}^{r} V_j^* V_j \in \mathcal{O}, \quad \rho \in \mathcal{S},\ A \in \mathcal{O}, \tag{4.25}$$

with the dual Kraus operator $K^\sharp : \mathcal{O} \to \mathcal{O}$ being defined as

$$K^\sharp(A) = \sum_{j=1}^{r} V_j^* A V_j, \quad A \in \mathcal{O} \cong \mathrm{Herm}(\mathcal{H}). \tag{4.26}$$

Proof. This is a direct application of Theorem 3.57. Observe that

$$K^\sharp(I) = \sum_{j=1}^{r} V_j^* V_j =: V,$$

thus obtaining the proposed expression. □

Now, consider the vector field W' which is a linear combination of three different vector fields with real coefficients, defined as follows.

$$W' = \widetilde{X}_H + \widetilde{Y}_F + Z_K, \quad H, F \in \mathcal{O}. \tag{4.27}$$

As before, the action of W' on expectation value functions can be directly computed:

$$W'(\epsilon_A)(\rho) = \epsilon_{[\![H,A]\!]}(\rho) + \epsilon_{F\odot A}(\rho) + \epsilon_A(K(\rho)) - \epsilon_F(\rho)\epsilon_A(\rho) - \epsilon_V(\rho)\epsilon_A(\rho), \quad \rho \in \mathcal{S},\ A \in \mathcal{O}. \tag{4.28}$$

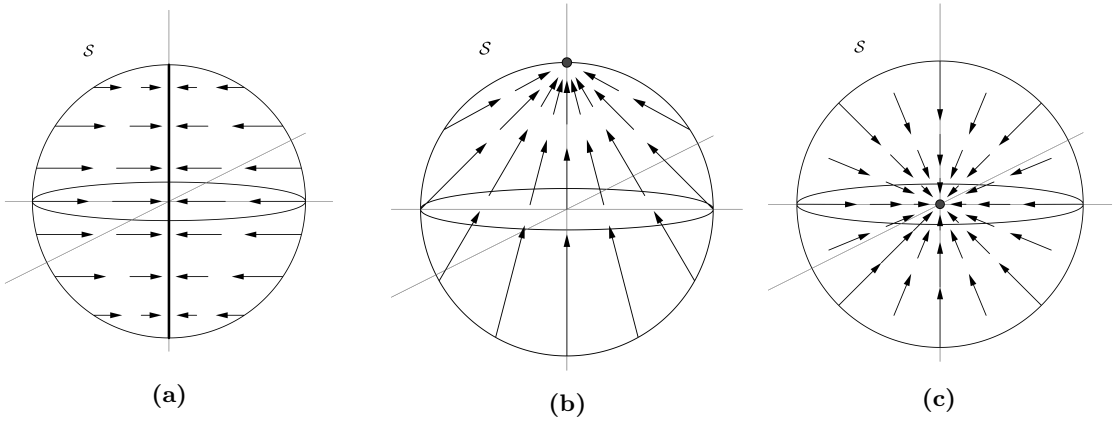


Figure 4.2: Representations of different Kossawkoski-Lindblad vector fields for the 2-level system on the Bloch ball introduced in Chapter 3. They correspond to **(a)** phase damping, **(b)** decay and **(c)** dissipation of the system. These examples will be fully explained in later sections.

The non-linearity of this vector field is now due to the last two terms. Thus, in contraposition to (4.23), linearity can be regained in this case by imposing a fine tuning between the last two summands in (4.28):

$$\epsilon_F(\rho) + \epsilon_V(\rho) = 0 \quad \forall \rho \in S. \tag{4.29}$$

This tuning can be achieved by considering the following expression for the observable F appearing in (4.27):

$$F = -V = -\sum_{j=1}^{r} V_j^* V_j. \tag{4.30}$$

Linearity is thus achieved. The resulting vector field is the generator of the Markovian dynamics associated with the Kossakowski-Lindblad equation.

Theorem 4.13. [72] *Let H be an observable and let K be the Kraus operator defined as in (4.24). The vector field Z_L on $\mathcal{S}$ defined as*

$$Z_L = \widetilde{X}_H - \widetilde{Y}_V + Z_K, \quad V = \sum_{j=1}^{n^2-1} V_j^* V_j = K^\sharp(I). \tag{4.31}$$

is such that the system of differential equations for its integral curves is given by the Kossakowski-Lindblad equation (4.18). Its action on expectation value functions is

$$Z_L(\epsilon_A)(\rho) = \epsilon_{[\![H,A]\!]}(\rho) - \epsilon_{V\odot A}(\rho) + \epsilon_{K^\sharp(A)}(\rho), \quad \rho \in \mathcal{S},\ A \in \mathcal{O} \tag{4.32}$$

where the dual map $K^\sharp : \mathcal{O} \to \mathcal{O}$ is defined as in (4.26).

The last two vector fields in the decomposition of Z_L given in (4.31) are not independent. The gradient vector field Y_V is uniquely determined for each possible vector field Z_K. Such relation follows, as indicated before, in order to obtain $\mathbb{R}$-linear transformations in the space of states. The resulting vector field is well defined in the whole set of states $\mathcal{S}$, but is not in general tangent to each stratum of the set, as a consequence of Theorem 4.9 proved in [141]. As seen above, this geometric approach to Markovian dynamics allows for an in-depth study of its properties, such as the importance of linearity. Observe that, due to Lemma 4.4, vector field Z_L is the more general linear positivity-preserving vector field that can be written on $\mathcal{S}$. Generalisations of this vector field could be easily described, mimicing the description of non-positive dynamical maps mentioned in 4.1.1. The geometric formalism, however, offers another possible generalisation. Non-linear maps could be described by dropping the constraint in the expression of the gradient vector field in (4.31). In this way, it is possible to extend the study of open quantum system to non-linear dynamics. This could have applications in cases in which the interaction with the environment is not negligible, such as spin chains or molecular systems.

4.1.4 Markovian dynamics for 2-level systems

In order to get some insight on the properties of the Kossakowski-Lindblad vector field, several simple examples can be computed. The coordinate expressions for the observables of a 2-level system have been presented in Sections 1.1.7 and 3.4. A basis of the algebra of observables $\mathcal{O} = \mathrm{Herm}(\mathbb{C}^2)$ is given by the three Pauli matrices and the identity matrix:

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4.33}$$

The Lie and Jordan product of the elements in these basis are the following:

$$\begin{aligned} &[\![\sigma_j, \sigma_k]\!] = 2\epsilon_{jkl}\sigma_l, \quad \sigma_j \odot \sigma_k = 2\delta_{jk}\sigma_0, && j,k = 1,2,3 \\ &[\![\sigma_0, \sigma_\mu]\!] = [\![\sigma_\mu, \sigma_0]\!] = 0, \quad \sigma_0 \odot \sigma_\mu = \sigma_\mu \odot \sigma_0 = 2\sigma_\mu, && \mu = 0,1,2,3. \end{aligned} \tag{4.34}$$

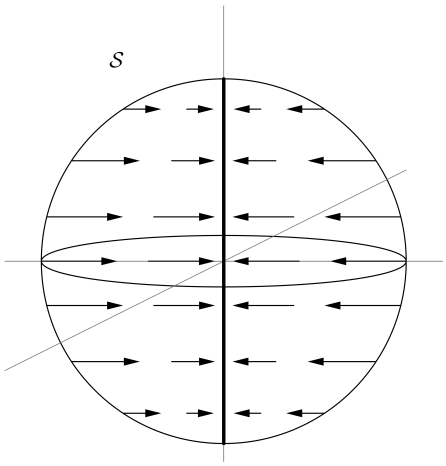


Figure 4.3: Vector field and limit manifold for the phase damping of a 2-level quantum system. The limit manifold is the intersection of the Bloch ball with the x_3-axis, as computed in (4.40).

The set of states $\mathcal{S}$ is a three-dimensional manifold. As stated in Proposition 3.58, states of the system can be written as

$$\rho = \sigma^0 + x_j \sigma^j = \frac{1}{2}\begin{pmatrix} 1+x_3 & x_1 - ix_2 \\ x_1 + ix_2 & 1-x_3 \end{pmatrix}, \quad x_1^2 + x_2^2 + x_3^2 \leq 1, \tag{4.35}$$

where $\sigma^\mu = \frac{1}{2}\sigma_\mu$, with $\mu = 0, 1, 2, 3$, is the dual basis to (4.33).

Phase damping of 2-level systems

As a first example, consider the phase damping of a 2-level system. Phase damping is a quantum process in which the interaction with an environment causes losses of quantum information, while the energy of the system does not vary. For the particular case of a 2-level system, the phase damping is modelised by the following Kossakowski-Lindblad operator [7, 92]:

$$L(\rho) = -\gamma(\rho - \sigma_3 \rho \sigma_3), \quad \rho \in \mathcal{S}. \tag{4.36}$$

In order to obtain the explicit expression for the associated vector field Z_L on $\mathcal{S}$, consider the basis for $\mathcal{O}$ given in (4.33). As L is a self-adjoint operator on matrices, i.e. $L = L^\sharp$, the following follows

$$L^\sharp(\sigma_1) = -2\gamma\sigma_1, \quad L^\sharp(\sigma_2) = -2\gamma\sigma_2, \quad L^\sharp(\sigma_3) = 0, \quad L^\sharp(I) = 0.$$

The coordinate expression of the vector field Z_L can be computed directly by Proposition 4.8:

$$Z_L = -2\gamma\left(x_1 \frac{\partial}{\partial x_1} + x_2 \frac{\partial}{\partial x_2}\right). \tag{4.37}$$

A plot of this vector field and its integral curves on the Bloch ball can be found in Figure 4.3. By direct integration, the following coordinate expression for the flow of Z_L can be found:

$$\Phi_t^L(x_{10}, x_{20}, x_{30}) = (e^{-2\gamma t}x_{10}, e^{-2\gamma t}x_{20}, x_{30}). \tag{4.38}$$

The limit manifold $\mathcal{S}_L$ of the evolution is defined as the subset of $\mathcal{S}$ towards which the whole states of the system evolve:

$$\mathcal{S}_L = \lim_{t\to\infty} \Phi_t^L(\mathcal{S}). \tag{4.39}$$

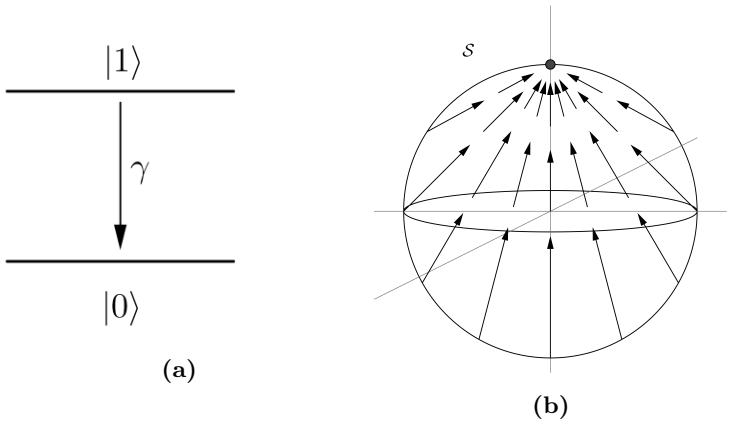


Figure 4.4: **(a)** Decay of a two level system. **(b)** Vector field and limit manifold for the decay of a 2-level quantum system. The limit manifold is the pure state corresponding to the ground state of the system.

From (4.37) and (4.38), the limit manifold coincides with the fixed points of the dynamics. This subset is

$$\mathcal{S}_L = \{\rho \in \mathcal{S} \mid \rho = \sigma^0 + x_3\sigma^3\}. \tag{4.40}$$

In the representation in terms of the Bloch ball, presented in Figure 4.3, the limit manifold corresponds to the intersection of the Bloch ball with the x_3-axis. Points in the ball evolve in such a way that they tend to this axis. Observe that the properties stated in Section 4.3 are present here. Recall that rank 1 states belong to the surface $\mathcal{S}_1$ of the ball, while rank 2 states are in the interior $\mathcal{S}_2$ of the ball. Evolution starting on the surface for $t = 0$ immediately enter the interior $\mathcal{S}_2$, except for the two fixed points on the surface. For any $t > 0$, evolution has to preserve the strata; in this case, evolution occurs inside $\mathcal{S}_2$. In this example, no change in rank occurs in the asymptotic limit.

Decay of 2-level systems

Other examples of Markovian evolution can be considered. Consider the decay of a 2-level system onto its ground state, as graphically represented in Figure 4.4. This phenomenon is modelled by the following Kossakowski-Lindblad operator [39]:

$$L(\rho) = J\rho J^\dagger - \frac{1}{2}(J^\dagger J\rho + \rho J^\dagger J), \quad J = \sqrt{\gamma}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \gamma > 0, \tag{4.41}$$

where the eigenstates of the Hamiltonian are taken as a basis for the Hilbert space of the system. The vector field Z_L associated to this operator is given by Proposition 4.8:

$$Z_L = -\frac{\gamma}{2}x_1\frac{\partial}{\partial x_1} - \frac{\gamma}{2}x_2\frac{\partial}{\partial x_2} + \gamma(1 - x_3)\frac{\partial}{\partial x_3}. \tag{4.42}$$

This vector field can be easily plotted on the Bloch ball, as seen in Figure 4.4. By direct integration, the flow of Z_L is

$$\Phi_t^L(x_{10}, x_{20}, x_{30}) = (e^{-\gamma\frac{t}{2}}x_{10}, e^{-\gamma\frac{t}{2}}x_{10}, 1 - e^{-\gamma t}(1 - x_{30})). \tag{4.43}$$

Clearly, the limit manifold of the dynamic is

$$\mathcal{S}_L = \left\{\rho = \sigma^0 + \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\right\}, \tag{4.44}$$

which corresponds to the ground state of the system. As in the previous example, the rank of states increases from $t = 0$ to $t > 0$ for starting points on the surface of the Bloch sphere, in agreement with Proposition 4.11. Strata are thus preserved by the evolution for $t > 0$.

Dissipation of 2-level systems

As a last example, consider the following Kossakowski-Lindblad operator:

$$L(\rho) = \sum_{j=1}^{2} \left(J_j \rho J_j^\dagger - \frac{1}{2}(J_j^\dagger J_j \rho + \rho J_j^\dagger J_j) \right), \tag{4.45}$$

where operators J_1, J_2 are defined as

$$J_1 = \sqrt{\gamma_1} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad J_2 = \sqrt{\gamma_2} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \gamma_1, \gamma_2 > 0, \tag{4.46}$$

This Kossakowski-Lindblad operator models the dissipation of a 2-level system [39]. Physically, there exist transitions between both energy levels, modelled by the parameters γ_1 and γ_2. Their values determine the limit of the evolution.

The vector field Z_L associated to this operator can be directly computed by Proposition 4.8. It can also be computed separately for each summand, thus obtaining:

$$\begin{aligned} Z_{L1} &= -\frac{\gamma_1}{2} x_1 \frac{\partial}{\partial x_1} - \frac{\gamma_1}{2} x_2 \frac{\partial}{\partial x_2} + \gamma_1 (1 - x_3) \frac{\partial}{\partial x_3}, \\ Z_{L2} &= -\frac{\gamma_2}{2} x_1 \frac{\partial}{\partial x_1} - \frac{\gamma_2}{2} x_2 \frac{\partial}{\partial x_2} - \gamma_2 (1 + x_3) \frac{\partial}{\partial x_3}. \end{aligned} \tag{4.47}$$

Define the quantities $\gamma := \gamma_1 + \gamma_2$ and $\delta := \gamma_1 - \gamma_2$. The total Kossakowski-Lindblad vector field Z_L is

$$Z_L = Z_{L1} + Z_{L2} = -\frac{\gamma}{2} x_1 \frac{\partial}{\partial x_1} - \frac{\gamma}{2} x_2 \frac{\partial}{\partial x_2} + (\delta - \gamma x_3) \frac{\partial}{\partial x_3}. \tag{4.48}$$

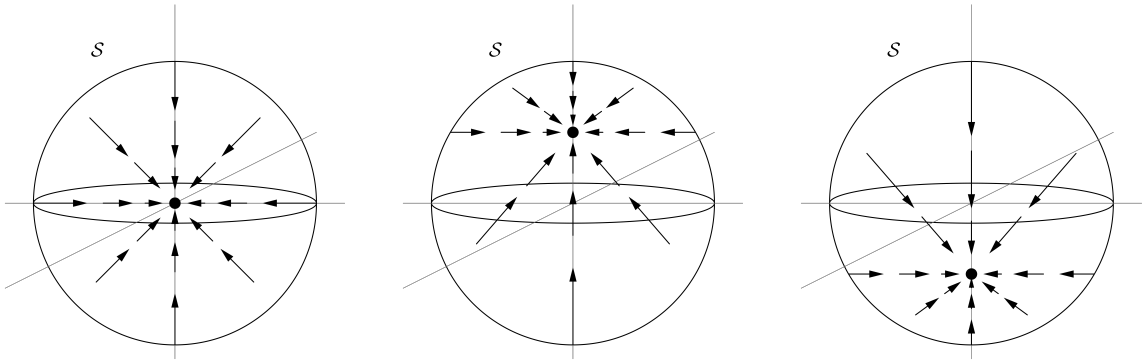


Figure 4.5: Dissipation of a 2-level system for different values of the parameters in (4.45). In the case $\gamma_1 = \gamma_2$, the limit of the evolution is the maximally mixed state.

The vector fields for different values of the parameters are represented in Figure 4.5. The limit set of the evolution is composed of a single point:

$$\mathcal{S}_L = \left\{ \rho \in \mathcal{S} \mid \rho = \sigma^0 + \frac{\delta}{\gamma} \sigma^3 \right\}. \tag{4.49}$$

For $\delta = \gamma$, i.e. for $\gamma_2 = 0$, the decay presented in the previous section is obtained. On the other hand, for $\delta = 0$, the limit of the evolution is σ^0, the maximally mixed state. This case corresponds to the complete dissipation of the state of the system, in the sense that the entropy of the system is maximised by the dynamics.

4.2 Contractions of finite-dimensional algebras

Once the behaviour of open quantum systems is understood, it is possible to apply the geometric formalims to the study of different properties of the system. A particularly interesting feature is the behaviour of observables under Markovian evolution. As recently proved by Chruściński, Marmo and co-workers, [7, 92, 158], the behaviour of the algebraic structures of the observables of an open quantum system is not trivial, and can in fact be explicitely computed. The algebra of observables is subject to a contraction, thus effectively leading in the asymptotic limit to a new algebra, hence to a quantum system with different properties. The contraction of algebras of quantum observables has recently been presented in a scientific paper [72]. For a complete characterisation of these contractions, the present section deals with the mathematical description of this procedure.

The motivation behind the study of contractions of algebras comes from physical problems, and in particlar of the study of the classical limit of Special Relativity. An algebraic characterisation of the problem shows that, when varying the speed of light c, the Poincaré group evolves in a specific way whose limit is precisely the Galileo group. In the 1950's, Segal [240] and independently Inönü and Wigner [159] aimed to describe this phenomenon in terms of Linear Algebra. They found that, when the parameters describing the properties of the algebra are changed, it is possible to obtain in the asymptotic limit a different algebraic structure. Such a procedure is nowadays known as a contraction of the algebra. The present section is devoted to the description of those characteristics of the theory of contractions that are relevant in connection with the study of quantum systems.

Consider an n-dimensional algebra $(V, *)$ and a basis $\{e_j\}_{j=1}^n$ for the algebra. The product $*$ can be described in terms of the corresponding structure constants c_{jk}^l, defined as

$$e_j * e_k = c_{jk}^l e_l, \quad j,k = 1,2,\dots,n. \tag{4.50}$$

A generic regular linear transformation $U : V \to V$ of the algebra amounts for a change of basis in V of the form

$$e'_j := Ue_j = U_j^k e_k, \quad j = 1,2,\dots,n, \tag{4.51}$$

being U_j^k the components of the matrix representation of the transformation U. The products of the elements in this new basis can be related to those of the initial ones (4.50) as follows:

$$e'_j * e'_k = U_j^p U_k^q e_p * e_q = c_{pq}^r U_j^p U_k^q e_r = \left(c_{pq}^r U_j^p U_k^q (U^{-1})_r^l\right) e'_l, \quad j,k = 1,2,\dots,n. \tag{4.52}$$

It is possible though to see the transformation U under a different light. Namely, as a way to introduce a new product $*_U$ in the linear space V. This product is defined as

$$a *_U b = U^{-1}\left(Ua * Ub\right), \quad a,b \in V. \tag{4.53}$$

By acting with U^{-1} on (4.52), the new product of elements in the basis can be obtained. Thus, the structure constants $(c_U)_{jk}^l$ of the new product are simply given by

$$e_j *_U e_k = (c_U)_{jk}^l e_l, \quad (c_U)_{jk}^l = c_{pq}^r U_j^p U_k^q (U^{-1})_r^l, \quad j,k,l = 1,2,\dots,n. \tag{4.54}$$

Lemma 4.14. *The regular linear transformation $U : V \to V$ is an algebra isomorphism between $(V, *)$ and $(V, *_U)$, with both products related by (4.53).*

Proof. By acting with U on (4.53), it is immediate to obtain that $U(a *_U b) = Ua * Ub$. □

Consider now a family of linear transformations $\{U(\epsilon) : V \to V \mid 0 \le \epsilon \le 1\}$ depending continuously on the parameter ϵ, with $U(1)$ being the identity transformation, and such that $U(\epsilon)$ is regular for $\epsilon > 0$ and $U(0)$ is singular. Thus, for every $\epsilon > 0$, there exists a new product $*_\epsilon$ on V given by

$$a *_\epsilon b = U^{-1}(\epsilon)\left(U(\epsilon)a * U(\epsilon)b\right), \quad a,b \in V, \quad 0 < \epsilon \le 1. \tag{4.55}$$

As a result, these transformations define a family $\{(V, *_\epsilon) \mid 0 < \epsilon \leq 1\}$ of algebras that are isomorphic among them. The structure constants $c^l_{jk}(\epsilon)$ for each product $*_\epsilon$ are

$$c^l_{jk}(\epsilon) = c^r_{pq} U^p_j(\epsilon) U^q_k(\epsilon) (U^{-1})^l_r(\epsilon), \quad j,k,l = 1,2,\ldots,n, \quad 0 < \epsilon \leq 1. \tag{4.56}$$

Observe that the definition (4.55) makes no sense for $\epsilon = 0$, as $U(0)$ is not invertible. However, once the family of algebras is obtained, it is possible to take into consideration the existence of an asymptotic limit when $\epsilon \to 0$.

Definition 4.15. *Consider the family of algebras $\{(V, *_\epsilon) \mid 0 < \epsilon \leq 1\}$ defined as above. If there exists an asymptotic limit for the family when $\epsilon \to 0$, let $*_0$ be the product defined as*

$$a *_0 b = \lim_{\epsilon \to 0} a *_\epsilon b, \quad a, b \in V. \tag{4.57}$$

The algebra $(V, *_0)$ is called a contraction of the algebra $(V, *)$.

The theory of contraction deals with the classification of algebras for which a contraction can be obtained, and with the characterisation of such contractions. Observe that, in general, the contraction $(V, *_0)$ of an algebra $(V, *)$ is not isomorphic to it. Thus, contractions are in a sense a way to establish a hierarchy between different algebras.

Characterisation and generalisation of contractions introduced by Segal, Inönü and Wigner have been studied in detail. Among other authors, important contributions are due to Saletan [231], who proposed a new type of algebra contraction; Weimar-Woods [268–271], who fully described the contraction of Lie algebras; and Cariñena, Grabowski and Marmo [77–79], who described the theory in a more geometric setting. Other contributions can be found in [107, 113, 189] and references therein.

4.2.1 Behaviour of properties of algebraic structures under contraction

The contraction procedure can be applied to any type of algebra. The particular case of Lie algebras has been fully described [268–271]. For the study of Quantum Mechanics, and due to the algebraic nature of the set of observables presented in Section 3.2, however, a more general setting is necessary. The description of contractions for generic algebras has been achieved by Cariñena, Grabowski and Marmo [78]. Concerning the case of Quantum Mechanics, one of the results presented in their work has particular importance. Namely, the nature and properties of a contracted algebra with respect to the initial one.

Consider a finite-dimensional algebra $(V, *)$ over a field K. The properties of any algebra can be described in term of a certain number N of properties $A_{*,1}, \ldots, A_{*,N}$. A property $A_{*,j}$ amounts to the determination of a function $\mu_{*,j} : V \times \cdots \times V \to K$, depending on the product $*$, that satisfies a certain condition. For example, a property can be expressed by writing

$$A_{*,j} : \quad \mu_{*,j}(a_1, \ldots, a_{r_j}) = 0, \quad \forall a_1, \ldots, a_{r_j} \in V, \tag{4.58}$$

with r_j a natural number. Such a property only uses universal quantifiers, and the equality is satisfied for any element in the algebra. This is the case of the associativity property,

$$A_{*,1} : \quad \mu_{*,1}(a_1, a_2, a_3) = (a_1 * a_2) * a_3 - a_1 * (a_2 * a_3) = 0, \quad \forall a_1, a_2, a_3 \in V,$$

or the skew-symmetry property,

$$A_{*,2} : \quad \mu_{*,2}(a_1, a_2) = a_1 * a_2 + a_2 * a_1 = 0, \quad \forall a_1, a_2 \in V.$$

Other properties, however, may be satisfied only for a particular element in the algebra, i.e. they depend on existential qualifiers:

$$A_{*,j} : \quad \exists e_1, \ldots, e_{s_j} \in V \ : \ \mu_{*,j}(e_1, \ldots, e_{s_j}, a_1, \ldots, a_{t_j}) = 0, \quad \forall a_1, \ldots, a_{t_j} \in V. \tag{4.59}$$

A typical example corresponds to the existence of an element unit:

$$\begin{array}{ll} A_{*,3}: & \exists 1 \in V \ : \mu_{*,3}(1,a) = 1 * a - a = 0, \\ A'_{*,3}: & \exists 1 \in V \ : \mu'_{*,3}(1,a) = a * 1 - a = 0, \end{array} \qquad \forall a \in V.$$

Theorem 4.16. *Consider an algebra satisfying certain properties with universal quantifiers, in the form of (4.58). Any contraction of this algebra satisfies the same properties.*

Proof. This result is proved in [78]. Given a family of linear transformations $\{U(\epsilon)\}$ satisfying the same properties as above, and due to Lemma 4.14, the algebras $(V, *)$ and $(V, *_\epsilon)$ are isomorphic, thus they satisfy the same properties in the form of (4.58). This is preserved in the limit $\epsilon \to 0$. □

Observe that existential qualifiers are not preserved by generic contractions. For example, the existence of a unit may not be satisfied for a contracted algebra if $U(\epsilon)^{-1}1$ is not defined in the limit $\epsilon \to 0$. This consideration, however, proves the following:

Corollary 4.17. *The contraction of a unital algebra is unital if the unity is preserved along the contraction.*

This result is relevant in the context of Quantum Mechanics. Observables of a finite-dimensional quantum system are elements of a unital real Lie-Jordan algebra. If this algebra is contracted, by Theorem 4.16 the contracted algebra will be again a Lie-Jordan algebra. It will also be unital if the contraction procedure preserves the unit observable. If such is the case, the contracted algebra can again be seen as the set of observables of a certain hypothetical quantum system.

4.2.2 Three-dimensional Lie algebras

In order to illustrate the theory of contractions of algebras, some simple examples will be considered. The contractions of three-dimensional Lie algebras have been classified by Weimar-Woods [269]. A relevant algebra in the context of Quantum Mechanics is the Lie algebra $\mathfrak{su}(2)$ of the special unitary group acting on $\mathbb{C}^2$. This algebra is isomorphic to the Lie algebra of traceless observables of a 2-level quantum system, as described in Section 1.1.7. Thus, the possible contractions of this algebra will be computed next.

Consider a basis $\{e_1, e_2, e_3\}$ for the Lie algebra $\mathfrak{su}(2) = (V, [\cdot,\cdot])$, with $V \cong \mathbb{R}^3$, such that the commutations relations are

$$[e_1, e_2] = e_3, \quad [e_2, e_3] = e_1, \quad [e_3, e_1] = e_2, \tag{4.60}$$

In order to obtain a contraction of this algebra, take a family $\{U(\epsilon)\}$ of linear transformations of the algebra such that

$$U(\epsilon)e_1 = \epsilon\, e_1, \quad U(\epsilon)e_2 = \epsilon\, e_2, \quad U(\epsilon)e_3 = e_3, \quad 0 \le \epsilon \le 1. \tag{4.61}$$

That is to say, the matrix representation of $U(\epsilon)$ in the given basis is

$$U(\epsilon) = \begin{pmatrix} \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad 0 \le \epsilon \le 1. \tag{4.62}$$

By (4.55), the product $[\cdot,\cdot]_\epsilon$ can be computed for each $\epsilon \in (0, 1]$. Thus, the products among the elements in the basis are

$$[e_1, e_2]_\epsilon = U^{-1}(\epsilon)[\epsilon\, e_1, \epsilon\, e_2] = \epsilon^2 e_3, \quad [e_2, e_3]_\epsilon = e_1, \quad [e_3, e_1]_\epsilon = e_2, \quad 0 \le \epsilon \le 1. \tag{4.63}$$

According to Definition 4.15, a contraction of the initial algebra is obtained if, when $\epsilon \to 0$, the asymptotic limits of these products exist. As this condition is satisfied, the given family of transformations does define a contraction of the $\mathfrak{su}(2)$ algebra. The contracted algebra has the following product:

$$[e_1, e_2]_0 = 0, \quad [e_2, e_3]_0 = e_1, \quad [e_3, e_1]_0 = e_2. \tag{4.64}$$

Observe the characteristics of this algebra. There exists an Abelian subalgebra generated by e_1 and e_2, which is additionally an ideal of the algebra. This is precisely the case of the Lie algebra $\mathfrak{e}(2)$ of the Euclidean group on the plane, which describes translations and rotations. Thus, the contracted algebra of $\mathfrak{su}(2)$ by (4.61) is $\mathfrak{e}(2)$. The contraction theory thus relates two Lie algebras that, at first sight, were independent. Observe that the main difference between $\mathfrak{su}(2)$ and $\mathfrak{e}(2)$ is the value of the product between e_1 and e_2. It is a key characteristics of contractions the fact that the algebras become 'more Abelian'.

The behaviour of algebras under a contraction procedure can be understood by inspecting the properties of the maps described in (4.61). Observe that the only invariant subset of $\mathfrak{su}(2)$ is the subalgebra generated by e_3. It is a standard result in the study of contractions of algebras, first proved by Inönü and Wigner [159], that a family of transformations such as (4.61) defines a contraction of the algebra if and only if the invariant subspace of the transformations is a subalgebra.

The contraction described by (4.63) and (4.64) is a case of an Inönü-Wigner contraction [159]. Other types of contractions are possible. Consider the following family $\{\hat{U}(\delta)\}$ of linear transformations of the $\mathfrak{su}(2)$ algebra

$$\hat{U}(\delta)e_1 = \delta\ e_1, \quad \hat{U}(\delta)e_2 = \delta\ e_2, \quad \hat{U}(\delta)e_3 = \delta^2 e_3, \quad \Leftrightarrow \quad \hat{U}(\delta) = \begin{pmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta^2 \end{pmatrix}, \quad 0 \leq \delta \leq 1. \tag{4.65}$$

As in the previous example, (4.55) gives the definition of a new product $[\cdot,\cdot]'_\delta$, which can be computed for each $\delta \in (0,1]$:

$$[e_1,e_2]'_\delta = \hat{U}^{-1}(\delta)[\delta e_1, \delta e_2] = \hat{U}^{-1}(\delta)(\delta^2 e_3) = e_3, \quad [e_2,e_3]'_\delta = \delta^2 e_1, \quad [e_3,e_1]'_\delta = \delta^2 e_2, \quad 0 \leq \delta \leq 1. \tag{4.66}$$

Again, there exist limits for these expression when $\delta \to 0$. The limit algebra is described by the following product:

$$[e_1,e_2]'_0 = e_3, \quad [e_2,e_3]'_0 = 0, \quad [e_3,e_1]'_0 = 0. \tag{4.67}$$

This algebra is isomorphic to the Lie algebra $\mathfrak{h}$ of the Heisenberg group H, defined as the group of real 3×3 upper triangular matrices of the following form [146]:

$$H(1) = \left\{ \begin{pmatrix} 1 & a & b \\ 0 & 1 & c \\ 0 & 0 & 1 \end{pmatrix} \middle| \, a,b,c, \in \mathbb{R} \right\}. \tag{4.68}$$

Such a group appears in the study of one-dimensional quantum systems. From the perspective of contractions, the Lie algebra $\mathfrak{h}$ is related with $\mathfrak{su}(2)$ by means of a contraction. Observe that, as in the previous case, the contracted algebra has more commuting elements than the initial one.

To conclude this characterisation of contractions of three-dimensional Lie algebras, consider the following facts. Any Lie algebra can be contracted onto an Abelian algebra by the family of transformations $\{U(\epsilon) = \epsilon \mathbb{I}\}$. It is also possible [269] to find a contraction from $\mathfrak{e}(2)$ to $\mathfrak{h}$. Thus, the contraction of algebras establish the following hierarchy of three-dimensional Lie algebras:

$$\mathfrak{su}(2) \longrightarrow \mathfrak{e}(2) \longrightarrow \mathfrak{h} \longrightarrow \text{Abelian}. \tag{4.69}$$

These contractions play an important role in the analysis of 2-level quantum systems that will be carried out in following sections.

4.3 Geometric description of Markovian dynamics

The contraction of algebras appear naturally in the study of Markovian open quantum systems [7, 72, 92, 158]. A geometric description of Markovian dynamics is particularly well suited for the description of this phenomenon. The present section details the geometric properties of such dynamics.

While the usual matrix mechanics describes the evolution of observables, the geometric formalism is more flexible. Given a vector field, as Z_L, one can obtain the evolution of any function or tensor field, for example, functions as concurrence, purity or entropies. This section will focus mainly on the evolution of the contravariant tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ under the action of the Kossakowski-Lindblad vector field Z_L and the corresponding semigroup $\{\Phi_t^L : \mathcal{S} \to \mathcal{S}, t \geq 0\}$ of $\mathbb{R}$-linear transformations. Observe that the flow of a generic vector field on $\mathcal{S}$ is indeed a semigroup, and not a group, as $\mathcal{S}$ is a manifold with boundary. The inverse of Φ_t^L is defined on the envolving manifold $\widehat{\mathcal{S}}$, but not necessarily on $\mathcal{S}$.

Consider a vector field X on a manifold M, whose flow is a semigroup of transformations $\{\Phi_t^X : \mathcal{S} \to \mathcal{S}, t \geq 0\}$. The change along the integral curves of X of tensor fields is determined by the Lie derivative with respect to X. As in the rest of this paper, the notation followed is the one of the book by Crampin and Pirani [104]. The expression for the Lie derivative of a contravariant tensor field T on M with respect to the vector field X is defined as

$$\mathcal{L}_X T = \lim_{t \to 0^+} \frac{1}{t} \left(T - \Phi_{t*}^X(T) \right). \tag{4.70}$$

By integration, it is possible to determine the push-forward by Φ_t^X of contravariant tensor fields. Therefore, given a vector field on a manifold, each contravariant tensor field T defines a family $\{\Phi_{t*}^X(T), t \geq 0\}$ of tensor fields on the manifold.

Definition 4.18. *Let $\mathcal{S}$ be the set of states of a quantum open system with a Markovian evolution. If Z_L is the Kossakowski-Lindblad vector field, the families $\{\Lambda_{\mathcal{S},t}, t \geq 0\}$ and $\{R_{\mathcal{S},t}, t \geq 0\}$ are defined as those obtained by the push-forward of the contravariant tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ that reproduces the algebraic structure of quantum observables:*

$$\begin{aligned} \Lambda_{\mathcal{S},t} =& e^{-t\mathcal{L}_{Z_L}} \Lambda_{\mathcal{S}} = \Lambda_{\mathcal{S}} - t\mathcal{L}_{Z_L}\Lambda_{\mathcal{S}} + \frac{t^2}{2!}(\mathcal{L}_{Z_L})^2\Lambda_{\mathcal{S}} - \cdots, \\ R_{\mathcal{S},t} =& e^{-t\mathcal{L}_{Z_L}} R_{\mathcal{S}} = R_{\mathcal{S}} - t\mathcal{L}_{Z_L} R_{\mathcal{S}} + \frac{t^2}{2!}(\mathcal{L}_{Z_L})^2 R_{\mathcal{S}} - \cdots, \end{aligned} \qquad t \geq 0, \tag{4.71}$$

These families have a huge relevance in the characterisation of the dynamics of quantum systems. Recall that, as proved in Chapter 3, contravariant tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ codify the algebraic structure of the quantum observables of the system. Thus, evolution of the tensor fields is in direct relation with changes in the algebraic properties of observables. This is precisely the main topic in the theory of contractions of algebras. The analysis of these families of tensor fields may provide with information on the behaviour of quantum systems, in particular of their observables. The relation between evolved tensor fields $\Lambda_{\mathcal{S},t}$ and $R_{\mathcal{S},t}$ is made explicit by the following result.

Proposition 4.19. *Consider the families $\{\Lambda_{\mathcal{S},t}, t \geq 0\}$ and $\{R_{\mathcal{S},t}, t \geq 0\}$ defined in (4.71). Then, for every $t \geq 0$, there exists a Lie-Jordan algebra of expectation value functions with composition laws defined by*

$$\{\epsilon_A, \epsilon_B\}_t(\rho) = \Lambda_{\mathcal{S},t}(\mathrm{d}\epsilon_A, \mathrm{d}\epsilon_B)(\rho), \quad (\epsilon_A, \epsilon_B)_t(\rho) = R_{\mathcal{S},t}(\mathrm{d}\epsilon_A, \mathrm{d}\epsilon_B)(\rho) + 2\epsilon_A(\rho)\epsilon_B(\rho), \quad \rho \in \mathcal{S}. \tag{4.72}$$

with $A, B \in \mathcal{O}$. All the resulting algebras are isomorphic for any finite time $t \geq 0$.

Proof. The transformations Φ_t^L defining the flow of the vector field Z_L is invertible for any finite t. Therefore, tensorial properties are preserved, as it is a point transformation. For any finite $t > 0$, the Lie-Jordan algebra of expectation value functions is isomorphic to the initial one. Hence all these algebras are isomorphic. □

The families may or may not have asymptotic limits when $t \to \infty$. If they exist, let them be denoted

$$\Lambda_{\mathcal{S},\infty} = \lim_{t \to \infty} \Lambda_{\mathcal{S},t}, \quad R_{\mathcal{S},\infty} = \lim_{t \to \infty} R_{\mathcal{S},t}. \tag{4.73}$$

The interest of these limits rests on the algebra in the space of functions that they define. As expected, a contraction of the algebra of expectation value functions is obtained.

Theorem 4.20. *Suppose that the limits $\Lambda_{\mathcal{S},\infty}$ and $R_{\mathcal{S},\infty}$ of the families presented in Proposition 4.19 do exit. Then, the set of expectation value functions $\mathcal{E}_{\mathcal{O}}(\mathcal{S})$ on $\mathcal{S}$ is a Lie-Jordan algebra with respect to the products $\{\cdot,\cdot\}_\infty$ and $(\cdot,\cdot)_\infty$ defined as*

$$\begin{aligned}\{\epsilon_A,\epsilon_B\}_\infty(\rho) &= \Lambda_{\mathcal{S},\infty}(\mathrm{d}\epsilon_A,\mathrm{d}\epsilon_B)(\rho),\\ (\epsilon_A,\epsilon_B)_\infty(\rho) &= R_{\mathcal{S},\infty}(\mathrm{d}\epsilon_A,\mathrm{d}\epsilon_B)(\rho)+2\epsilon_A(\rho)\epsilon_B(\rho),\end{aligned}\qquad \rho\in\mathcal{S}. \tag{4.74}$$

This algebra gives rise to an associative complex algebra with respect to the product

$$\epsilon_A *_\infty \epsilon_B = (\epsilon_A,\epsilon_B)_\infty + \mathrm{i}\{\epsilon_A,\epsilon_B\}_\infty,\quad A,B\in\mathcal{O}. \tag{4.75}$$

Proof. The new algebra is by definition a contraction of the initial algebra of expectation value functions (which was isomorphic to $\mathcal{O}$). As proved in Theorem 4.16, algebraic properties depending on universal qualifiers (skew-symmetry, Jacobi identity, etc.) are preserved by the contraction procedure. Thus, the contracted algebra satisfies the same properties as the initial one, i.e. it is a Lie-Jordan algebra. Observe that the unity element $\epsilon_I = 1$ is preserved by the contraction procedure. Thus, the condition of Corollary 4.17 is satisfied, and the contracted algebra is also unital. Finally, complex associative algebras can always obtained from real Lie-Jordan algebras, as is the case. □

Observe that there exists a one-to-one correspondence between expectation value functions and quantum observables. Thus, the new algebra thus obtained immediately defines a contraction of the algebra of observables of the system. Notice that, from an algebraic point of view, the contracted Poisson and symmetric brackets no longer represent the commutator or anti-commutator of observables. In fact, products in (4.74) define a new pair of operations $[\![\cdot,\cdot]\!]_\infty$ and $\odot_\infty$ on the set of observables,

$$\epsilon_{[\![A,B]\!]_\infty} := \{\epsilon_A,\epsilon_B\}_\infty,\quad \epsilon_{A\odot_\infty B} := (\epsilon_A,\epsilon_B)_\infty,\quad A,B\in\mathcal{O}. \tag{4.76}$$

which are different from the initial ones. Thus, a contraction of the algebra of observables is obtained. Due to the nature of the contraction procedure, some non-commuting observables $[A,B]\neq 0$ in the initial algebra may satisfy $[A,B]_\infty = 0$. Similarly, the non-associativity of the Jordan product may disappear, obtaining $A\odot_\infty B = AB$. Thus, the contraction of the algebra is connected with the transition from quantum to classical observables. The physical implications of the contraction procedure is a promising topic that will be discussed in future works.

4.3.1 Contractions for open 2-level systems

In order to illustrate the described contraction of algebras, consider the Markovian evolutions of 2-level systems described in Section 4.1.4. With the given coordinate system, it is immediate to write the coordinate expressions for the tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$, as proved in 3.59:

$$\Lambda_{\mathcal{S}} = \sum_{j,k,l=1}^{3}\epsilon_{jkl}\,x_l\frac{\partial}{\partial x_j}\wedge\frac{\partial}{\partial x_k},\qquad R_{\mathcal{S}} = 2\sum_{j=1}^{3}\frac{\partial}{\partial x_j}\otimes\frac{\partial}{\partial x_j} - 2\sum_{j,k=1}^{3}x_jx_k\frac{\partial}{\partial x_j}\otimes\frac{\partial}{\partial x_k}. \tag{4.77}$$

Contractions for the phase damping of 2-level systems

The phase damping of a 2-level system is described by (4.37):

$$Z_L = -2\gamma\left(x_1\frac{\partial}{\partial x_1}+x_2\frac{\partial}{\partial x_2}\right). \tag{4.78}$$

The 2-level system has great advantages from a computational point of view. Namely, the Lie derivatives of $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ with respect to this vector field can be directly computed:

$$\mathcal{L}_{Z_L}(\Lambda_{\mathcal{S}}) = 8\gamma x_3\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_2},\quad \mathcal{L}_{Z_L}(R_{\mathcal{S}}) = 8\gamma\frac{\partial}{\partial x_1}\otimes\frac{\partial}{\partial x_1}+8\gamma\frac{\partial}{\partial x_2}\otimes\frac{\partial}{\partial x_2}.$$

In order to compute the coordinate expressions of the families $\Lambda_{\mathcal{S},t}$ and $R_{\mathcal{S},t}$, consider the expansion given in Proposition 4.19. Thus, the resulting t-dependent tensor fields are

$$\begin{aligned}\Lambda_{\mathcal{S},t} =& 2e^{-4\gamma t}x_3\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_2}+2x_1\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_3}+2x_2\frac{\partial}{\partial x_3}\wedge\frac{\partial}{\partial x_1},\\ R_{\mathcal{S},t} =& 2e^{-4\gamma t}\left(\frac{\partial}{\partial x_1}\otimes\frac{\partial}{\partial x_1}+\frac{\partial}{\partial x_2}\otimes\frac{\partial}{\partial x_2}\right)+2\frac{\partial}{\partial x_3}\otimes\frac{\partial}{\partial x_3}-2\sum_{j,k=1}^{3}x_jx_k\frac{\partial}{\partial x_j}\otimes\frac{\partial}{\partial x_k},\end{aligned}\qquad t\geq 0. \tag{4.79}$$

Theorem 4.21. *There exist asymptotic limits $\Lambda_{\mathcal{S},\infty}$ and $R_{\mathcal{S},\infty}$ for the families of tensor fields given in (4.79), determined by the Markovian evolution generated by the vector field (4.37). The limits are*

$$\begin{aligned}\Lambda_{\mathcal{S},\infty} &= 2x_1\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_3}+2x_2\frac{\partial}{\partial x_3}\wedge\frac{\partial}{\partial x_1},\\ R_{\mathcal{S},\infty} &= 2\frac{\partial}{\partial x_3}\otimes\frac{\partial}{\partial x_3}-2\sum_{j,k=1}^{3}x_jx_k\frac{\partial}{\partial x_j}\otimes\frac{\partial}{\partial x_k}.\end{aligned} \tag{4.80}$$

Consider the products of smooth functions on $\mathcal{S}$ defined by

$$\{f,g\}_\infty=\Lambda_{\mathcal{S},\infty}(\mathrm{d}f,\mathrm{d}g),\quad (f,g)_\infty=R_{\mathcal{S},\infty}(\mathrm{d}f,\mathrm{d}g)+fg. \tag{4.81}$$

The product $\{\cdot,\cdot\}_\infty$ is a Poisson bracket, while $(\cdot,\cdot)_\infty$ is a symmetric product.

Proof. The existence of the limits to (4.79) is clear by direct inspection. Tensorial properties are preserved in the family, as in Theorem 4.20. Thus the resulting tensor fields define the same type of products as the initial ones. □

It is immediate to check that the set of expectation value functions $\mathcal{E}_{\mathcal{O}}(\mathcal{S})$ on $\mathcal{S}$ is a Lie-Jordan algebra with respect to the products $\{\cdot,\cdot\}_\infty$ and $(\cdot,\cdot)_\infty$. Recall from (3.126) that the relation between observables and expectations value functions is the following:

$$a=a^\mu\sigma_\mu\ \Leftrightarrow\ \epsilon_a=e^0+a^jx_j. \tag{4.82}$$

As the products are $\mathbb{R}$-linear, it is enough to describe the products of constant and linear functions. The unit function satisfies $\{f,1\}_\infty=0$ and $(f,1)_\infty=f$ for any smooth function f on $\mathcal{S}$. Regarding linear functions, they satisfy the following products:

$$\begin{aligned}&\{x_1,x_3\}_\infty=-2x_2,\quad \{x_2,x_3\}_\infty=2x_1,\quad \{x_1,x_2\}_\infty=0,\\ &(x_1,x_1)_\infty=(x_2,x_2)_\infty=0,\quad (x_3,x_3)_\infty=2,\end{aligned} \tag{4.83}$$

and the rest of the products vanish identically. It is immediate to check that these products define a Lie-Jordan algebra.

Similarly, the $*_\infty$-product of functions introduced in Theorem 4.20 can be computed. The constant unit function acts as the unit element, as $\epsilon_a *_\infty 1=1*_\infty\epsilon_a=a$ for any expectation value function. The products of linear functions are

$$\begin{aligned}&x_1*_\infty x_1=0, && x_1*_\infty x_2=0, && x_1*_\infty x_3=-2\,\mathrm{i}x_2,\\ &x_2*_\infty x_1=0, && x_2*_\infty x_2=0, && x_2*_\infty x_3=2\,\mathrm{i}x_1,\\ &x_3*_\infty x_1=2\,\mathrm{i}x_2, && x_3*_\infty x_2=-2\,\mathrm{i}x_1, && x_3*_\infty x_3=2.\end{aligned} \tag{4.84}$$

It can be check by direct computation that the $*_\infty$-product is associative.

One can conclude that the phase damping of a 2-level system defines a contraction of the algebra of expectation values. That is, starting from the algebra given by (3.130), the evolution defines a transformation of the products. In the asymptotic limit, the algebra described in (4.83) is obtained. This new

algebra is not isomorphic to the initial one, however it is still a Lie-Jordan algebra, and it gives rise to a complex associative product. Notice that the contraction defines new products over the same linear space: the functions are not modified, and they are still expectation value functions on $\mathcal{S}$.

For the sake of completeness, observe that Lie algebra $(\mathcal{E}_{\mathcal{O}}(\mathcal{S}), \{\cdot,\cdot\}_\infty)$ is isomorphic to the Lie algebra on the plane. This result is in agreement with previous works [7, 92], which obtain similar results from an algebraic computation. The tensorial description presents the advantage of dealing directly with the algebraic structures codified in terms of tensor fields. As seen in the example, it is not necessary to compute the evolution of expectation value functions in order to obtain the results. As fewer objects are to be dealt with, a possible generalisation to more abstract settings can thus be more easily achieved in the tensorial description.

Contractions for the dissipation of 2-level systems

Consider now the dissipation of the 2-level system, described by (4.48):

$$Z_L = -\frac{\gamma}{2}x_1\frac{\partial}{\partial x_1} - \frac{\gamma}{2}x_2\frac{\partial}{\partial x_2} + (\delta - \gamma x_3)\frac{\partial}{\partial x_3}. \tag{4.85}$$

The families $\Lambda_{\mathcal{S},t}$ and $R_{\mathcal{S},t}$ of contravariant tensor fields are determined by the expansions in Proposition (4.19). The terms in the expansions can be computed directly. The Lie derivatives of the Poisson tensor fields $\Lambda_{\mathcal{S}}$ are

$$\begin{aligned}
\mathcal{L}_{Z_L}(\Lambda_{\mathcal{S}}) &= 2\delta\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_2} + 2\gamma x_1\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_3} + 2\gamma x_2\frac{\partial}{\partial x_3}\wedge\frac{\partial}{\partial x_1},\\
\mathcal{L}^2_{Z_L}(\Lambda_{\mathcal{S}}) &= 2\gamma\delta\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_2} + 2\gamma^2 x_1\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_3} + 2\gamma^2 x_2\frac{\partial}{\partial x_3}\wedge\frac{\partial}{\partial x_1},\\
\mathcal{L}^3_{Z_L}(\Lambda_{\mathcal{S}}) &= 2\gamma^2\delta\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_2} + 2\gamma^3 x_1\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_3} + 2\gamma^3 x_2\frac{\partial}{\partial x_3}\wedge\frac{\partial}{\partial x_1},\\
&\dots
\end{aligned}$$

On the other hand, the terms in the expansion of $R_{\mathcal{S},t}$ are the following:

$$\begin{aligned}
\mathcal{L}_{Z_L}(R_{\mathcal{S}}) =& 2\gamma\frac{\partial}{\partial x_1}\otimes\frac{\partial}{\partial x_1} + 2\gamma\frac{\partial}{\partial x_2}\otimes\frac{\partial}{\partial x_2} + 4(\gamma-\delta x_3)\frac{\partial}{\partial x_3}\otimes\frac{\partial}{\partial x_3}\\
&- 2\delta x_1\frac{\partial}{\partial x_1}\otimes_S\frac{\partial}{\partial x_3} - 2\delta x_2\frac{\partial}{\partial x_2}\otimes_S\frac{\partial}{\partial x_3},\\
\mathcal{L}^2_{Z_L}(R_{\mathcal{S}}) =& 2\gamma^2\frac{\partial}{\partial x_1}\otimes\frac{\partial}{\partial x_1} + 2\gamma^2\frac{\partial}{\partial x_2}\otimes\frac{\partial}{\partial x_2} + 4(2\gamma^2-\delta^2-\gamma\delta x_3)\frac{\partial}{\partial x_3}\otimes\frac{\partial}{\partial x_3}\\
&- 2\gamma\delta x_1\frac{\partial}{\partial x_1}\otimes_S\frac{\partial}{\partial x_3} - 2\gamma\delta x_2\frac{\partial}{\partial x_2}\otimes_S\frac{\partial}{\partial x_3},\\
\mathcal{L}^3_{Z_L}(R_{\mathcal{S}}) =& 2\gamma^3\frac{\partial}{\partial x_1}\otimes\frac{\partial}{\partial x_1} + 2\gamma^3\frac{\partial}{\partial x_2}\otimes\frac{\partial}{\partial x_2} + 4(4\gamma^3-3\gamma\delta^2-\gamma^2\delta x_3)\frac{\partial}{\partial x_3}\otimes\frac{\partial}{\partial x_3}\\
&- 2\gamma^2\delta x_1\frac{\partial}{\partial x_1}\otimes_S\frac{\partial}{\partial x_3} - 2\gamma^2\delta x_2\frac{\partial}{\partial x_2}\otimes_S\frac{\partial}{\partial x_3},\\
&\dots
\end{aligned}$$

Integration of these derivatives by (4.71) is immediate. The only complication may arise from the (x_3, x_3) terms in the Lie derivatives of $R_{\mathcal{S}}$. This term is easily integrated by considering the following property concerning the vector field Z_L and Lie derivatives:

$$\mathcal{L}^n_{Z_L}\left((a+bx_3)\frac{\partial}{\partial x_3}\otimes\frac{\partial}{\partial x_3}\right) = (2\gamma)^n a + (2^n-1)\gamma^{n-1}\delta b + \gamma^n b x_3, \quad n = 1, 2, \dots, \tag{4.86}$$

which is proved by direct computation from (4.85). Substituting all these results in (4.71), the following families of tensor fields are obtained:

$$\begin{aligned}
\Lambda_{\mathcal{S},t} =& \left(2x_3 + \frac{2\delta}{\gamma}(e^{-\gamma t}-1)\right)\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_2} + 2e^{-\gamma t}x_1\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_3} + 2e^{-\gamma t}x_2\frac{\partial}{\partial x_3}\wedge\frac{\partial}{\partial x_1},\\
R_{\mathcal{S},t} =& 2e^{-2\gamma t}\left(\frac{\partial}{\partial x_1}\otimes\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2}\otimes\frac{\partial}{\partial x_2}\right) - \frac{2\delta x_1}{\gamma}(e^{-\gamma t}-1)\frac{\partial}{\partial x_1}\otimes_S\frac{\partial}{\partial x_3}\\
&- \frac{2\delta x_2}{\gamma}(e^{-\gamma t}-1)\frac{\partial}{\partial x_2}\otimes_S\frac{\partial}{\partial x_3} - 2\sum_{j,k=1}^{3}x_jx_k\frac{\partial}{\partial x_j}\otimes\frac{\partial}{\partial x_k}\\
&+\left[2\left(1-\frac{\delta^2}{\gamma^2}\right)e^{-2\gamma t} + 4\frac{\delta}{\gamma}\left(\frac{\delta}{\gamma}-x_3\right)e^{-\gamma t} - \frac{2\delta^2}{\gamma^2} + \frac{4\delta}{\gamma}x_3\right]\frac{\partial}{\partial x_3}\otimes\frac{\partial}{\partial x_3}.
\end{aligned} \tag{4.87}$$

In this example, asymptotic limits for these tensor fields also exist. A new contraction of the algebra of expectation functions, hence of the algebra of quantum observables, is obtained.

Theorem 4.22. *There exist asymptotic limits $\Lambda_{\mathcal{S},\infty}$ and $R_{\mathcal{S},\infty}$ for the families of tensor field given in (4.87), determined by the Markovian evolution generated by the vector field (4.48). The limits are*

$$\begin{aligned}
\Lambda_{\mathcal{S},\infty} =& 2\left(x_3-\frac{\delta}{\gamma}\right)\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_2},\\
R_{\mathcal{S},\infty} =& \frac{2\delta}{\gamma}x_1\frac{\partial}{\partial x_1}\otimes_S\frac{\partial}{\partial x_3} + \frac{2\delta}{\gamma}x_2\frac{\partial}{\partial x_2}\otimes_S\frac{\partial}{\partial x_3}\\
&+\frac{2\delta}{\gamma}\left(2x_3-\frac{\delta}{\gamma}\right)\frac{\partial}{\partial x_3}\otimes\frac{\partial}{\partial x_3} - 2\sum_{j,k=1}^{3}x_jx_k\frac{\partial}{\partial x_j}\otimes\frac{\partial}{\partial x_k}.
\end{aligned} \tag{4.88}$$

The product $\{f,g\}_\infty = \Lambda_{\mathcal{S},\infty}(\mathrm{d}f,\mathrm{d}g)$ and $(f,g)_\infty = R_{\mathcal{S},\infty}(\mathrm{d}f,\mathrm{d}g)+fg$ of smooth functions are a Poisson bracket and a symmetric product

In the particular case $\delta = 0$, the limit manifold of the evolution is, as computed before, the maximally mixed state of the system. In this case, the limit tensor fields are much simpler:

$$\Lambda_{\mathcal{S},\infty} = 2x_3\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_2},\quad R_{\mathcal{S},\infty} = -2\sum_{j,k=1}^{3}x_jx_k\frac{\partial}{\partial x_j}\otimes\frac{\partial}{\partial x_k}. \tag{4.89}$$

In this particular case, it is immediate to characterise the new Lie-Jordan algebra of expectation value functions, defined by the products

$$\{x_1,x_2\}_\infty = 2x_3,\quad \{x_1,x_3\}_\infty = \{x_2,x_3\}_\infty = 0;\qquad (x_j,x_k) = 0,\quad j,k=1,2,3. \tag{4.90}$$

the remaining products vanishing identically. Regarding the product $f *_\infty g = (f,g)_\infty + \mathrm{i}\{f,g\}_\infty$, the only non-zero products of x_j functions are

$$x_1 *_\infty x_2 = -(x_2 *_\infty x_1) = 2\mathrm{i}x_3. \tag{4.91}$$

Thus, the $*_\infty$-product is associative.

It can be concluded from (4.90) that contracted Lie algebra $(\mathcal{E}_{\mathcal{O}}(\mathcal{S}),\{\cdot,\cdot\}_\infty)$ is isomorphic to the Heisenberg algebra. As proved in [269], the only non-trivial contractions of the $\mathfrak{su}(2)$ Lie algebra are the Euclidean algebra and the Heisenberg algebra. It is thus possible to describe all the possible contractions of this algebra by means of Markovian evolution of the corresponding quantum system. Also, with our approach, the Jordan algebra is also contracted, thus obtaining all the non-trivial contractions of the Lie-Jordan algebra of observables of a 2-level quantum system.

4.3.2 Contractions for open 3-level systems

The manifold of states of a 3-level system presents a richer structure than that of 2-level systems. While the later is composed of two strata, manifolds of states of 3-level systems are decomposed in three strata, two of them composing the boundary. It is therefore of interest to consider evolution of a 3-level system. The structure of the set $\mathcal{S}$ of pure and mixed states of a 3-level system is summarised in Appendix A. A detailed description of this set can be found in the work by Goyal and coworkers [140].

Regarding contractions, consider the model of decoherence for massive particles, presented in [7, 92]:

$$L_M(\rho) = -\gamma[X,[X,\rho]], \quad \rho \in \mathcal{S}, \quad \gamma > 0. \tag{4.92}$$

where X is the position operator. This model can be discretised by considering a finite number d of positions $\vec{x}_m$ along a circle. The positions are given by

$$\vec{x}_m = (\cos\phi_m, \sin\phi_m), \quad \phi_m = \frac{2\pi m}{d}, \quad m = 1, 2, \ldots, d. \tag{4.93}$$

Let $\{|m\rangle\}_{m=1}^{d}$ denote the basis of eigenstates of the position operator. In this basis, the Kossakowski-Lindblad operator L_M takes the form

$$L_M|m\rangle\langle n| = -\gamma\,|\vec{x}_m - \vec{x}_n|\,|m\rangle\langle n| = -4\gamma\sin^2\left(\frac{\pi(m-n)}{d}\right)|m\rangle\langle n|, \tag{4.94}$$

for $m, n = 1, 2, \ldots, d$.

Taking $d = 3$, a Markovian evolution for the 3-level system is obtained. Starting from the operator defined in (4.92), it is immediate to obtain the corresponding vector field Z_L on $\mathcal{S}$ by Proposition 4.8:

$$Z_L = -3\gamma\left(x_1\frac{\partial}{\partial x_1} + x_2\frac{\partial}{\partial x_2} + x_4\frac{\partial}{\partial x_4} + x_5\frac{\partial}{\partial x_5} + x_6\frac{\partial}{\partial x_6} + x_7\frac{\partial}{\partial x_7}\right). \tag{4.95}$$

Computations similar to those carried out in the previous section are necessary in order to determine the families of tensor fields $\Lambda_{\mathcal{S},t}$ and $R_{\mathcal{S},t}$. The corresponding Lie derivatives are

$$\begin{aligned}
\mathcal{L}^n_{Z_L}\Lambda_{\mathcal{S}} =& (6\gamma)^n\left(2x_3\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_2} + (x_3+\sqrt{3}x_8)\frac{\partial}{\partial x_4}\wedge\frac{\partial}{\partial x_5} + (\sqrt{3}x_8 - x_3)\frac{\partial}{\partial x_6}\wedge\frac{\partial}{\partial x_7}\right)\\
&+ (3\gamma)^n\left(x_7\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_4} - x_6\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_5} + x_5\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_6} - x_4\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_7}\right.\\
&\quad + x_6\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_4} + x_7\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_5} - x_4\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_6} - x_5\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_7}\\
&\quad \left.+x_2\frac{\partial}{\partial x_4}\wedge\frac{\partial}{\partial x_6} + x_1\frac{\partial}{\partial x_4}\wedge\frac{\partial}{\partial x_7} - x_1\frac{\partial}{\partial x_5}\wedge\frac{\partial}{\partial x_6} + x_2\frac{\partial}{\partial x_5}\wedge\frac{\partial}{\partial x_7}\right),\\
\mathcal{L}^n_{Z_L}R_{\mathcal{S}} =& (6\gamma)^n\left(\frac{2\gamma}{3}(2+\sqrt{3}x_8)\left(\frac{\partial}{\partial x_1}\otimes\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2}\otimes\frac{\partial}{\partial x_2}\right)\right.\\
&\quad + \frac{\gamma}{3}(4+3x_3-\sqrt{3}x_8)\left(\frac{\partial}{\partial x_4}\otimes\frac{\partial}{\partial x_4} + \frac{\partial}{\partial x_5}\otimes\frac{\partial}{\partial x_5}\right)\\
&\quad \left.+\frac{\gamma}{3}(4-3x_3-\sqrt{3}x_8)\left(\frac{\partial}{\partial x_6}\otimes\frac{\partial}{\partial x_6} + \frac{\partial}{\partial x_7}\otimes\frac{\partial}{\partial x_7}\right)\right)\\
&+ (3\gamma)^n\left(x_6\frac{\partial}{\partial x_1}\otimes_S\frac{\partial}{\partial x_4} + x_7\frac{\partial}{\partial x_1}\otimes_S\frac{\partial}{\partial x_5} + x_4\frac{\partial}{\partial x_1}\otimes_S\frac{\partial}{\partial x_6} + x_5\frac{\partial}{\partial x_1}\otimes_S\frac{\partial}{\partial x_7}\right.\\
&\quad - x_7\frac{\partial}{\partial x_2}\otimes_S\frac{\partial}{\partial x_4} + x_6\frac{\partial}{\partial x_2}\otimes_S\frac{\partial}{\partial x_5} + x_5\frac{\partial}{\partial x_2}\otimes_S\frac{\partial}{\partial x_6} - x_4\frac{\partial}{\partial x_2}\otimes_S\frac{\partial}{\partial x_7}\\
&\quad \left.+x_1\frac{\partial}{\partial x_4}\otimes_S\frac{\partial}{\partial x_6} - x_2\frac{\partial}{\partial x_4}\otimes_S\frac{\partial}{\partial x_7} + x_2\frac{\partial}{\partial x_5}\otimes_S\frac{\partial}{\partial x_6} + x_1\frac{\partial}{\partial x_5}\otimes_S\frac{\partial}{\partial x_7}\right).
\end{aligned} \tag{4.96}$$

Even for a simple vector field as the one presented in (4.95), expressions become much complex when the dimension of the quantum system increases. For this reason, the use of mathematical software is necessary in order to study quantum systems with 3 or more energy levels. For this particular case, given these expressions, it is possible to deduce from (4.71) that the families of tensor fields $\Lambda_{\mathcal{S},t}$ and $R_{\mathcal{S},t}$ have an asymptotic limit when t goes to infinity.

Theorem 4.23. *The limit tensor fields $\Lambda_{\mathcal{S},\infty}$ and $R_{\mathcal{S},\infty}$ of the families induced by vector field (4.95) exists, being their coordinate expressions*

$$\begin{aligned}\Lambda_{\mathcal{S},\infty} =& \frac{1}{2}\sum_{j,k,l=1}^{8} c^{\infty}_{jkl} x_l \frac{\partial}{\partial x_j}\wedge\frac{\partial}{\partial x_k},\\ R_{\mathcal{S},\infty} =& \sum_{j,k=1}^{8}\left(d^{\infty}_{jk0}+\sum_{l=1}^{8} d^{\infty}_{jkl}x_l\right)\frac{\partial}{\partial x_j}\otimes\frac{\partial}{\partial x_k} - 2\sum_{j,k=1}^{8} x_j x_k \frac{\partial}{\partial x_j}\otimes\frac{\partial}{\partial x_k},\end{aligned} \tag{4.97}$$

where the new constants c^{∞}_{jkl} and d^{∞}_{jkl} are respectively antisymmetric and symmetric on the first two indexes. Their non-zero values are

$$\begin{gathered} c^{\infty}_{312}=c^{\infty}_{231}=2,\quad c^{\infty}_{345}=c^{\infty}_{534}=c^{\infty}_{376}=c^{\infty}_{637}=1,\quad c^{\infty}_{845}=c^{\infty}_{584}=c^{\infty}_{867}=c^{\infty}_{786}=\sqrt{3},\\ d^{\infty}_{000}=2.,\quad d^{\infty}_{330}=d^{\infty}_{880}=\frac{4}{3},\\ d^{\infty}_{181}=d^{\infty}_{282}=d^{\infty}_{383}=d^{\infty}_{338}=\frac{2}{\sqrt{3}},\quad d^{\infty}_{344}=d^{\infty}_{355}=1,\quad d^{\infty}_{366}=d^{\infty}_{377}=-1,\\ d^{\infty}_{484}=d^{\infty}_{585}=d^{\infty}_{686}=d^{\infty}_{787}=-\frac{1}{\sqrt{3}},\quad d^{\infty}_{888}=-\frac{2}{\sqrt{3}}.\end{gathered} \tag{4.98}$$

and their respective permutations.

These new structure constants define a contraction of the Lie-Jordan algebra of observables, presented in Appendix A. Observe that there exist differences between both algebras. For example, the new structure constants are no longer totally symmetric or antisymmetric. The identification of this new algebra is not obvious, and its properties are yet to be studied.

4.4 Analysis on the limit of Markovian evolution

In the analysis of Markovian evolutions presented in Sections 4.1 and 4.3, several common features have been presented. In the examples, the limit of the evolution is described by a subset of $\mathcal{S}$, which coincides with the set of fixed points of the dynamics. The general case is similar, although a bit more complex, as the flows of many vector fields, in particular Hamiltonian ones, do not have a well-defined limit. This problem is solved with the concept of limit manifolds.

Definition 4.24. *Consider an evolution on a differentiable manifold M described by a family of diffeomorphisms $\{\Phi_t : M\to M, t\in\mathbb{R}\}$. If it exists, the subset*

$$M_L := \lim_{t\to\infty}\Phi_t(M) \tag{4.99}$$

is called the limit set of the evolution. If, in addition, M_L is a submanifold of M, then it is called the limit manifold of the evolution.

The main reference for the description of limit manifold is the book by Hirsch, Pugh and Schub [155]. Observe that, with this definition, periodic evolutions are easily dealt with. The analysis of limit manifold is an interesting topic, with many applications in the study of open quantum systems and, in general physical problems. The affine structure of the set $\mathcal{S}$ of pure and mixed states of a quantum systems

allows for the description of affine and projective vector fields on $\mathcal{S}$ [104, 147, 193, 228, 277], with direct application to the characterisation of Markovian evolution [168].

For the purpose of this dissertation, however, a much simpler description can be offered. The set $\mathcal{S}$ is a convex subset of the linear space $\mathcal{O}^*$. It is a simple matter to combine this linear structure with the Kossakowski-Lindblad equation (4.17), in order to obtain a characerisation of the limits of the Markovian evolution of open quantum systems. This section presents an analysis of these limits, followed by a discussion on their impact on the behaviour of tensor fields, in particular $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$, when subject to Markovian evolution.

4.4.1 Limit manifolds for Markovian evolution

Let V be a real linear space. Consider the differential equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = Ax, \tag{4.100}$$

with $A \in GL(V)$. For the initial condition $x(0) = x_0 \in V$, the solution of this equation is

$$x(t) = e^{tA}x_0, \quad t \in \mathbb{R}. \tag{4.101}$$

Stability and unstability of this solution can be easily considered. In fact, this equation is usually the first example studied in the analysis of dynamical systems. The analysis of the spectrum of A is enough in order to determine the properties of asymptotic limits.

Theorem 4.25. *Consider the map $\Phi_t^A : V \to V$, with $t \in \mathbb{R}$. defined by (4.101):*

$$\Phi_t^A(x) = e^{tA}x, \tag{4.102}$$

The asymptotic limit

$$V_L = \lim_{t\to\infty} \Phi_t^A(V) \tag{4.103}$$

exists if and only if A has no eigenvalue with positive real part. In this case, V_L is a linear subspace of V.

Proof. As mentioned, differential equation (4.100) is a simple case of a dynamical system. As such, the theory of Lyapunov exponents gives the solution to the stability problem. For simplicity, consider an eigenvalue λ of A such that $\mathrm{Re}\,\lambda > 0$, and an eigenvector $v_\lambda \in V$ such that $Av_\lambda = \lambda v_\lambda$. Then,

$$\Phi_t^A(v_\lambda) = e^{t\lambda}v_\lambda \Rightarrow \nexists \lim_{t\to\infty} \Phi_t^A(v_\lambda).$$

Identical behaviours are obtained for generalised eigenvectors of A with eigenvalue λ. Thus, non-positivity of real parts of eigenvectors is a necessary condition for the existence of the limit V_L. If $\mathrm{Re}\,\lambda < 0$, the limit of $\Phi_t^A(v_\lambda)$ is the origin $0 \in V$, while purely complex eigenvectors define oeriodic trajectories. For both cases, the limit of $\Phi_t^A(V)$ does exist, thus proving the theorem. For a full characterisation of dynamical systems and Lyapunov exponents, see [90, 253, 273] and references therein.

Assuming that this conditions are satisfied, it is immediate to determine that V_L is in fact a subspace of V. Consider the generalised eigenspaces E_λ of A associated to a purely complex eigenvalue λ (including zero). As all their elements belong to periodic integral curves of (4.100), they are necessarily in V_L. On the other hand, if $\mathrm{Re}\,\lambda < 0$, then there is no element in $v \in V - \{0\}$ such that the asymptotic limit of $\Phi_t^A(v)$ belongs to E_λ, as can be checked by inverting the sign of t in (4.101). As a consequence, the limit set V_L is spanned by the generalised eigenspaces E_λ with purely complex eigenvalues, hence it is a subspace of V. □

This result has a direct application to the study of Markovian dynamics of quantum systems. Observe that the Kossawkoski-Lindblad equation (4.17) is determined by a linear operator $L : \mathcal{O}^* \to \mathcal{O}^*$. Theorem 4.25 characterises the properties of the solutions to the Kossakowski-Lindlbad equation on $\mathcal{O}^*$. They can be then projected onto $\mathcal{S}$ by the map described in Figure 3.2. Then, the following result is obtained.

Theorem 4.26. *Consider the Kossakowski-Lindblad vector field $Z_L \in \mathfrak{X}(\mathcal{S})$ determined by the linear operator $L : \mathcal{O}^* \to \mathcal{O}^*$ given in (4.18), and let $\Phi_t^Z : \mathcal{S} \to \mathcal{S}$ be its flow. The limit set S_L, defined as*

$$\mathcal{S}_L := \lim_{t\to\infty}(\Phi_t^Z(\mathcal{S})), \tag{4.104}$$

does exist. It is a convex subset of $\mathcal{S}$. Furthermore, there exists an affine subspace $\widehat{S}_L \subset \widehat{S}$ such that $\mathcal{S}_L = \widehat{S}_L \cup \mathcal{S}$.

Proof. The existence of the limit set $\mathcal{S}_L$ is obvious, as $\mathcal{S}$ is a compact manifold. As seen in Theorem 4.25, limit sets always exist as long as vectors are not mapped into the infinity. However, such thing is not possible in $\mathcal{S}$, hence $\Phi_t^Z(\mathcal{S})$ has an asymptotic limit. Its characterisation is a direct consequence of Theorem 4.25. The linear map $L : \mathcal{O}^* \to \mathcal{O}^*$ defines a limit subspace $(\mathcal{O}^*)_L$ of the dynamics, which has to be projected onto $\mathcal{S}$. However, from $L(I) = 0$, it is clear that the result of this projection is $\mathcal{S}_L = \mathcal{S} \cup (\mathcal{O}^*)_L$, which is clearly convex. The last property comes from the fact that $\widehat{S}$ is an affine subspace of $\mathcal{O}^*$, hence $\widehat{S}_L = \widehat{\mathcal{S}} \cup (\mathcal{O}^*)_L$ is an affine subspace of $\widehat{S}$. □

Important consequences can be extracted from this result. For any Markovian evolution $\Phi_t^Z : \mathcal{S} \to \mathcal{S}$, the limit manifold $\mathcal{S}_L$ is a manifold with boundary in $\widehat{\mathcal{S}}$. It is thus possible to carry out differential calculus in the limit manifold, with the usual limitiations of the boundary. This boundary already has played a role in the existence of the limit of Markovian evolution. The study of limit manifolds in affine spaces may offers useful results in the analysis of the dynamics of open quantum systems.

4.4.2 Contractions of tensor fields

Once the limit manifolds of Markovian evolution have been determined, some interesting results can be obtained concerning the behaviour of contravariant tensor fields. These results are particularly interesting in the analysis of the contractions of algebras of observables in the study of open quantum systems, presented in Section 4.3. For this reason, the following results are concieved for vector fields determining Markovian-like evolutions.

In the following, consider a vector field $Z \in \mathfrak{X}(\widehat{\mathcal{S}})$ on the differentiable manifold $\widehat{S}$. Let $\Phi_t^Z : \widehat{\mathcal{S}} \to \widehat{\mathcal{S}}$, with $t \in \mathbb{R}$, denote its flow, and assume that, as in the case of Markovian evolution, there exists a limit manifold

$$\widehat{S}_L := \lim_{t\to\infty}(\Phi_t^Z(\widehat{S})). \tag{4.105}$$

For simplicity, assume that this manifold coincides with the set of fixed point of the dynamics. Because of Theorem (4.25), this is equivalent to the assumption that the Lyapunov exponents of the evolution either are zero, or have negative real part. From a physical perspective, this evolution can always be obtained by adding a controlled unitary evolution to the system, typically by a laser acting on the system.

As mentioned, it is interesting to characterise the behaviour of contravariant tensor fields with respect to the flow of Z. Any r-contravariant tensor field T defines a family of tensor fields on $\widehat{\mathcal{S}}$ by

$$T_t := \Phi_{t*}^X(T), \quad t \geq 0. \tag{4.106}$$

When the limit of the family exists,

$$T_\infty := \lim_{t\to\infty} T_t, \tag{4.107}$$

it is called the contraction of T. The aim of this section is to obtain some sufficient conditions that ensure the existence of this contraction. With the assumed properties for Z, the following results can be obtained.

Proposition 4.27. *If T_∞ exists, then the vector field Z is a Lie symmetry of T_∞, i.e. $\mathcal{L}_Z T_\infty = 0$.*

Proof. As the flow Φ_t^Z is a diffeomorphism for every $t \in \mathbb{R}$ and T_∞ is assumed to exist, it follows that:

$$\Phi_{s*}^Z T_\infty = \Phi_{s*}^Z \left(\lim_{t\to\infty} \Phi_{t*}^Z T \right) = \lim_{t\to\infty} \Phi_{t+s*}^Z T = T_\infty, \qquad \forall s \in \mathbb{R}.$$

Substituting the above in the definition of the Lie derivative $\mathcal{L}_Z T_\infty$, it can be concluded that Z is a symmetry of T_∞. □

Proposition 4.28. *The value of T_∞ on $\mathcal{S}_L$ is determined by its value on any open set $U \supset \mathcal{S}_L$.*

Proof. Since Φ_{t*}^Z is invertible for each $t \in \mathbb{R}$, it follows that

$$\Phi_{-t*}^Z(T_\infty)(\alpha_1,\dots,\alpha_r)(x) = T_\infty(\Phi_{-t}^{Z*}(\alpha_1),\dots,\Phi_{-t}^{Z*}(\alpha_r))(\Phi_t^Z(x)), \quad \forall \alpha_1,\dots,\alpha_r \in \textstyle\bigwedge^1(\widehat{\mathcal{S}}), \quad \forall x \in \widehat{\mathcal{S}}.$$

Proposition 4.27 establishes that $\Phi_{t*}^Z(T_\infty) = T_\infty$ for any $t \in \mathbb{R}$. Thus, this expression can be rewritten as

$$T_\infty(\alpha_1,\dots,\alpha_r)(x) = T_\infty(\Phi_{-t}^{Z*}(\alpha_1),\dots,\Phi_{-t}^{Z*}(\alpha_r))(\Phi_t^Z(x)), \quad \forall \alpha_1,\dots,\alpha_r \in \textstyle\bigwedge^1(\widehat{\mathcal{S}}), \quad \forall x \in \widehat{\mathcal{S}}. \tag{4.108}$$

By assumption, there exists a limit manifold $\mathcal{S}_L$. As a consequence, there always exists a value τ_x such that, for any $t > \tau_x$, the evolution $\Phi_t^Z(x)$ is arbitrarily close to $\widehat{\mathcal{S}}_L$, e.g. $\Phi_t^Z(x) \in U$. In view of this and (4.108), the value of T_∞ at $x \notin \widehat{\mathcal{S}}_L$ is completely determined by its value at $\Phi_t^Z(x) \subset U$. Hence, T_∞ on the whole $\widehat{\mathcal{S}}$ is determined by its value on U. □

Theorem 4.29. *The family of tensors at $x_L \in \widehat{\mathcal{S}}_L$ given by $\{(T_t)_{x_L},\, t \geq 0\}$, has a well defined asymptotic limit $t \to \infty$, which coincides with $(T_\infty)_{x_L}$ when the asymptotic tensor field T_∞ does exist.*

Proof. For every $t \geq 0$ the tensor $(T_t)_{x_L}$ is defined by its action on covector fields at x_L. By hypothesis, any $x_L \in \widehat{\mathcal{S}}_L$ is a fixed point of the diffeomorphisms Φ_t^Z. Hence, for any $\alpha_1,\dots,\alpha_r \in T_{x_L}^*\widehat{\mathcal{S}}$,

$$(T_t)_{x_L}(\alpha_1,\dots,\alpha_r) = T_{x_L}((\Phi_t^{Z*})_{x_L}(\alpha_1),\dots,(\Phi_t^{Z*})_{x_L}(\alpha_r)).$$

The pull-back $(\Phi_t^{Z*})_{x_L}$ has an asymptotic limit when $t \to \infty$, which proves the existence of the limit of the family of tensors $\{(T_t)_{x_L},\, t \geq 0\}$. □

Proposition 4.28 and Theorem 4.29 present an interesting idea. When restricted to the limit manifold, the contraction of a contravarian tensor field always exists. Observe that this is precisely the case of the second example presented in Section 4.3.2. On the other hand, if the contraction exists on points arbitrarily close to the limit manifold, then by Proposition 4.28 it exists on the whole manifold. These facts how the path to follow. As presented schematically in Figure 4.6, it is necessary to investigate the behaviour of the tensor field in directions which are not tangent to the limit manifold. Thus, the relevant objects in this analysis are the Lie derivatives of the tensor field with respect to vector fields that are not tangent to $\widehat{\mathcal{S}}_L$. These objects are characterised in the following results.

Theorem 4.30. *Consider a set $\mathfrak{W} \subset \mathfrak{X}(\widehat{\mathcal{S}})$ generating the tangent space to $\mathcal{S}$ at every $x \in \widehat{\mathcal{S}}_L$, i.e.*

$$\operatorname{span}\{W_x \mid W \in \mathfrak{W}\} = T_x\widehat{\mathcal{S}}, \quad \forall x \in \widehat{\mathcal{S}}_L. \tag{4.109}$$

Given a contravariant tensor field T on $\widehat{\mathcal{S}}$, for every $x \in \widehat{\mathcal{S}}_L$ and every $W \in \mathfrak{W}$ consider the families $\{(\mathcal{L}_W T_t)_x \mid t \in \mathbb{R}\}$ of tensors at x. Then, the contraction T_∞ of the contravariant tensor field T exists if and only if there exist asymptotic limits to all these families when $t \to \infty$.

Proof. Consider the integral curves $\gamma_W(x_0,\tau)$ of every $W \in \mathfrak{W}$, with $\gamma_W(x_0,0) = x_0 \in \widehat{S}_L$. Because of condition (4.109), for every $\epsilon > 0$ the set

$$U_\epsilon = \{\gamma_W(x_0,\delta) | x_0 \in \widehat{\mathcal{S}}_L, -\epsilon < \delta < \epsilon\} \tag{4.110}$$

is an open set in $\widehat{S}$ containing $\widehat{\mathcal{S}}_L$. For arbitrarily small values of ϵ, it is possible to determine the value of any tensor on U_ϵ simply by its value on S_L and its Lie derivatives with respect to tensor fields $W \in \mathfrak{W}$. In particular, this gives the value of T_t on U_ϵ, hence on $\widehat{\mathcal{S}}$ by Proposition 4.28. By continuity, if the families of Lie derivatives have an asymtotic limit, then the family $\{T_t\}$ has an asymptotic limit T_∞. □

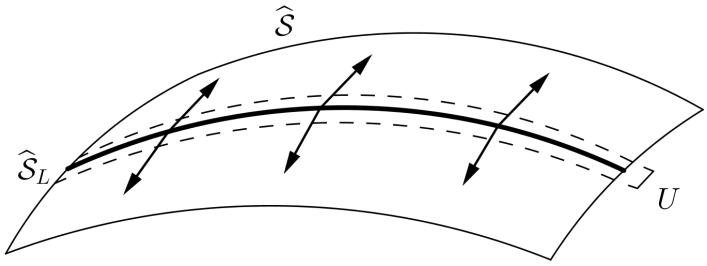


Figure 4.6: Consider a Markovian evolution in $\widehat{\mathcal{S}}$ whose limit manifold is $\widehat{\mathcal{S}}_L$. Because of Theorem 4.29, the asymptotic limit of any family of contravariant tensor field T_t, as defined in (4.107), exists when restricted to $\widehat{\mathcal{S}}_L$. Also, Proposition 4.28 shows that the value of T_t on $\widehat{\mathcal{S}}$ is determined by its value on an open set U containing $\widehat{\mathcal{S}}_L$. Therefore, the analysis of the global existence of T_∞ is done by considering the directions going out of $\widehat{\mathcal{S}}_L$, as in Theorem 4.30.

The result of this theorem allows to check the existence of the asymptotic tensor field by computing the evolution of the tensor fields $\mathcal{L}T_t$. In particular examples, these tensor fields have simple expressions. The computations are easier if the set $\mathfrak{W}$ is wisely chosen.

Lemma 4.31. *Let W be a vector field such that $[Z, W] = \lambda W$, for some $\lambda \in \mathbb{R}$. The following relation holds:*

$$\mathcal{L}_W T_t = e^{\lambda t} \Phi^Z_{t*}(\mathcal{L}_W T). \tag{4.111}$$

Proof. With the hypothesis $[Z, W] = \lambda W$, the Lie derivative with respect to W and Z satisfy the relation $\mathcal{L}_W \mathcal{L}_Z = (\mathcal{L}_Z - \lambda)\mathcal{L}_W$. By integrating this expression, the relation between $\mathcal{L}_W$ and the flow of Z is

$$\mathcal{L}_W \circ \Phi^Z_{t*} = e^{-t(L_Z - \lambda)} \circ \mathcal{L}_W = e^{\lambda t} \Phi^Z_{t*} \circ \mathcal{L}_W.$$

When applied to the tensor field T, the result follows. □

In general, it is possible to compute $\Phi^Z_{t*}(\mathcal{L}_W T)$ by knowing the values of $\mathcal{L}_W T$ and $\mathcal{L}_Z \mathcal{L}_W T$, which can have relatively simple expressions. This gives the value of $\mathcal{L}_W T_t$, and it is easy to compute the existence of the asymptotic limit when $t \to \infty$.

Theorem 4.32. *Given a contravariant field T and a symmetry W of Z, then a necessary condition for the existence of its contraction T_∞ is that the limit of $\Phi_{t*}(\mathcal{L}_W T)$ exists. If such contraction T_∞ exists, then*

$$\lim_{t\to\infty} \Phi_{t*}(\mathcal{L}_W T) = \mathcal{L}_W T_\infty. \tag{4.112}$$

Proof. Let W be a Lie symmetry of Z, i.e. $[W, Z] = 0$. Then, $[\mathcal{L}_W, \mathcal{L}_Z] = \mathcal{L}_{[W,Z]} = 0$, which implies that $\mathcal{L}_W T_t = \Phi_{t*}(\mathcal{L}_W T)$. If the contraction T_∞ exists, then, because of the linearity of the Lie derivative, $\mathcal{L}_W T_\infty$ is the limit of the family of tensors $\{\mathcal{L}_W T_t\}$. Hence the family $\{\Phi_{t*}(\mathcal{L}_W T)\}$ has a well-defined limit. □

Theorem 4.33. *Let f be a function such that $\mathrm{d}(Zf) = 0$. Given a bivector field T, let us denote its contraction with f as $\tau_f = \iota(df)T$. A necessary condition for the existence of the limit T_∞ is the convergence of the family of vector fields $\{\tau_{t,f}\}$ given by*

$$\tau_{t,f} = \iota(\mathrm{d}f) T_t = \Phi_{t*}(\tau_f). \tag{4.113}$$

If the limit T_∞ exists, then

$$\lim_{t\to\infty} \tau_{t,f} = \iota(\mathrm{d}f) T_\infty. \tag{4.114}$$

Proof. For any bivector field T, the definition of Lie derivative gives

$$(\mathcal{L}_Z T)(\mathrm{d}f, \mathrm{d}g) = \mathcal{L}_Z(\iota(\mathrm{d}f)T)(\mathrm{d}g) - T(\mathrm{d}Z(f), g).$$

If f satisfies $\mathrm{d}(Zf) = 0$, then $\iota(\mathrm{d}f)\mathcal{L}_Z T = \mathcal{L}_Z(\iota(\mathrm{d}f)T)$. Therefore, the evolution by the flow of Z gives

$$\tau_{t,f} := \iota(\mathrm{d}f)\Phi_{t*}(T_t) = \Phi_{t*}(\iota(\mathrm{d}f)T) = \Phi_{t*}(Z_f).$$

If the limit T_∞ exists, then this family has a limit given by $\tau_{\infty,f} = \iota(\mathrm{d}f)T_\infty$. □

Theorem 4.34. *Let $f, g \in \mathcal{F}(M)$ be such that $\mathrm{d}(Zf) = \mathrm{d}(Zg) = 0$. The existence of T_∞ requires the existence of the asymptotic limit of the family of functions $\{\Phi^*_{-t}(T(\mathrm{d}f, \mathrm{d}g)),\ t \geq 0\}$ when $t \to \infty$.*

Proof. If a function f satisfy the hypothesis $\mathrm{d}(Zf) = 0$, then $\mathrm{d}f$ is constant along the integral curves of Z. For such function f, g,

$$T_t(\mathrm{d}f, \mathrm{d}g)(x) = T(\mathrm{d}f, \mathrm{d}g)(\Phi_{Z,-t}(x)) = \Phi^*_{Z,-t}\big(T(\mathrm{d}f, \mathrm{d}g)\big)(x).$$

The limit of T_t can therefore be studied by considering the family of functions $\{\Phi^*_{Z,-t}\big(T(\mathrm{d}f, \mathrm{d}g)\big),\ t \geq 0\}$. □

These results offer several useful tools for the geometric analysis of contractions. The main result of this section is Theorem 4.29, as it proves that, when restricted to the limit manifold, there always exists the contraction of any contravariant tensor field. From a physical perspective, this result has a huge impact. It proves that, when dealing with non-unitary evolutions, quantum observables preserve their properties in the limit of the evolution. That is, if a quantum system evolves into a subset of the manifold of states $\mathcal{S}$, then the observables of the system, restricted to this limit subset, still conform an algebra. This will no longer be, as shown in the example, the same algebra as the one for the initial state. The characterisation of these contracted algebras, restricted to limit manifolds, is an interesting topic that could help to describe the properties of open quantum systems.

4.4.3 Application to the phase damping of a 2-level system

In order to finish this approach to the field of geometric contractions and limit manifold, the phase damping of a 2-level system is revisited, with the purpose of illustrating the above results. As shown in Section 4.1.4, the phase damping is determined by the vector field given by (4.37):

$$Z_L = -2\gamma\left(x_1\frac{\partial}{\partial x_1} + x_2\frac{\partial}{\partial x_2}\right). \tag{4.115}$$

As before, consider the Bloch ball for the 2-level system. The limit manifold S_L for Z_L is precisely the set of fixed points, as computed in (4.40) and represented again in Figure 4.7:

$$\mathcal{S}_L = \{(0, 0, x_3) \mid x_3 \in [-1, 1]\}. \tag{4.116}$$

It is possible to apply the theorems presented along this section in order to study the evolution of the contravariant tensor fields $\Lambda_\mathcal{S}$ and $R_\mathcal{S}$. As proved in Proposition 3.59, their coordinate expressions are the following:

$$\Lambda_\mathcal{S} = \sum_{j,k,l=1}^{3} \epsilon_{jkl}\, x_l \frac{\partial}{\partial x_j} \wedge \frac{\partial}{\partial x_k}, \qquad R_\mathcal{S} = 2\sum_{j=1}^{3} \frac{\partial}{\partial x_j} \otimes \frac{\partial}{\partial x_j} - 2\sum_{j,k=1}^{3} x_j x_k \frac{\partial}{\partial x_j} \otimes \frac{\partial}{\partial x_k}. \tag{4.117}$$

Consider the restrictions to $\mathcal{S}_L$ of the contravariant tensor fields $\Lambda_\mathcal{S}$ and $R_\mathcal{S}$:

$$\Lambda_\mathcal{S}|_{\mathcal{S}_L} = 2x_3 \frac{\partial}{\partial x_1} \wedge \frac{\partial}{\partial x_2}, \quad R_\mathcal{S}|_{\mathcal{S}_L} = 2\frac{\partial}{\partial x_1} \otimes \frac{\partial}{\partial x_1} + 2\frac{\partial}{\partial x_2} \otimes \frac{\partial}{\partial x_2} + 2(1 - x_3^2)\frac{\partial}{\partial x_3} \otimes \frac{\partial}{\partial x_3}. \tag{4.118}$$

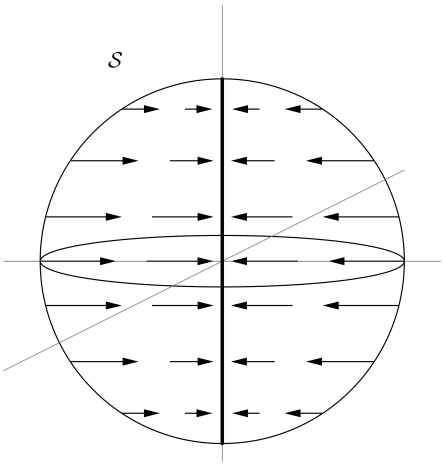


Figure 4.7: Vector field and limit manifold for the phase damping of a 2-level quantum system.

By Theorem 4.29, both $\Lambda_{\mathcal{S},t}$ and $R_{\mathcal{S},t}$ have well-defined limits when evaluated on $\mathcal{S}_L$, Their contractions with 1-forms generate vector fields tangent to $\mathcal{S}_L$. Therefore, as a direct computation shows, the asymptotic tensor fields on $\mathcal{S}_L$ are

$$\Lambda_{\mathcal{S},\infty}|_{\mathcal{S}_L} = 0, \quad R_{\mathcal{S},\infty}|_{\mathcal{S}_L} = 2(1-x_3^2)\frac{\partial}{\partial x_3}\otimes\frac{\partial}{\partial x_3}. \tag{4.119}$$

It can be easily proved by Theorem 4.30 that the asymptotic tensor fields $\Lambda_{\mathcal{S},\infty}$ and $R_{\mathcal{S},\infty}$ exist on all the manifold $\mathcal{S}$. Consider the following family $\mathfrak{W} = \{W_1, W_2, W_3\}$ of vector fields:

$$W_1 = \frac{\partial}{\partial x_1}, \quad W_2 = \frac{\partial}{\partial x_2}, \quad W_3 = \frac{\partial}{\partial x_3}. \tag{4.120}$$

These vector fields generate the tangent space to the manifold at every point. They satisfy the following commutation relations with the Kossakowski-Lindblad vector field:

$$[Z, W_1] = \gamma W_1, \quad [Z, W_2] = \gamma W_2, \quad [Z, W_3] = 0. \tag{4.121}$$

Therefore, these vector fields satisfy the condition of Proposition 4.31. As a result, computations required in Theorem 4.30 are much simpler. For example,

$$\mathcal{L}_{W_1}\Lambda_{\mathcal{S}} = 2\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_3}, \quad \mathcal{L}_Z\mathcal{L}_{W_1}\Lambda_{\mathcal{S}} = 2\gamma\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_3} \Rightarrow \Phi^Z_{t*}(\mathcal{L}_{W_1}\Lambda_{\mathcal{S}}) = 2e^{-\gamma t}\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_3}.$$

Similar computation can be done for the remaining vector fields, and also for their actions on the tensor field $R_{\mathcal{S}}$. Substituting the results in equation (4.111) and taking into account the eigenvalues found in (4.121), the following is obtained:

$$\mathcal{L}_{W_1}(\Lambda_{\mathcal{S},t}) = 2\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_3}, \quad \mathcal{L}_{W_2}(\Lambda_{\mathcal{S},t}) = 2\frac{\partial}{\partial x_3}\wedge\frac{\partial}{\partial x_1}, \quad \mathcal{L}_{W_3}(\Lambda_{\mathcal{S},t}) = 2e^{-2\gamma t}\frac{\partial}{\partial x_1}\wedge\frac{\partial}{\partial x_2}, \tag{4.122}$$

$$\mathcal{L}_{W_1}(R_{\mathcal{S},t}) = -2\frac{\partial}{\partial x_1}\otimes_S\Delta, \quad \mathcal{L}_{W_2}(R_{\mathcal{S},t}) = -2\frac{\partial}{\partial x_2}\otimes_S\Delta, \quad \mathcal{L}_{W_3}(R_{\mathcal{S},t}) = -2\frac{\partial}{\partial x_3}\otimes_S\Delta. \tag{4.123}$$

All of these families of tensor fields have an asymptotic limit when $t\to\infty$. Therefore, the asymptotic tensor fields $\Lambda_{\mathcal{S},\infty}, R_{\mathcal{S},\infty}$ do exist. Their values can be obtained by integrating the limits of (4.122) and (4.123) along the integral lines of W_1, W_2, W_3, with initial conditions (4.119). The result is

$$\Lambda_{\mathcal{S},\infty} = 2x_1\frac{\partial}{\partial x_2}\wedge\frac{\partial}{\partial x_3} + 2x_2\frac{\partial}{\partial x_3}\wedge\frac{\partial}{\partial x_1}, \quad R_{\mathcal{S},\infty} = 2\frac{\partial}{\partial x_3}\otimes\frac{\partial}{\partial x_3} - 2\Delta\otimes\Delta, \tag{4.124}$$

which coincide with the results presented in Theorem 4.21. The advantage of the procedure presented here is clear. The evolution of tensor fields is decomposed along different directions on the manifold. Along each particular direction, tensor fields can be easily studied. It is thus possible to compute the contraction, if it exists, of a contravariant tensor field. And if this contraction is not possible, the procedure presented here offers information on the problematic directions and the nature of the divergence.

4.5 Geometric control of Markovian evolution

The description of open quantum systems leads in a natural way to consider its controllability properties. Experimentally, control of quantum systems is carried out by means of external fields such as lasers, mathematically represented by unitary evolutions. The control of quantum systems has a broad set of applications, and in particular has a great importance in relation with quantum information theory. Controllability of the Kossakowski-Lindblad equation has been addressed in several works [17, 18, 20, 21]. This section presents the fundamentals of this approach and its application to the study of controllabioity of open quantu systems.

4.5.1 Basic concepts of geometric control theory

A control system is a dynamical system whose dynamical laws depend on arbitrary parameters, called controls

$$X(u) = X_0 + \sum_{k=1}^{q} u_k X_k, \quad X_0, X_1, \dots, X_q \in \mathfrak{X}(M), \quad u = (u_1, \dots u_q) \in U \subset \mathbb{R}^q. \tag{4.125}$$

The set U is called the set of admissible controls. The controls of the system are usually given by a time-dependent function $u : I \subset \mathbb{R} \to U$, which can be determined according to different strategies. This control function is responsible of the changes in the behaviour of the system.

Control theory is a large subject with many applications in physical and engineering problems. It is also a very interesting topic in the study of differential geometry. In particular, the present section focuses on the application of control theory to Lie groups, and its relevance in the analysis of open quantum systems. Deeper descriptions of control of Lie groups can be found in the book by Jurdjevic [170] and in the review by Sachkov [229]. In particular, affine systems have also been studied in geometric terms [171].

The geometric description of a control system is based on the following approach. The states space of the system is considered to be a differentiable manifold M. The action of controls on the system is easily represented in a geometric setting by means of vector fields. For simplicity, assume that the controlled vector field $X(u)$ is complete and smooth. Given a control function $u(t)$, the solution for the control problem with initial condition $x_0 \in M$ is a trajectory $x(t)$ on M satisfying the following differential equation:

$$\frac{\mathrm{d}}{\mathrm{d}t} x(t) = X(u(t))_{x(t)}, \quad x(0) = x_0. \tag{4.126}$$

In order to obtain the optimal control function, requirements are usually established on this trajectory. For example, a control problem may ask for a trajectory that transfers the state of the system between two prescribed states. Instead, it may be required that the trajectory is close enough to some fixed states, while a certain function is minimised, such as the length of the trajectory or the time of transition.

Some additional concepts are required in order to solve control problems. The concept of reachable set determines which transitions are allowed in a control problem [170].

Definition 4.35. *The reachable set $\mathcal{R}(x,t)$ of a point $x \in M$ at a time $t > 0$ is the set of points $x_R \in M$ such that, for some control function $u(t)$, the integral curve of $X(u(t))$ starting at x reaches the point x_R at time t. The reachable set of x is*

$$\mathcal{R}(x) = \bigcup_{t>0} \mathcal{R}(x,t). \tag{4.127}$$

Definition 4.36. *Consider a control system on a manifold M.*

1. *The system is controllable if $\mathcal{R}(x) = M$ for any $x \in M$.*
2. *The system is small-time controllable if any $x \in M$ belongs to the interior of its reachable sets, $x \in \operatorname{int} \mathcal{R}(x,t)$ for any $t > 0$.*
3. *The system is accessible if $\mathcal{R}(x, \leq t)$ contains non-empty open sets of M for any $t > 0$.*

Small-time controllability is equivalent to reversibility of controlled dynamics. It is important to notice that it is a sufficient, although not necessary, condition for controllability [170]. Also, in relation to the application to open quantum systems, recall that the set of states of the system is compact, which implies that limit points of the dynamics are not reached in finite time. Also, as it will be seen, it is not always possible to reach points in the boundary with finite controls; however in most cases, if the controls are not bounded, the system can evolve to a state arbitrarily close to the boundary. Summing all, the following definition will be useful in the description of controlled open quantum systems.

Definition 4.37. *A control system is called almost controllable if the closure of $R(x)$ is $\operatorname{cl} \mathcal{R}(x) = M$ for any $x \in M$.*

The geometric analysis of control problems allows for a deep understanding of the behaviour of the systems. Accessibility is the key for the description of the direction in which the system may be controlled. Even if the evolution is not invertible, it may be possible to analyse closed trajectories that allow for controllability of the system. This is the case of most controllable open quantum systems. The following theorem makes possible a geometric description of accessibility.

Theorem 4.38. [170] *A control system determined by a vector field $X(u)$ as in (4.125) is accessible if and only if $\operatorname{Lie}(X_0, X_1, \ldots, X_q)$ generates the tangent space to M at each point of the manifold.*

There are many other interesting properties of control systems that are easily described in geometric terms. In the following, these properties will be applied to the study of controlled Markovian evolution of quantum systems. The results prove that the geometric formalism of Quantum Mechanics has a broad range of applications to the study of many different problems.

4.5.2 Control of open quantum systems

The application of control theory to Quantum Mechanics has been an interesting topic of study for decades. As the ability to manipulate matter and light at microscopic scales increases, the relevance of these problems has been growing. Many works have been devoted to the analysis of these systems [17–21, 58, 60, 85, 96, 175].

The control of open quantum systems is an important topic in many fields. In particular, it has a great relevance in the realm of quantum computing. The set of vector fields which are necessary to make the system controllable correspond to a set of universal quantum gates, as they can implement any quantum algorythm on the given system. Geometric control theory has great potential in the analysis of controlled quantum systems. It is possible to combine this theory with the geometric formalism presented in this dissertation in order to characterise control problems in Quantum Mechanics. The control of pure states of quantum systems can be described by means of the Schrödinger picture, as developed in Chapters 1 and 2. This leads to the concept of quantum splines, smooth curves on the manifold of pure states of a quantum system that evolves in a controlled way [60]. The manifold of pure states has the advantage of being controllable by unitary vector fields, thus allowing for many different control strategies.

The control of open quantum systems is a more complex topic. Pure and mixed states have to be considered, and in general the evolution is hard to describe. As a first approach to the problem, consider unitary evolution on the manifold of states $\mathcal{S}$, generated by a Hamiltonian vector field X_{H_0}. Control of the system is modelled by perturbations of this vector field. Physically, this corresponds to the action on the quantum system by external agents. Such an action is usually achieved by an external electromagnetic

field, e.g. a laser, which can be turned on and off at will. The action of electromagnetic fields on a quantum system is represented by Hamiltonian vector fields on the manifold of states [21]. Thus, the controlled dynamics is governed by the following control vector field

$$X(u) = X_{H_0} + \sum_{j=1}^{q} u_k X_{H_k}, \quad u = (u_1, \ldots, u_q) \in U, \tag{4.128}$$

where $H_0, H_1, \ldots, H_q$ are observables of the quantum system. Some results can be proved for this controlled system.

Proposition 4.39. *The control system with vector field (4.128) is small-time controllable by unitary controls.*

Proof. It is possible to take some H_k proportional to H_0 and a large enough set U of admissible parameters such that $X(u) = 0$ for some $u \in U$. Hence every point in $\mathcal{S}$ belongs to the set of reachable states, as it is stable for some control. □

Proposition 4.40. *The control system defined by the vector field*

$$X(u) = X_{H_0} + uX_H, \quad u \in \mathbb{R}, \tag{4.129}$$

is accessible and controllable on each of the symplectic leaves of $\mathcal{S}$ if and only if $[X_{H_0}, X_H] \neq 0$.

Proof. For an n-level system, the algebra of Hamiltonian vector fields on $\mathcal{S}$ is isomorphic to $\mathfrak{su}(n)$, which is a simple Lie algebra. Thus, any two non-commuting elements generate the whole algebra. Thus, if $[X_{H_0}, X_H] \neq 0$, then $\mathrm{Lie}(X_{H_0}, X_H) \simeq \mathfrak{su}(n)$. Symplectic leaves are by definition orbits of the Hamiltonian vector field on $\mathcal{S}$. The tangent space of each leaf is generated by Hamiltonian vector fields, thus satisfying Theorem 4.38 and proving accessibility. Finally, unitary evolution is invertible, therefore controllable. □

The case of Markovian evolution is more complex and it is difficult to establish global results. The geometric formalism offers a nice description of the dynamics, as seen in Section 4.3. Control of Markovian evolution has been object of study in recent years; see the works by Altafini and co-workers [17–21] and references therein. As before, control will be assumed to be achieved by Hamiltonian vector fields. The controlled vector field takes the following form:

$$X(u) = Z_L + \sum_{j=1}^{q} u_k X_{H_k} = X_{H_0} + \sum_{j=1}^{q} u_k X_{H_k} + Y_V + Z_K, \quad u = (u_1, \ldots, u_q) \in \mathcal{U}, \tag{4.130}$$

where $H_0, H_1, \ldots, H_q$ are observables of the quantum system.

Proposition 4.41. *A generic Markovian evolution of a quantum system is neither small-time controllable nor controllable by unitary controls.*

Proof. As shown in Theorem 4.13, the Kossakowski-Lindblad vector field is not (in general) a Hamiltonian vector field. Thus, there exists no combination of Hamiltonian vector fields and controls such that generic points in $\mathcal{S}$ are stable under the controlled dynamics. In other words, $X(u)_\rho \neq 0$ for every $u \in U$ and generic points $\rho \in \mathcal{S}$, hence the system is not small-time controllable. Regarding controllability, recall from Theorem 4.9 and Corollary 4.10 that rank of states cannot increase in finite-time. Thus, the reachable set $\mathcal{R}(\rho)$ for any $\rho \in \mathcal{S}$ consists necessarily of elements with rank equal or less than ρ, plus those in the limit manifold of the dynamics. As Hamiltonian vector fields do not change the rank, it is never possible to achieve controllability of open quantum systems by unitary controls. □

Although controllability is not possible, open quantum systems may be almost controllable, in the sense of Definition 4.37. While no controlled dynamics may cause a transition from a mixed state to a generic pure state, it is sometimes possible to reach a mixed state infinitesimally close to such a pure state. In this sense, almost controllability is a nice property for open quantum systems. The following results describe the conditions that those systems have to satisfy.

Theorem 4.42. *An open quantum system evolving under generic Markovian dynamics with generic unitary controls is accessible.*

Proof. This theorem has been proved in detail from an algebraic formalims by Altafini [19, 20]. In the geometric setting, consider Theorem 4.38. It has to be proved that the tangent space to $\mathcal{S}$ at each point can be obtained by elements in the associated algebra $\mathfrak{g} = \mathrm{Lie}(Z_L, X_{H_1}, \ldots, X_{H_q})$ to (4.130). This tangent space is necessarily generated by all the transformations of states that preserve positivity. Therefore, by direct application of the results by Gorini, Kossakowski, Sudarshan [139] and Lindblad [191], it is enough to prove that all possible Kossakowski-Lindblad vector fields are elements of $\mathfrak{g}$. Recall that the expressionf of the Kossakowski-Lindblad operator is

$$L(\rho) = -\mathrm{i}[H_0, \rho] - \frac{1}{2}\sum_{j=1}^{r}[V_j^\dagger V_j, \rho]_+ + K(\rho), \quad K(\rho) = \sum_{j=1}^{r} V_j \rho V_j^\dagger, \tag{4.131}$$

with $\rho \in \mathcal{S}$, $H_0 \in \mathcal{O} = \mathrm{Herm}(\mathcal{H})$, $V_1, \ldots, V_r \in \mathfrak{sl}(\mathcal{H})$, $\mathrm{tr}(H_0) = 0$ and $\mathrm{tr}(V_j^\dagger V_k) = 0$ if $j \neq k$, for $j, k = 1, 2, \ldots, r \leq n^2 - 1$.

Observe that the algebra $\mathfrak{g}$ involves Lie brackets of vector fields on $\mathcal{S}$, which may not preserve the positivity condition of states. Thus, for the description of accessibility, the envolving differentiable manifold $\widehat{\mathcal{S}}$ of the manifold with boundary $\mathcal{S}$ will be considered (see Section 3.3.2).

Proposition 3.51 gives the commutation relations between Hamiltonian and gradient vector fields; in particular:

$$[X_A, X_B] = X_{[\![A,B]\!]}, \quad A, B \in O.$$

The commutator of the Kossakowski-Lindblad vector field Z_L with a generic Hamiltonian vector field X_H is

$$[X_H, Z_L] = [X_H, X_{H_0}] + [X_H, Y_V] + [X_H, Z_K] = -X_{[\![H,H_0]\!]} - Y_{[\![H,V]\!]} - Z_{[\mathrm{coad}_H, K]},$$

where the last term is obtained by (3.118). The value of the operator $[\mathrm{coad}_H, K]$ can be computed by its action on a generic state:

$$[\mathrm{coad}_H, K](\rho) = \sum_{j=1}^{r}[\![H, V_j]\!]\rho V_j^\dagger + \sum_{j=1}^{r} V_j \rho([\![H, V_j]\!])^\dagger = \sum_{j=1}^{r} A_j \rho A_j^\dagger - \sum_{j=1}^{r} B_j \rho B_j^\dagger, \tag{4.132}$$

where $A_j = V_j + [\![H, V_j]\!]$ and $B_j = V_j - [\![H, V_j]\!]$. Observe that this is not a Kraus operator, but an element in the linear space of operators generated by them. Thus, it does not preserve positivity and cannot be restricted to $\mathcal{S}$. This is the reason why accessibility has to be studied on the envolving differentiable manifold $\widehat{\mathcal{S}}$.

The algebra $\mathfrak{sl}(\mathcal{H})$ is a semisimple algebra, hence $\mathrm{Lie}(H, V_1, \ldots, V_r) = \mathfrak{sl}(\mathcal{H})$ for generic $H, V_1, \ldots, V_r \in \mathfrak{sl}(\mathcal{H})$. As a consequence, by (4.132), every possible Kraus operator is contained in $\mathrm{Lie}(\mathrm{coad}_H, K)$. As generic Markovian dynamics are determined by arbitrary elements $V_1, \ldots, V_{n^2-1} \in \mathfrak{sl}(\mathcal{H})$, the algebra $\mathfrak{g} = \mathrm{Lie}(Z_L, X_H)$ contains all possible Kossakowski-Lindblad vector fields, hence by the above argument the system is accessible by unitary controls. □

Proposition 4.43. *Assume that the Markovian evolution of a quantum system preserves the maximally mixed state. Then, the system is neither controllable nor almost controllable by unitary controls.*

Proof. This result is a direct consequence of the fact that the vector field describing a unital Markovian evolution never increases the purity on $\mathcal{S}$. Therefore, for any $\rho_0 \in \mathcal{S}$, the reachable set has no points with purity larger than that of ρ_0:

$$\forall \rho \in \mathcal{R}(\rho_0),\ P(\rho) \leq P(\rho_0). \tag{4.133}$$

If $P(\rho_0) < 1$, then $\mathrm{cl}\mathcal{R}(\rho_0) \neq \mathcal{S}$ and the system is not almost controllable. □

This result indicates that decoherence-like process, such as the phase damping, cannot be fully controlled. Evolution of the system always tends towards the increase in the degree of mixture of the system. Other systems, however, can be adequately controlled. This is the case of those systems for which the behaviour is precisely the opposite: they increase the purity of the system. The next result describes this property.

Theorem 4.44. *Consider an open quantum system evolving under Markovian evolution and whose limit manifold is a subset of the boundary of the manifold of states. Then, the system is almost controllable by unitary controls.*

In order to prove this theorem, it is interesting to consider first the following particular case.

Proposition 4.45. *An accessible open quantum system evolving under Markovian evolution whose limit manifold is a single pure state,*

$$S_L = \{\rho_L \in S_1\}, \tag{4.134}$$

is almost controllable by unitary controls.

Proof. Recall that $\mathcal{S}$ is a convex set, i.e. any internal point is a convex combination of two points in the boundary. In particular, given a fixed point in the boundary, say ρ_L, all the possible convex combinations with points in the boundary generate the whole manifold $\mathcal{S}$. Assume that the quantum system is in fact an n-level system. Any point $\rho_n \in \mathcal{S}$ of rank n can thus be describe as a convex combination of two states:

$$\rho_n = a\rho_L + b\rho', \quad a, b > 0,\ a + b = 1, \tag{4.135}$$

where ρ' is a state of rank at most $n-1$. Almost controllability is proved if every n-rank state can be reached.

Regarding Markovian dynamics, the integral curves of the Kossakowski-Lindblad vector field with no Hamiltonian term are straight lines, as seen in the examples of Section 4.1.4. Any straight line with points in the interior of a compact convex set meets the boundary at two points. Therefore, integral curves starting at the boundary of $\mathcal{S}$ cover the whole manifold $\mathcal{S}$. From the point of view of control theory, in order to prove that the system is controllable, it is enough to describe how to reach every point in the boundary.

Within this line of reasoning, the proposition can be proved by induction. Consider firstly the 2-level system, as in [19]. It is known that the boundary coincides with the set of pure states, and therefore all the points in the boundary are reachable from the limit point ρ_L by unitary controls. Following the above reasoning, the 2-level system is controllable.

Consider now the case of an n-level system, and take any state ρ_B on the boundary of $\mathcal{S}$. It has rank at most $n-1$, and it is either a pure state or a convex combination of a pure state ρ'_B and some other state. Recall pure states are almost reachable from ρ_L, as they are a leaf of the foliation generated by Hamiltonian vector fields. If ρ_B is pure, it is almost reachable. Else, unitary controls allow to almost reach ρ'_B. And if it is assumed by hypothesis that the $(n-1)$-level system is almost reachable, then any state ρ_B on the boundary can be almost reached. Thus, the n-level system is almost controllable. □

Proof of Theorem 4.44. Let S_L be the limit manifold, and choose a pure state $\rho_L \in \mathcal{S}_L$. It is possible to design a Hamiltonian vector field on $\mathcal{S}$ such that every other element in $\mathcal{S}_L$ is not stable. Thus, by controlling the system with this vector field, the problem reduces to the one presented in Proposition 4.45, with $\{\rho_L\}$ as the limit manifold, thus proving almost-controllability. □

These results offer the possibility to study control strategies in quantum systems. Below some simple examples are presented in which the controllability is analysed. They offer a good starting point for the geometric characterisation of controlled Markovian dynamics.

4.5.3 Control of the decay of the 2-level system

In order to illustrate the results of the previous section, the decay of a 2-level system will be considered. This example has been presented in Section 4.1.4. By application of the above results, and in particular Theorem 4.42, the system is proved to be accessible if adequate unitary controls are chosen. Recall that the Kossakowski-Lindlbad vector field of the system is

$$Z_L = -\gamma x_1\partial_1 - \gamma x_2\partial_2 + 2\gamma(1-x_3)\partial_3, \quad \gamma > 0. \tag{4.136}$$

Consider then the following controlled vector field:

$$X(u) = Z_L + uX_1, \quad X_1 = x_3\partial_2 - x_2\partial_3, \quad u \in \mathbb{R}. \tag{4.137}$$

The associated algebra $\mathfrak{g} = \mathrm{Lie}(Z_L, X_1)$ can be directly computed, thus proving accessibility by Theorem 4.38. The following computation relations are satisfied

$$\begin{aligned}&[Z_L, X_1] = \gamma(2-3x_3)\partial_2 + 3\gamma x_2\partial_3 = 2\gamma\partial_2 - 3\gamma X_1,\\ &[Z_L,\partial_2] = \gamma\partial_2, \quad [X_1,\partial_2] = \partial_3, \quad [Z_L,\partial_3] = \gamma\partial_3, \quad [X_1,\partial_3] = -\partial_2.\end{aligned}$$

Thus, the generated Lie algebra is

$$\mathfrak{g} = \mathrm{Lie}(Z_L, X_1) = \mathrm{span}\{Z_L, X_1, \partial_2, \partial_3\}. \tag{4.138}$$

The system is accessible everywhere except in the plane $x_1 = 0$. Global accessibility can be achieved by considering a more general unitary control:

$$X(u) = Z_L + u_1X_1 + u_2X_2, \quad X_2 = x_1\partial_3 - x_3\partial_1, \quad u_1, u_2 \in \mathbb{R}. \tag{4.139}$$

An identical computation shows that these vectors generate the algebra

$$\mathfrak{g} = \mathrm{Lie}(Z_L, X_1, X_2) = \mathrm{span}\{Z_L, X_1, X_2, X_3, \partial_1, \partial_2, \partial_3\}, \tag{4.140}$$

and the system is accessible.

The limit manifold of this evolution is a single point, $S_L = \{(0,0,1)\}$. Thus, by Proposition 4.45, the system is almost controllable. This has been already shown graphically in [19]. It is possible to obtain, by unitary control, closed trajectories on the Bloch ball. By the same procedure, it is possible to design trajectories that connect any two mixed states. Controlled trajectories are shown in Figure 4.8.

Regarding pure states, Theorem 4.9 and Corollary 4.10 rule out the possibility of reaching any point on the boundary in finite time. However, if no constraints are imposed on the set of admissible controls, then it is possible to reach points arbitrarily close to any pure state. Thus, $\mathrm{cl}\mathcal{R}(\rho) = \mathcal{S}$ for any $\rho \in \mathcal{S}$, and the system is almost controllable.

Another interesting aspect of the unitary control is the change of the limit point. Consider the case presented in (4.137). For $u \neq 0$, the limit point is no longer $(0,0,1)$; instead, the following equation has to be solved:

$$Z(u) = 0 \Rightarrow \begin{cases} -\gamma x_1 = 0 \\ ux_3 - \gamma x_2 = 0 \\ 2\gamma(1-x_3) - ux_3 = 0 \end{cases} \Rightarrow x_1 = 0,\ x_2 = \frac{2u\gamma}{u^2+2\gamma^2},\ x_3 = \frac{2\gamma^2}{u^2+2\gamma^2}. \tag{4.141}$$

The limit point is a mixed state for $u \neq 0$, and evolves towards ρ_0 when $u \to \infty$.

4.6 Outlook of the geometric description of Markovian evolution

Open quantum systems are one of the more relevant topics in the development of modern Quantum Physics. They appear in a gret variety of fields: Chemistry, Solid State Physics, Quantum Optics, etc.

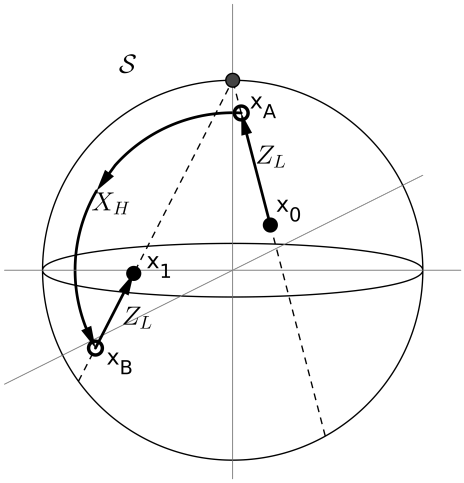


Figure 4.8: Unitary control of the decay of a 2-level system. Any mixed state can be reached from any initial one, thus proving the almost-reachability of the system. The plot shows how to evolve from any states x_0 to any mixed states x_1. Markovian evolution, determined by vector field Z_L, drives the system to the ground state. Hence, the state of a system with initial state x_0 changes along the dashed line until it reaches x_A. At that situation, an appropriate Hamiltonian vector field X_H changes the state to x_B (ideally in zero time). From it, the system evolves again along a straight line determined by Z_L, thus reaching x_1

Therefore, it is interesting to develop new description of these systems if they offer the possibility to analyse them from a different perspective. The geometric formalism of Quantum Mechanics is succesful in this task. The set of pure and mixed states of a quantum system, described in Chapter 3, can be characterise geometrically, which provides a suitable setting for the characterisation of non-unitary dynamics. In particular, Markovian dynamics can be given a simple description in terms of vector fields, which reproduce the Kossakowski-Lindblad equation [139, 191]. From these vector fields, it is immediate to reproduce the dynamics.

Two main applications of this geometric description of Markovian dynamics have been considered: the contractions of algebras of observables and the unitary control of the dynamics. The contractions of algebras is a mathematical construction with a great relevance in the analysis of physical systems. In fact, it was the analysis of the classical limit of Special Relativity that led Inönü, Wigner [159] and Segal [240] to the description of the contractions of algebras. In the realm of Quantum Mechanics, contractions of algebras of observables of open quantum systems were recently observed by Chruściński, Marmo and co-workers [7, 92, 158]. This phenomenon can easily be described in geometric terms [72]. Thus, the Kossakowski-Lindblad vector field induces a transformation in the relevant tensor fields on the manifold of states, which may end up in a contraction of the algebra. The geometric formalism presents here an advantage over the algebraic description of quantum systems. It is possible to characterise the Kossakowksi-Lindblad vector field in order to analyse the properties of its limit manifold. This allows to determine if contractions may exist. Instead, an algebraic approach requires always the explicit computation of the evolution, and no *a priori* arguments for the presence of contractions exist. The procedure developed here can also be extended to other kinds of evolutions and manifolds [168]. Thus the geometric formalism is easily adapted to more general quantum systems.

The other relevant application discussed here is the control of Markovian dynamics. Differential geometry offers many tools that allow for the analysis and characterisation of control systems. Thus, the formalism presented here can be combined with the results of Altafini [17, 18, 20, 21] in order to shed some light on the controllability properties of open quantum systems. The main conclusion is that most systems can be easily controlled by unitary evolutions, such as those induced by interactions with lasers. As proved, the reason for this property is the possibility to move along the boundary of the manifold of

states by unitary evolutions, which again can be easily understood from a geometric perspective. Future development of the control theory of open quantum systems may involve the incorporation of Lie systems, in a similar way to Chapter 2, and the analysis of time-dependent Kossakowski-Lindblad equations, as introduced by Rivas and Huelga [226].

Chapter 5

Hybrid quantum-classical dynamics

Open quantum systems are ubiquitous in the description of Nature. No system is isolated from its environment, and thus an appropriate description of this interaction is relevant. As seen in Chapter 4, Markovian evolution is a particular case in which quantum systems evolve in a very specific way. However, there are other examples of quantum systems that have great interest in many different areas, such as Chemistry and Biology. This is the case of hybrid quantum-classical systems.

Molecular modelling has been a challenging problem for a long time. Since the early days of Quantum Mechanics, the proposal of efficient descriptions of full molecules constitutes one of the boundaries of the discipline. Indeed, the Schrödinger equation for a combined system of electrons and nuclei is generally impossible to solve explicitly and approximations are necessary.

Typically, molecular dynamical models take advantage of the different behaviour of light and heavy particles. The approximations are based on the consideration of classical evolutions for the nuclei, while electrons retain their quantum nature [55,56]. Dynamics of classical and quantum particles are obviously interrelated. These characterisations of molecular systems are known as hybrid quantum-classical models. They are widely used in the description of molecular dynamics.

Hybrid quantum-classical models are introduced as approximations to the Schrödinger equation of a molecular system. See references such as the book by Marx and Hutter [198], the review by Yonehara, Hanasaki and Takatsuka [276] and references therein for a full description of these models. One of the fundamental hypothesis in the development of the models is the validity of the Born-Oppenheimer approximation [52, 54], according to which the evolution of electrons and nuclei can be separated. It is thus possible to characterise the electronic dynamics for fixed configurations of the nuclei, which are assumed to evolve more slowly. This is the basis of the so-called time-dependent self-consistent field method [108], which is a close approximation to the actual molecular system. The computation cost of this method, however, is usually large. Thus, the dynamics is further simplified by considering classical evolutions for the nuclei. Depending on the constraints imposed on the evolution, different models are obtained. For example, Born-Oppenheimer dynamics considers that electrons always stay at the ground state for any nuclear configuration [198]. Instead, the present chapter focuses on the analysis of the Ehrenfest model, which allows for transitions between electronic energy levels. The Ehrenfest model is discussed in detail in Section 5.1.

Despite its many advantages, the Ehrenfest model does not offer a good description of decoherence. This is a purely quantum phenomenon, which has a huge importance in the characterisation of molecular systems [261, 279]. Hybrid quantum-classical models, however, are deterministic, and thus coherence of quantum states is always preserved. It is thus a relevant topic the appropriate modification of these models in order to incorporate decoherence-like effects. Several approaches have been proposed, such as trajectory surface hopping algorithms by Tully and co-workers [184, 257, 262–264], stochastic mean field by Prezhdo [222] or the methods proposed by Subotnik [255, 256] by Neria and Nitzan [213] and others [40, 43, 238].

All these approaches share some common features. Namely, they propose algorithms that force a

decoherence-like behaviour into Ehrenfest dynamics. There exists, however, an alternative approach based on statistical ensembles that incorporates these effects in a more natural way. As proposed by Alonso, Clemente-Gallardo and collaborators, the author among them [8–10,14,15], a statistical extension of Ehrenfest dynamics can be achieved by means of a proper geometric characterisation of the model. The path led by the aforementioned works is followed here, thus combining the geometric formalism developed along this dissertation with the description of hybrid quantum-classical systems. This approach has clear advantages, such as allowing for an intrinsic formulation of the model, independent of coordinates. The geometric characterisation of statistical molecular ensembles, evolving under Ehrenfest dynamics, shows that decoherence-like effects, such as changes in purity, appear.

The chapter is organised as follows. Section 5.1 offers a first approach to the Ehrenfest model, by summarising the hypothesis and approximations made in the Schrödinger equation in order to obtain the model. The geometric characterisation of the dynamics is presented in Section 5.2. With this formalism, it is possible to develop a statistical model, as proved in Section 5.3. The thermodynamic limit is also analysed, as presented in [9, 15]. Finally, Section 5.4 focuses on the applications of the formalism to practical examples. In particular, to the simulation of the dynamics of diatomic molecules. Numerical results thus obtained are in agreement with the theory.

5.1 Derivation of hybrid quantum-classical models

Molecular systems, even the smallest ones, are characterised by a huge number of degrees of freedom. Even supercomputers have great difficulties in the exact computation of their dynamics. It is necessary to consider approximations to the Schrödinger equation in order to describe, at least partially, the dynamics of molecular systems. This section presents the derivation of hybrid quantum-classical models from molecular Schrödinger equations. As a result of the implemented approximations, nuclei follow classical laws of motion, while dynamics of electrons is still quantum. For further details, see [10, 55, 56, 134, 135, 197, 198] and references therein.

The motivation for the derivation of hybrid quantum-classical models can be found in the Ehrenfest theorem [56,124]. This theorem, first presented by Ehrenfest in 1927 [118], describes the change in time of the expectation values of observables. In its most simple case, consider a wave function $\psi(r,t)$ describing a massive particle on a one-dimensional space, moving in a scalar potential $V(r)$. As proved by Ehrenfest, the expectation values of the position r and momentum p operators satisfy the following relations:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle r\rangle = \frac{1}{M}\langle p\rangle, \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle p\rangle = -\left\langle \frac{\partial V}{\partial r}\right\rangle, \tag{5.1}$$

with M the mass of the particle. The form of these equations is similar to that of Hamilton equations appearing in Classical Mechanics. As first noted by Moyal [211], a power expansion of the scalar potential $V(r)$, followed by some modifications and approximations, is the key point in the computation of a classical limit for the model [198]. The idea behind the development of hybrid quantum-classical models in molecular dynamics is the extension of these approximations to some particles conforming the molecular system.

Consider a molecule with m atoms. Chemistry models show that the valence electrons are responsible for the properties of the molecule. The remaining electrons, which occupy the inner orbitals with lower energies, stay always close to their respective nuclei. For this reason, it is advisable to consider a nucleus and its inner electrons as a single entity, which shall be called a core. Therefore, a molecule is comprised of m cores and a certain number n of valence electrons. The state of a molecule at a time t is described by a wave function $\Psi(r,R,t)$ on the configuration space of valence electrons and cores, where

$$r = (\mathbf{r}_1,\dots,\mathbf{r}_n) \in \mathbb{R}^{3n}, \quad R = (\mathbf{R}_1,\dots,\mathbf{R}_m) \in \mathbb{R}^{3m}. \tag{5.2}$$

Each particle is characterised by its mass and its charge. In atomic units, every electron has mass equal to 1 and charge equal to -1, while the mass and charge of the J-th core are respectively M_J and Z_J.

Only Coulomb interactions are considered, modelled by the following potential:

$$V(r,R)=\sum_{J<K}^{m}\frac{Z_J Z_K}{|\mathbf{R}_J-\mathbf{R}_K|}+\sum_{j<k}^{n}\frac{1}{|\mathbf{r}_j-\mathbf{r}_k|}-\sum_{J=1}^{m}\sum_{j=1}^{n}\frac{Z_J}{|\mathbf{R}_J-\mathbf{r}_j|} \tag{5.3}$$

The evolution of the state of the molecule is determined by the Schrödinger equation:

$$\mathrm{i}\frac{\partial}{\partial t}\Psi(r,R,t)=H(r,R)\Psi(r,R,t), \tag{5.4}$$

where $H(r,R)$ is the standard molecular Hamiltonian. It is useful to write this operator as

$$H(r,R)=-\sum_{J=1}^{m}\frac{1}{2M_J}\nabla_J^2+H_e(r,R). \tag{5.5}$$

where $H_e(r,R)$ is called the electronic Hamiltonian of the system and is defined as

$$H_e(r,R)=-\frac{1}{2}\sum_{j=1}^{n}\nabla_j^2+V(r,R). \tag{5.6}$$

The classical behaviour of cores can now be introduced in different ways, each leading to a different model. The traditional approach is based in the computation of the eigenvectors of $H_e(r,R)$ for fixed positions of the cores [114,198]. This approach is based in the factorisation of the wave function according to the Born ansatz [52, 183]. By use of the Born-Oppenheimer approximation [52, 54], and considering the classical limit for the cores, a hybrid quantum-classical description of the molecule is obtained. This approach is usually known as the Born-Oppenheimer model, and is characterised by restricting the state of the quantum part to a fixed eigenvector of the electronic Hamiltonian, computed for each configuration of the cores. See in particular [198, p. 11] and references therein for a detailed description of the model.

It is possible to consider a different derivation of quantum-classical dynamics that retains a quantum evolution for the electronic subsystem. As before, some ansatzs and approximations have to be made. The resulting equations conform the so-called Ehrenfest model, due to its resemblance with the differential equations deduced in the Ehrenfest theorem. The derivation of the model presented here is based in the works by Tully [263, 264]; see also the works by Marx and Hutter [197, 198] and by Bornemann, Nettensheim and Schütte [55, 56] for further details.

In order to derive the Ehrenfest model, the following hypothesis are considered [56]:

- The cores are localised at a certain time t_0. In terms of operators, the variance of their position operators R_J, for $J=1,2,\ldots,m$, is considered to be small.
- The mass of cores is much larger than that of the electrons, i.e. $M_J \geq 1$ for every $J=1,2,\ldots,m$.

Due to the first hypothesis, the molecular wave function is separable at a time t_0 in a nuclear and an electronic parts [55]:

$$\Psi(r,R,t_0)\simeq\psi(r,t_0)\chi(R,t_0), \tag{5.7}$$

with ψ and χ normalised over $\mathbb{R}^{3n}$ and $\mathbb{R}^{3m}$, respectively. The separability of the wavefunction was first proposed by Dirac in 1930 [110]. This property is preserved along time evolution; thus, it is possible to approximate $\Psi(r,R,t)$ by a product of a nuclear and an electronic wavefunctions. Their respective differential equation are obtained by a variational principle, as shown by McLahlan [203]. For simplicity, it is advisable to add a time-dependent factor. Thus, the molecular wavefunction is approximated as

$$\Psi(r,R,t)\simeq\psi(r,t)\chi(R,t)\exp\left[\mathrm{i}\int_{t_0}^{t}E(t')\mathrm{d}t'\right], \tag{5.8}$$

where the function $E(t)$ is the expectation value function of the electronic Hamiltonian H_e at time $t \geq t_0$:

$$E(t) = \iint \psi^*(r,t)\chi^*(R,t)H_e(r,R)\psi(r,t)\chi(R,t)\mathrm{d}r\,\mathrm{d}R. \tag{5.9}$$

Observe that, due to this separability, the model thus obtained limits the interaction between particles, as it ignores the possible entangled states of cores and electrons that could appear along evolution [156].

The factorisation of the molecular wavefunctions is an important element in the derivation of molecular models. For this reason, it has been a topic of study for many years. It is remarkable the work by Abedi, Maitra and Gross on the exact factorisation of the wavefunction [1]; technical details on this topic were addressed by Alonso, Clemente-Gallardo, Echenique-Robba and the author, which were in turn responded [2, 16].

The differentiable equations for ψ and χ can be obtained either by a variational function or by direct substitution of (5.8) into the Schrödinger equation (5.4). Due to the extra exponential factor in (5.8), it is possible to obtain the following system of coupled differential equations:

$$\begin{aligned}
\mathrm{i}\,\frac{\partial}{\partial t}\psi(r,t) &= -\frac{1}{2}\sum_{j=1}^{n}\nabla_j^2\psi(r,t) + \left(\int |\chi(R,t)|^2 V(r,R)\ \mathrm{d}R\right)\psi(r,t),\\
\mathrm{i}\,\frac{\partial}{\partial t}\chi(R,t) &= -\sum_{J=1}^{m}\frac{1}{2M_J}\nabla_J^2\chi(R,t) + \left(\int \psi(r,t)^* H_e(r,R)\psi(r,t)\ \mathrm{d}r\right)\chi(R,t).
\end{aligned} \tag{5.10}$$

Each equation describes the quantum dynamics of the corresponding subsystem. Observe that the equations are coupled, as the effective potential acting on the cores depends on the state of the electronic subsystem, and vice versa. These equations are the basis of the time-dependent self-consistent field (TDSCF) method, a powerful tool in the description of molecular systems. Descriptions of the method can be found in numerous woks [134, 198].

From the TDSCF equation, it is possible to derive the Ehrenfest model by imposing the second hypothesis mentioned above. The assumption of large masses for the cores amounts to considering the classical limit on their dynamics [144]. As a result, as shown in [56, 198], the nuclear wavefunction can be written as

$$\chi(R,t) \simeq A(R,t)\exp(\mathrm{i}\,S(R,t)), \tag{5.11}$$

where the real functions $A(R,t)$ and $S(R,t)$ satisfy the following differential equations:

$$\begin{aligned}
&\frac{\partial}{\partial t}A^2(R,t) + \sum_{J=1}^{m}\frac{1}{M_J}\nabla_J\left(A^2(R,t)\nabla_J S(R,t)\right) = 0,\\
&\frac{\partial}{\partial t}S(R,t) + \sum_{J=1}^{m}\frac{1}{2M_J}\nabla_J^2 S(R,t) + \left(\int \psi(r,t)^* H_e(r,R)\psi(r,t)\ \mathrm{d}r\right)S(R,t) = 0.
\end{aligned} \tag{5.12}$$

The first equation is a continuity equation for the probability density of the nuclear wavefunction. In particular, if χ is assumed to be localised at t_0, then it is also localised at posterior times. In the limit of zero variance, the expectation values of the positions of the cores are identified with their classical positions.

The second equation in (5.12) is a Hamilton-Jacobi equation for $S(R,t)$. The solution for this equation is obtained by means of the Huygens principle [29, p. 255]. The linear momenta associated to the wavefunction $\chi(R,t)$ are

$$\mathbf{P}_J = \nabla_J S(R,t), \quad J = 1,2,\ldots,m. \tag{5.13}$$

At this point, it is possible to consider the classical limit of this formulation. Nuclear wave function is assumed to be localised, hence the state of cores are determined by their positions R. No explicit equation for the evolution of these positions is given yet. Instead, it is possible to identify the values $\mathbf{P}_1,\ldots,\mathbf{P}_m$ with the classical momenta of the cores. It is thus possible to obtain a classical dynamical system for

the cores. Observe that the described procedure is similar to the WKB approximation [145, 230], a common approximation in the resolution of the Schrödinger equation. Notice also the change in the dimensionality of the space describing the states of the cores, as the infinite-dimensional Hilbert space of nuclear wave functions is approximated by the finite-dimensional phase space of the cores. The reduction in the dimension is due to the assumption of a very specific kind of nuclear wave functions, namely localised functions (i.e. Dirac deltas). Summarising, it is possible to go from a quantum description of the whole system to the following hybrid quantum-classical dynamical system.

Theorem 5.1. *The evolution of the classical and quantum degrees of freedom of the described hybrid quantum-classical system is governed by the following differential equations:*

$$\begin{aligned} \frac{\mathrm{d}\mathbf{R}_J}{\mathrm{d}t}(t) &= \frac{1}{M_J}\mathbf{P}_J(t), \\ \frac{\mathrm{d}\mathbf{P}_J}{\mathrm{d}t}(t) &= -\nabla_J \left(\int \psi(r,t)^* H_e(r,R(t))\psi(r,t)\ \mathrm{d}r \right), \\ \mathrm{i}\,\frac{\partial}{\partial t}\psi(r,t) &= H_e(r,R(t))\psi(r,t), \end{aligned} \tag{5.14}$$

for $J = 1, 2, \ldots, m$ *and* $H_e(r,R)$ *given by* (5.6).

Proof. The Hamilton-Jacobi equation (5.12) for $S(R,t)$ is transformed into Hamilton equations for $\mathbf{R}_1, \ldots, \mathbf{R}_m$ and $\mathbf{P}_1, \ldots, \mathbf{P}_m$. On the other side, regarding the electronic degrees of freedom, the proposed equation is obtained from (5.10). □

Equations (5.14) define collectively the Ehrenfest model for molecular systems. It is important to notice correlations between evolutions of classical and quantum degrees of freedom. Cores follow classical laws of motion under a potential depending on the electronic state, often called the Eherenfest potential. Similarly, the electronic Hamiltonian is determined by the positions of the cores. Observe that, in contrast with the Born-Oppenheimer model, transitions between electronic states are allowed [198].

5.2 Geometric characterisation of the Ehrenfest model

In spite of formal similarities, Ehrenfest model, as presented in (5.14), is not a Hamiltonian system. While evolution of classical degrees of freedom is governed by Hamilton-like equations, there are other requirements that need to be fulfilled, such as the existence of a Poisson bracket. This in turn implies that a global phase-space description is necessary, encompassing both classical and quantum degrees of freedom.

The geometric formalism for Quantum Mechanics presented along this dissertation offers a suitable framework for a Hamiltonian description of Ehrenfest model. Classical Mechanics can be formulated as a theory on Poisson manifolds. The same is true for Quantum Mechanics. These formulations can be combined in the same way as when different classical systems are considered. Following previous works [8, 10, 14], this section presents a geometric description of hybrid quantum-classical systems and of dynamics described by Ehrenfest model.

5.2.1 The quantum-classical manifold

The geometric formulation of Classical Mechanics was fully described by Abraham and Marsden in their well-known book [3]. The phase space of the system is identified with the cotangent bundle of a differentiable manifold, which in its more simple description is the configuration space of the system. It is a well-known property of differentiable geometry that any cotangent bundle carries a canonical symplectic form. This in turn determines the dynamics of the system, as the trajectories of classical systems are the integral curves of Hamiltonian vector fields with respect to such structure.

Particularising to the case of molecular system, the phase space of the classical particles is

$$M_C = \overbrace{\mathbb{R}^6 \times \cdots \times \mathbb{R}^6}^{m} = \mathbb{R}^{6m}. \tag{5.15}$$

Points in the manifold M_C determine positions and momenta of the classical particles with the following notation:

$$\xi = (R, P) = (\mathbf{R}_1, \ldots, \mathbf{R}_m, \mathbf{P}_1, \ldots, \mathbf{P}_m) \in M_C. \tag{5.16}$$

with each position and momentum vector being

$$\mathbf{R}_J = (R_{J,1}, R_{J,2}, R_{J,3}) \in \mathbb{R}^3, \quad \mathbf{P}_J = (P_{J,1}, P_{J,2}, P_{J,3}) \in \mathbb{R}^3, \quad J = 1, 2, \ldots, m. \tag{5.17}$$

The classical phase space is a symplectic manifold (M_C, ω_C), with a Poisson bracket denoted as $\{\cdot,\cdot\}_C$. Its action on differentiable functions f, g is

$$\{f, g\}_C = \sum_{J=1}^{m} \sum_{k=1}^{3} \left(\frac{\partial f}{\partial R_{J,k}} \frac{\partial g}{\partial P_{J,k}} - \frac{\partial f}{\partial P_{J,k}} \frac{\partial g}{\partial R_{J,k}} \right), \quad f, g \in C^\infty(M_C). \tag{5.18}$$

The quantum subsystem can be described also in geometric terms. As presented in Chapter 1, the Hilbert space of the quantum system, and more specifically its projective space, is identified with a differentiable manifold $\mathcal{P}$. This manifold carries additional structures derived from the Hermitian product in the Hilbert space. Thus, the configuration space of a quantum system is a Kähler manifold $(\mathcal{P}, \omega_\mathcal{P}, g_\mathcal{P}, J_\mathcal{P})$. Kähler manifolds are particular cases of symplectic manifolds, and for the description of hybrid quantum-classical systems it is enough to consider the symplectic manifold $(\mathcal{P}, \omega_\mathcal{P})$, with $\{\cdot,\cdot\}_\mathcal{P}$ its Poisson bracket. Dynamics of quantum systems is also described by Hamiltonian vector fields.

A requisite for the geometrisation of the quantum description is the discretisation of the Hilbert space of electronic wavefunctions. As explained before, geometric characterisation on infinite dimensional quantum systems is a challenging problem that lays beyond the scope of this dissertation. A description in terms of finite dimensional systems is, nevertheless, accurate enough for the case of molecular systems. It is common, for example, to describe the states of the electronic subsystem in term of Slater determinants. These are generated by a large enough, although finite, set of eigenvectors for the electronic Hamiltonian. As a result, electronic states are approximated by elements in a finite dimensional manifold.

An alternative approach takes advantage of the spatial distribution of electrons. If the value of the electronic wavefunction far away from the cores is assumed to be negligible, then it is possible to bound the domain of wavefunctions. By discretising this domain, wavefunctions are determined by their values over a grid of points on $\mathbb{R}^{3n}$, thus spanning a finite dimensional Hilbert space. The dimension of the Hilbert space is equal to the number of points in the space grid. Obviously, large number of points allows for a good approximation to the continuum case. For computational purposes, this approach is the one chosen in following sections. Regardless of the actual discretisation procedure, the resulting finite dimensional Hilbert space and its projective space can be described geometrically as usual.

The geometric description of hybrid quantum-classical systems combines these two approaches. Thus, the configuration space of a hybrid quantum-classical system is assumed to be the following product manifold [8, 10, 14]:

$$M_{QC} = M_C \times \mathcal{P}. \tag{5.19}$$

Observe that, with this definition, it is implicitely assumed that there exists no entanglement between the classical and quantum subsystems.

Proposition 5.2. *The product manifold M_{QC} is a symplectic manifold, being its Poisson bracket defined as*

$$\{f, g\}_{QC} = \{f, g\}_C + \{f, g\}_\mathcal{P}. \tag{5.20}$$

Proof. The manifold M_{QC} is defined as the direct product of two symplectic manifolds. Hence, it is also a symplectic manifold. See the book by Abraham and Marsden [3] for a proof of this property. □

Observe that the reduced Planck constant $\hbar$ is not included in (5.20), unlike the product proposed in [10]. The reason is that, with the definitions presented in Chapter 1, this important constant is already contained in the quantum Poisson bracket $\{\cdot,\cdot\}_{\mathcal{P}}$. See in particular Section 1.2.5 for an analysis of the role of $\hbar$ in the geometric description of Quantum Mechanics.

5.2.2 The observables of the hybrid quantum-classical system

Both in geometric Classical and Quantum Mechanics, observables are represented by functions on the corresponding manifolds. The same happens in the product manifold M_{QC}. It is however necessary to describe in detail these observables.

In Classical Mechanics, observables are smooth functions $f_C : M_C \to \mathbb{R}$ that assign results of measurements to points on the manifold. Thus, the set of observables on M_C is simply $C^\infty(M_C)$, the associative algebra of smooth functions. Observe that this algebra is obviously closed under the classical Poisson bracket $\{\cdot,\cdot\}_C$.

The case of the quantum subsystem is different. As seen in Chapter 1, observables of a quantum system are the set $\mathcal{O} = \mathrm{Herm}(\mathcal{H})$ of Hermitian operators on the Hilbert space of the system. When dealing with the projective manifold $\mathcal{P}$, observables are represented by the set $\mathcal{E}_{\mathcal{O}}(\mathcal{P})$ of expectation value functions:

$$\mathcal{E}_{\mathcal{O}}(\mathcal{P}) = \{\epsilon_A,\ A \in \mathcal{O}\}, \quad \epsilon_A([\psi]) = \frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle}, \quad [\psi] \in \mathcal{P}. \tag{5.21}$$

The set of expectation value functions is thus a subset of all the possible smooth functions on $\mathcal{P}$. It is note, unlike in the classical case, an associative algebra, but a Lie-Jordan algebra with respect to the Poisson and symmetric products on $\mathcal{P}$ defined by the Kähler structure (see Chapters 1 and 3).

Observables on the hybrid system have to represented by functions on M_{QC} that keep some relation with these two cases. Let $\mathcal{O}_{QC}$ represent the set of such functions. Due to the geometric structure present in M_{QC}, and following the properties of observables in Classical and Quantum Mechanics, the set $\mathcal{O}_{QC}$ is required to be closed under the Poisson bracket $\{\cdot,\cdot\}_{QC}$.

The extension of $C^\infty(M_C)$ and of $\mathcal{E}_{\mathcal{O}}(\mathcal{P})$ to the product manifold are the subsets of $\mathcal{O}_{QC}$ representing, respectively, purely classical and quantum observables. Futhermore, these are Poisson subalgebras with respect to the Poisson bracket $\{\cdot,\cdot\}_{QC}$, defined in (5.20). Examples of these operators are one-particle operators such as positions and momenta of each particle. Arbitrary linear combinations of these functions also represent observables. This is the case, for example, of the total linear momentum of the molecule.

More complex combinations have to be considered in order to properly describe the properties of hybrid systems. Consider a classical-quantum observable A on the molecular system. According to the geometric formalism, it is represented by a smooth function $\epsilon_A : M_{QC} \to \mathbb{R}$. It is possible to determine the formal expression of these functions. Observe that the restriction of ϵ_A to $\mathcal{P}$ is necessarily an expectation value function, with the specific form (5.21). Thus, it is natural to consider ξ-dependent observables $A(\xi) \in \mathcal{O}$ and define the function ϵ_A as

$$\epsilon_A(\xi,[\psi]) = \frac{\langle\psi|A(\xi)|\psi\rangle}{\langle\psi|\psi\rangle}, \quad (\xi,[\psi]) \in M_{QC}. \tag{5.22}$$

The linear space generated by these functions is denoted as $\mathcal{E}_{QC}(M_{QC})$. This set, however, is not closed under the Poisson bracket $\{\cdot,\cdot\}_{QC}$ [10]. In fact, consider two hybrid observables A, B. The classical and quantum Poisson bracket of their respective functions are

$$\begin{aligned}
\{\epsilon_A,\epsilon_B\}_C(\xi,[\psi]) &= \sum_{J=1}^{m}\sum_{k=1}^{3}\left(\frac{\langle\psi|\frac{\partial A}{\partial R_{J,k}}|\psi\rangle}{\langle\psi|\psi\rangle}\frac{\langle\psi|\frac{\partial B}{\partial P_{J,k}}|\psi\rangle}{\langle\psi|\psi\rangle} - \frac{\langle\psi|\frac{\partial A}{\partial P_{J,k}}|\psi\rangle}{\langle\psi|\psi\rangle}\frac{\langle\psi|\frac{\partial B}{\partial R_{J,k}}|\psi\rangle}{\langle\psi|\psi\rangle}\right), \\
\{\epsilon_A,\epsilon_B\}_Q(\xi,[\psi]) &= \frac{\langle\psi|[\![A(\xi),B(\xi)]\!]|\psi\rangle}{\langle\psi|\psi\rangle}.
\end{aligned} \tag{5.23}$$

By combining both results as in (5.20), it can be concluded that $\{\epsilon_A,\epsilon_B\}_{QC} \notin \mathcal{E}_{QC}(M_{QC})$. For the set $\mathcal{O}_{QC}$ of observable functions to close a Poisson algebra, it is necessary to consider all smooth functions

on the product manifold:

$$\mathcal{O}_{QC} = C^\infty(M_{QC}). \tag{5.24}$$

The set $\mathcal{O}_{QC}$ includes therefore functions without a clear physical interpretation, as their restrictions to the quantum subsystems are not expectation value functions. This is however a natural feature of Ehrenfest dynamics, which stems from the interaction between both subsystems. In a sense, the quantum subsystem can be regarded as an open quantum system, whose evolution is influenced by an external system (the classical part) and whose properties are not entirely equivalent to those of isolated quantum systems.

Two considerations can be made with respect to this issue. Firstly, this feature resembles in a way the entanglement of quantum particles, in which the description of the system as a whole is intrinsically different than that of each constituent part. Similarly, in molecular systems, there exists new features (in this case, new functions) that do not appear when the quantum subsystem is considered alone. Surprisingly, the classical system presents no difficulties. Thus, the entanglement-like behaviour of molecular systems appears only in the quantum part, not in the classical one, of the system.

The other main consideration has to do with the geometric characterisation of quantum systems. As seen above, this geometric formalism allows for a join description of the classical and quantum subsystems of the molecule. But in the case of the observables, the relevance of this description is greater. The set of functions $\mathcal{O}_{QC}$ defined in (5.24) makes sense only on a geometric setting, and has no direct correlation with any object in a algebraic formalism. Thus, the geometric characterisation allows for an extension of the concept of observables to any smooth function on the manifold.

5.2.3 Ehrenfest model as Hamiltonian dynamics

Consider in particular, the function ϵ_H associated to the Hamiltonian of the system. Its value at each point $(\xi, [\psi]) \in M_{QC}$ gives as a result the energy of the molecule for a configuration $\xi \in M_C$ of the nuclei and a state of the electrons described by $[\psi] \in \mathcal{P}$. The value of this function is given by considering the discrete expression of (5.5):

$$\epsilon_H(\xi, [\psi]) = \frac{\langle\psi|H(\xi)|\psi\rangle}{\langle\psi|\psi\rangle} = \sum_{J=1}^{m} \frac{1}{2M_J}\mathbf{P}_J^2 + \frac{\langle\psi|H_e(R)|\psi\rangle}{\langle\psi|\psi\rangle}, \tag{5.25}$$

where $H_e(R)$ is the discrete version of the electronic Hamiltonian (5.6). By using this function and the Poisson bracket (5.20), it is possible to define a Hamiltonian vector field on M_{QC} whose integral curves are the solutions to the equations of the Ehrenfest model [10].

Theorem 5.3. *Let X_H^{QC} be the vector field on M_{QC} defined as*

$$X_H^{QC}(f) = -\{\epsilon_H, f\}_{QC}, \quad f \in C^\infty(M_{QC}). \tag{5.26}$$

The integral curves of this vector field are the solution to the set of differentiable equations (5.14) associated to the Ehrenfest model.

Proof. Equation (5.26) can be rewritten according to the expression (5.20) of the classical-quantum Poisson bracket:

$$X_H^{QC}(f) = -\{\epsilon_H, f\}_C - \{\epsilon_H, f\}_{\mathcal{P}}, \quad f \in C^\infty(M_{QC}). \tag{5.27}$$

The second term is, by (1.138) and (5.25), the Hamiltonian vector field on $\mathcal{P}$ associated to $H_e(R)$. Its integral curves are, by Theorems 1.48 and 1.65, the projection onto $\mathcal{P}$ of the solutions to the Schrödinger equation for $H_e(R)$. Regarding the classical degrees of freedom, consider an integral curve for the vector field X_H^{QC}. By (5.26), the differential equations for the classical coordinates of this integral curve are:

$$\begin{aligned} \frac{\mathrm{d}R_{J,k}}{\mathrm{d}t} &= -\{\epsilon_H, R_{J,k}\}_{QC} = \frac{\partial \epsilon_H}{\partial P_{J,k}} = \frac{1}{M_J} P_{J,k}, \\ \frac{\mathrm{d}P_{J,k}}{\mathrm{d}t} &= -\{\epsilon_H, P_{J,k}\}_{QC} = -\frac{\partial \epsilon_H}{\partial R_{J,k}} = -\frac{\partial}{\partial R_{J,k}} \frac{\langle\psi|H_e(R)|\psi\rangle}{\langle\psi|\psi\rangle}, \end{aligned} \qquad J = 1, 2, \ldots, m; \ k = 1, 2, 3, \tag{5.28}$$

which are precisely the equations in (5.14). □

This Theorem proves that the Ehrenfest model is recovered as a Hamilton system on the hybrid quantum-classical manifold M_{QC}. Evidently, the set $\mathcal{O}_{QC}$ of observable functions is preserved under evolution, as it is closed under the Poisson bracket. Observe also that it is impossible to obtain any kind of entanglement between classical and quantum degrees of freedom by means of Ehrenfest dynamics. By taking M_{QC} as the differentiable manifold of the system, this entanglement is intrinsically ruled out. This and the deterministic property of the evolution are the main reasons of the lack of decoherence-like effects in Ehrenfest dynamics. While several methods exist to include in some way these effects (see the introduction to this chapter), the geometric description of the dynamics offers another alternative. A statistical treatment of the theory is possible thanks to the presence of symplectic volumes. As seen in following sections, theorietical computations and numerical simulations prove the emergence of decoherence-like effects in this statistical setting, thus expanding the possibilities of Ehrenfest dynamics.

5.3 Ehrenfest statistical model

After writing it in the appropriate way, Ehrenfest equations are Hamiltonian with respect to the symplectic structure on the manifold M_{QC}. Therefore, from Liouville theorem, there exists a volume $\mathrm{d}\mu_{QC}$ on M_{QC} which is invariant under the dynamics. Such a volume is obtained as the product of the symplectic volumes on the classical and quantum manifolds:

$$\mathrm{d}\mu_{QC} = \mathrm{d}\mu_C \otimes \mathrm{d}\mu_{\mathcal{P}}. \tag{5.29}$$

This makes possible the definition of a Statistical Mechanical model where Ehrenfest equations defines the dynamics of the microstates. The results presented here are based on previous works by Alonso, Clemente-Gallardo and co-workers, the author among them [8–10, 14, 15].

Consider a probability density function on the manifold M_{QC}, i.e. a function satisfying a normalisation condition:

$$\int_{M_{QC}} \mathrm{d}\mu_{QC} F_{QC}(\xi, [\psi]) = 1, \tag{5.30}$$

From an empirical point of view, probability densities are needed in order to describe any molecular system. Indeed, in a laboratory, any macroscopic system interacting with the molecule has a certain distribution of states, associated to thermal motion or to a simple uncertainty of the exact state of the particles.

Recall that M_{QC} is a product manifold, and integration over the manifold can be solved by iterated integrals, firstly over M_C and secondly over $\mathcal{P}$, or vice versa. Thus, it is natural to consider the corresponding marginal probability density functions F_C and F_Q, which encode respectively the uncertainties of the classical and quantum degrees of freedom.

$$F_C(\xi) := \int_{\mathcal{P}} \mathrm{d}\mu_Q F_{QC}(\xi, [\psi]), \qquad F_Q([\psi]) := \int_{M_C} \mathrm{d}\mu_C F_{QC}(\xi, [\psi]), \qquad \xi \in M_C, \quad [\psi] \in \mathcal{P}. \tag{5.31}$$

A probability density function defines expectation values for any magnitude measured on the manifold, either classical, quantum or hybrid. The expectation value of a hybrid A observable, represented by a function $\epsilon_A(\xi, [\psi])$ on M_{QC}, is thus defined as

$$\langle A \rangle = \int_{M_{QC}} \mathrm{d}\mu_{QC} F_{QC}(\xi, [\psi]) \epsilon_A(\xi, [\psi]). \tag{5.32}$$

Consider the particular cases of a purely classical magnitude A_C, or on the contrary a purely quantum one A_Q. In these cases, the expectation values of the magnitudes can be computed by means of the corresponding marginal distributions:

$$\langle A_C \rangle = \int_{M_C} \mathrm{d}\mu_C F_C(\xi) f_{A_C}(\xi), \quad \langle A_Q \rangle = \int_{\mathcal{P}} \mathrm{d}\mu_Q F_Q([\psi]) \epsilon_{A_Q}([\psi]), \tag{5.33}$$

Thus, classical and quantum Statistical Mechanics are recovered. In fact, observe that the second equation gives the expectation value for a quantum observable, which can therefore written in a more standard way [14]. By Gleason's theorem, there exists a density matrix $\hat{\rho}$ such that

$$\langle A_Q \rangle = \mathrm{Tr}(\widehat{\rho} A_Q). \tag{5.34}$$

This density matrix can be explicitly obtained by averaging the projectors on the quantum states by the distribution F_{QC}:

$$\widehat{\rho} = \int_{M_{QC}} \mathrm{d}\mu_{QC} F_{QC}(\xi, [\psi]) \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} = \int_{\mathcal{P}} \mathrm{d}\mu_Q F_Q([\psi]) \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}. \tag{5.35}$$

As presented in Section (3.1.5), when dealing with statistical quantum ensemble, density matrices are correct object that describes their properties. The reason has to do with the superposition principle of Quantum Mechanics. Pure states, represented by points in the quantum manifold $\mathcal{P}$, are not independent. Thus, for any probability density function on $\mathcal{P}$ there exist equivalent functions which give the same expectation value for any observables of the system. All of them are represented by the same density matrix.

Hybrid classical-quantum system present analogous characteristics. By (5.35), quantum marginal distributions are represented by density matrices for the quantum subsystem. This concept can be extended to properly describe the total probability distribution F_{QC}, which also presents some ambiguity in the quantum degrees of freedom.

Proposition 5.4. *For every probability distribution F_{QC} on M_{QC} and every $\xi \in M_C$, let $\widehat{\rho}(\xi)$ be the operator defined as*

$$\widehat{\rho}(\xi) := \int_{\mathcal{P}} \mathrm{d}\mu_Q F_{QC}(\xi, [\psi]) \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}. \tag{5.36}$$

This is a Hermitian, positive operator whose trace gives the classical marginal distrubition functions,

$$F_C(\xi) = \mathrm{Tr}(\rho(\xi)), \quad \forall \xi \in M_C, \tag{5.37}$$

If a quantum-classical observable A defines for every $\xi \in M_C$ a quantum observable $A(\xi) \in \mathcal{O}_Q$, then the expectation value of A is

$$\langle A \rangle = \int \mathrm{d}\mu_C \mathrm{Tr}(\widehat{\rho}(\xi) A(\xi)). \tag{5.38}$$

Proof. The expression of $F_C(\xi)$ is deduced from (5.31) and (5.36). Regarding the expectation values of observables, if A defines a ξ-dependent quantum observable, then its corresponding function ϵ_A on M_{QC} is given by (5.22). This expression, together with (5.32) and (5.36), proves the result. □

Observe that the operator $\rho(\xi)$ is not of unit trace, thereforeit is not a density matrix. It is however a positive, Hermitian operator, and it is related with the density matrix $\widehat{\rho}$ of the quantum subsystem by the following relation:

$$\widehat{\rho} = \int_{M_C} \mathrm{d}\mu_C \ \widehat{\rho}(\xi) = \int_{\mathcal{P}} \mathrm{d}\mu_Q F_Q([\psi]) \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}. \tag{5.39}$$

In order to understand the difference between these objects, consider Gleason's theorem. For each $\xi \in M_C$, it is possible to apply the theorem to the probability density defined by $F_{QC}(\xi, [\psi])$, in order to obtain a density matrix describing the expectation values of quantum observables. For this reason, $\widehat{\rho}(\xi)$ is Hermitian and positive for every $\xi \in M_C$. It is not, however, of unit trace, as $F_{QC}(\xi, [\psi])$ is not normalised for a fixed value of ξ. Normalisation only occurs for the whole manifold M_{QC}; indeed, it is immediate to prove that

$$\int_{M_C} \mathrm{d}\mu_C \mathrm{Tr}(\widehat{\rho}(\xi)) = \mathrm{Tr}(\widehat{\rho}) = 1. \tag{5.40}$$

Some examples are useful in order to illustrate the introduced concepts. The simplest distribution on M_{QC} is given by Dirac's delta functions:

$$F_{QC}(\xi,[\psi]) = \delta(\xi-\xi_0)\delta([\psi]-[\psi_0]), \quad (\xi_0,[\psi_0]) \in M_{QC}. \tag{5.41}$$

The corresponding density matrix representation is

$$\widehat{\rho}(\xi) = \delta(\xi-\xi_0)\frac{|\psi_0\rangle\langle\psi_0|}{\langle\psi_0|\psi_0\rangle}. \tag{5.42}$$

The next step is to consider some uncertainty on the initial conditions of any of the two subsystems. For example, if the uncertainty is presented in the classical subsystem, then the distribution is

$$F_{QC}(\xi,[\psi]) = f(\xi)\delta([\psi]-[\psi_0]), \quad [\psi_0] \in \mathcal{P}. \tag{5.43}$$

The corresponding density matrix is

$$\widehat{\rho}(\xi) = f(\xi)\frac{|\psi_0\rangle\langle\psi_0|}{\langle\psi_0|\psi_0\rangle}. \tag{5.44}$$

This case describes a flat distribution of molecules whose quantum degrees of freedom are at the initial state ψ_0 but whose classical subsystems are described by a distribution $f(\xi)$. This is the case studied in [14] for a simplified model where the distribution was chosen as

$$f(\xi) = \frac{1}{N}\sum_{k=1}^{N}\delta(\xi-\xi_k), \quad \xi_1,\ldots,\xi_N \in M_C. \tag{5.45}$$

Another physically relevant case, namely the canonical ensemble of hybrid quantum-classical systems [9, 10, 15], are considered in Section 5.5.

Once that the statistical model is describe, it is possible to incorporate dynamics. Consider the Ehrenfest dynamics on the product manifold $M_{QC} = M_C \times \mathcal{P}$. As the dynamics is Hamiltonian with respect to the function f_H defined in (5.25) , the volume element $d\mu_{QC}(\xi,\psi)$ is invariant with respect to the evolution. This makes possible to consider the Liouville equation [33, 34], which determines trajectories $F_{QC}(t)$ on the space of distributions:

$$\frac{\mathrm{d}}{\mathrm{d}t}F_{QC}(t) = \{\epsilon_H, F_{QC}(t)\}_{QC}, \tag{5.46}$$

As dynamics preserves the volume, the evolution $F_{QC}(t)$ of a distribution defines in turn an evolution for the density matrix of the quantum subsystem:

$$\widehat{\rho}(t) = \int_{M_{QC}} \mathrm{d}\mu_{QC} F_{QC}(\xi,[\psi];t)\frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}. \tag{5.47}$$

This evolution is, in general, quite complicated from a mathematical point of view, and certainly can not be written as the solution of von Neumann master equation, even if Ehrenfest electronic equation in (5.14) were linear [14].

From this point of view, the statistical version of Ehrenfest dynamics is powerful enough to incorporate at least some of the correlation between nuclear and electronic degrees of freedom that is lost in the purely dynamical Ehrenfest model. Furthermore, the geometric approach, which does not depend on any particular choice of basis for the system, makes possible to consider an intrinsic definition of decoherence time. For a system losing coherence along evolution, it shall be consider that such decoherence time is reached when its purity stabilises.

5.4 Decoherence-like effects for diatomic molecules

The geometric description of the Ehrenfest model and its extension to statistical ensembles has considerable potential. In order to illustrate the theory, particular examples have been studied. Namely, the evolution of statistical ensembles of diatomic molecules under the Ehrenfest dynamics. This section presents a detailed description of the problem and the method used in order to obtain significant results. The initial statistical ensemble is constructed in such a way that all the uncertainty is on the classical degrees of freedom. Therefore, the quantum density matrix corresponds to a pure state. This choice of the initial conditions allows for an optimal characterisation of the decoherence effects appearing along evolution.

Recall that the geometric formalism used to describe hybrid quantum-classical systems is the reason why statistics and dynamics can be successfully combined. It is thus possible to consider the evolution of the initial distribution, which in turns defines a time-dependent density matrix for the quantum subsystem, which is in general not pure. Explicit computations of the purity of the quantum system along time are also presented.

5.4.1 Modellisation of diatomic molecules

According to the Ehrenfest model, diatomic molecules are divided in a classical and a quantum subsystem. The quantum subsystem is composed of the valence electrons, while the cores of the molecule form the classical subsystem. In this case, there are only 2 cores, thus the classical phase space is $M_C = \mathbb{R}^{12}$. Classical degrees of freedom are the position $\mathbf{R}_1, \mathbf{R}_2$ and momenta $\mathbf{P}_1, \mathbf{P}_2$ of the cores.

In order to simplify the model, the atoms composing the molecule are assumed to be identical and of unit valence. Thus, the masses of the cores are $M_1 = M_2 := M$, while their electric charge is $Z_1 = Z_2 = 1$. There are many physical examples of such molecules: $H_2, Na_2, \ldots$

Regarding the quantum subsystem, a further simplification is made. For practical reasons that will be made clear later, the molecule is assumed to be ionised. Thus, there is a single valence electron in the quantum subsystem. The evolution of the system is determined by equations (5.14) of the Ehrenfest model, with electronic Hamiltonian given by

$$H_e(R) = -\frac{\hbar^2}{2m_e}\nabla^2 + \frac{1}{4\pi\epsilon_0}\frac{1}{|\mathbf{R}_1 - \mathbf{R}_2|} - \frac{1}{4\pi\epsilon_0}\sum_{J=1}^{2}\frac{1}{|\mathbf{R}_J - \mathbf{r}|}. \tag{5.48}$$

The initial statistical ensemble of molecules is defined as follows. The valence electron is assumed to be in a completely determined state $[\psi_0] \in \mathcal{P}$, while the cores are described by a distribution over a set of N equally probable discrete points $\xi_1, \ldots, \xi_N \in M_C$. The initial distribution is thus:

$$F_{QC}(\xi, [\psi]; 0) = \frac{1}{N}\sum_{k=1}^{N}\delta(\xi - \xi_k)\delta\big([\psi] - [\psi_0]\big). \tag{5.49}$$

This is a natural assumption, as in practice it is impossible to determine with complete precision the initial state of the particles.

The evolution of this statistical system is computed by solving the Ehrenfest dynamics N times. For the initial condition $(\xi_k, [\psi_0])$, with $k = 1, 2, \ldots, N$, the corresponding solution of the Ehrenfest equations (5.14) are denoted as $(\xi_k(t), [\psi_k(t)])$. The resulting set of trajectories determine the distribution $F_{QC}(\xi, [\psi]; t)$ at any time as

$$F_{QC}(\xi, [\psi]; t) = \frac{1}{N}\sum_{k=1}^{N}\delta(\xi - \xi_k(t))\delta\big([\psi] - [\psi_k(t)]\big), \quad t \geq 0. \tag{5.50}$$

Observe that, unlike (5.49), this distribution is no longer separable in classical and quantum degrees of freedom.

The evolution of the density matrix ρ for the quantum subsystem is immediately computed as

$$\widehat{\rho}(t) = \int_{M_{QC}} \mathrm{d}\mu_{QC}\ F_{QC}(\xi,[\psi];t)\frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} = \frac{1}{N}\sum_{k=1}^{N}\frac{|\psi_k(t)\rangle\langle\psi_k(t)|}{\langle\psi_k(t)|\psi_k(t)\rangle}. \tag{5.51}$$

The quantum state described by this density matrix is, in general, mixed.

5.4.2 Characterisation of the numerical simulations

In order to explicitly solve the Ehrenfest dynamics, numerical methods are required. Simulations have been performed using the Octopus code. As described in its web page[1],

> 'Octopus is a scientific program aimed at the ab initio virtual experimentation on a hopefully ever-increasing range of system types. Electrons are described quantum-mechanically within density-functional theory, in its time-dependent form when doing simulations in time. Nuclei are described classically as point particles. Electron-nucleus interaction is described within the pseudopotential approximation'.

The code for Octopus has been developed for the last years by Andrade, Castro, Rubio and many others [24, 25, 89, 195]. It is a powerful tool in the analysis and characterisation of molecular systems, from simple systems to the most complex ones. It thus offers great possibilities for the statistical analysis of molecular systems, in particular the Ehrenfest model.

The computations of Octopus have been performed with the avaliable resources at the BIFI institute[2], in Zaragoza (Spain), of which the author is member. BIFI hosts, among many other computational resources, the computer Tesla, composed of two 12-core Xeon processors, together with a 24 GB common RAM. This is the computer on which the simulations have been implemented.

Observe that the description offered by Octopus is not the one offerd by the Ehrenfest model. Octopus implements density-functional theory simulations, based on the Kohn-Sham model. Without entering into details, it so happens that both models are identical for the case in which the quantum subsystem of the molecular system is composed of a single valence electron [13]. This is the practical reason why the model described in section 5.4.1 considers ionised molecules, thus having only one valence electron.

The simulations with Octopus are based on a discretisation of the three-dimensional space that describes the position of the valence electron. Thus, the wave function describing the state of the quantum subsystem takes values on a three-dimensional bounded grid, hence the corresponding Hilbert space is finite-dimensional. The grid is composed of equispaced points in $\mathbb{R}^3$, with the additional constraint of belonging to the bulk of a sphere of radius r_G, centred at the origin. Hence points in the grid take the form

$$(a\delta, b\delta, c\delta) \in \mathbb{R}^3, \quad (a^2+b^2+c^2)\delta^2 \leq r_G^2, \quad a,b,c \in \mathbb{Z}, \tag{5.52}$$

with δ the grid parameter. This parameter is to be taken small enough, and the radius large enough, so that the accuracy of the results is not compromised.

For practical purposes, the electrostatic potential between cores cannot be modelled directly by the Coulomb potential. The divergence in the potential when the distance between cores goes to zero presents computational problems. Octopus offers the possibility of using user-defined electrostatic potential. Thus, instead of the Coulomb potential in (5.6), the following approximate potential is used in the simulations:

$$V_a(\mathbf{R}_1,\mathbf{R}_2) = -\frac{1}{4\pi\epsilon_0}\left(a^2+|\mathbf{R}_1-\mathbf{R}_2|^2\right)^{-1/2}, \tag{5.53}$$

with a a positive parameter that has to be specified.

[1] www.tddft.org/programs/octopus.

[2] BIFI is the short name for the 'Instituto de Computación y Física de Sistemas Complejos' (*Institute for Biocomputation and Physics of Complex Systems*), located at Edificio I+D, c/Mariano Esquillor, 50.018 Zaragoza (Spain).

Octopus allows for the computation of the spectrum and eigenvectors of the electronic Hamiltonian $H_e(\xi)$ for a given configuration of the cores. This makes possible a further simplification in the computations, and mainly in the storage, of simulations. The n_H lower eigenvalues of the spectrum, are computed for the initial configuration of the cores. Their corresponding eigenvectors are used as a truncated bases for the Hilbert space of the quantum system. Thus, the states of the quantum subsystem are described by elements in $\mathcal{H} \cong \mathbb{C}^{n_H}$ (or rather in its projective space). By taking adequate values of n_H, simulation time and required storage space are significantly reduced without compromising the accuracy of the results.

In order to characterise the cores, their mass, initial positions and initial momenta have to be determined. A consideration has to be done regarding masses. Observe that the model described in Section 5.4.1 accurately described a ionised hydrogen molecule H_2^+. It is not advisable, however, to consider this system as a model. The reason has to do with the small mass of the hydrogen atom. It has been proved in literature that hybrid quantum-classical systems are not accurate enough to describe such small atoms. A larger mass is thus preferable. For the simulations, the atomic mass of the sodium is used, thus $M = 23$ a.u.. For practical purposes, the parameter $a = 0.4$ in (5.53) is chosen.

In order to finish the description of the simulations, the initial conditions of the cores have to be described. It is advisable to consider identical initial positions of the cores for a given statistical ensemble. Thus, the basis of $\mathcal{H}$ given by the electronic Hamiltonian is common for all the simulations. The evolution under the Ehrenfest dynamics consists of vibrations of the cores around the equilibrium positions of the cores for the given state of the electron. These are taken as the initial positions $\mathbf{R}_{1,0}$ and $\mathbf{R}_{2,0}$ of the cores.

5.4.3 Parameter fitting

Numerical computations can be performed with Octopus in order to obtain the equilibrium energy of the molecular system for each configuration of the cores and each value of the parameters δ, r_G and a in (5.52) and (5.53). These simulations, in turn, allow for the determination of the optimal values for these parameters.

The grid parameters δ and r_G determine the number of points in the grid. If this number is not large enough, the electronic wave functions is not accurately computed and numerical problems arise. In order to fix the values of the parameters, ground state computations may be performed.

Recall that the electronic Hamiltonian $H_e(R)$ depends parametrically on the classical degrees of freedom of the system. A ground state computation gives, for each $R \in \mathbb{R}^6$, the ground state energy $E_0(R)$ of the electronic Hamiltonian. The cores are seized in rest; thus, the total energy $E_T(R)$ of the molecular system is obtained by evaluating (5.25):

$$E_T(R) = \frac{1}{4\pi\epsilon_0}(a^2 + |\mathbf{R}_1 - \mathbf{R}_2|^2)^{-1/2} + E_0(R). \tag{5.54}$$

A large number of grid points is necessary in order to obtain valid results. Figure 5.1 shows the ground state energy $E_0(R)$ for some ground state computations. These are performed for fixed positions of the cores and with different values δ and r_G. By examining these graphics, the following values for the parameters are chosen:

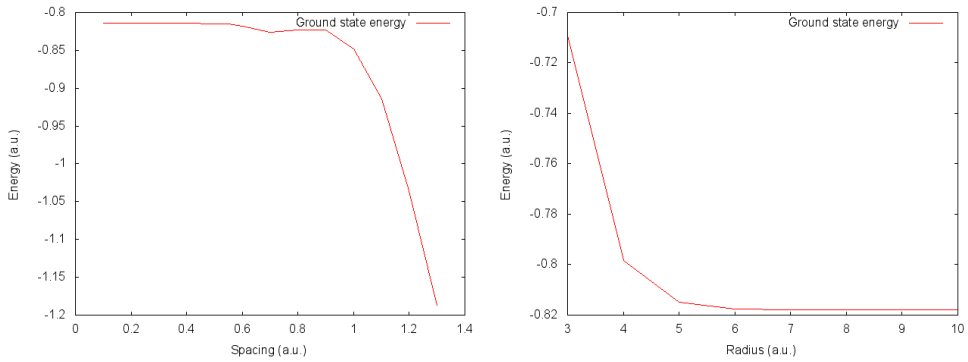
$$\delta = 0.6 \text{ a.u.}, \quad r_G = 6.5 \text{ a.u.} \tag{5.55}$$

The value for a models the radius of the cores, as it represents the repulsion among the inner atomic electrons. Figure 5.2 shows, for $a = 0.4$ a.u., the total energy $E_T(R)$ of the molecular system (5.54) in terms of the distance between the cores. The minimum total energy corresponds to a distance of 2.69554 a.u..

If the x-axis is chosen along the line linking the cores and the centre os mass is take and the origin of coordinates, then the equilibrium positions of the cores for the ground state energy are approximately taken as

$$\mathbf{R}_1 = (1.3 \text{ a.u.}, 0, 0), \quad \mathbf{R}_2 = (-1.3 \text{ a.u.}, 0, 0). \tag{5.56}$$

With this choice, the centre of mass of the classical subsystem is at the centre of the grid.



(a) Ground state energy for $r_G = 6.5$ a.u. **(b)** Ground state energy for $\delta = 0.6$ a.u.

Figure 5.1: Ground state simulations for $a = 0.4$. The cores are in positions $\mathbf{R}_{1,0} = (1.3 \text{ a.u.}, 0, 0)$ and $\mathbf{R}_{2,0} = (-1.3 \text{ a.u.}, 0, 0)$. Graphic (a) represents the ground state energy of simulations performed by varying the grid parameter δ, with a fixed grid radius $r_G = 6.5$ a.u. Conversely, simulations whose ground state energies are represented in (b) are performed varying the grid radius r_G, while keeping fixed the grid parameter as $\delta = 0.6$ a.u. In both graphics, the ground state energy stabilises for large numbers of grid points.

5.4.4 Initial statistical ensembles

Different statistical ensembles are characterised by the initial state $[\psi_0] \in \mathcal{P}$ of the quantum subsystem and the set of initial classical degrees of freedom $\xi_1, \ldots, \xi_N \in M_C$, as seen in (5.49). Large enough statistical samples are obtained for $N = 40$. In order to simplify the computations, the positions of the cores are taken constant; thus, the initial classical degrees of freedom are of the form

$$\xi_j = (\mathbf{R}_{1,0}, \mathbf{R}_{2,0}, \mathbf{P}_{1,j}, \mathbf{P}_{2,j}), \quad j = 1, 2, \ldots, 40. \tag{5.57}$$

In the following, the initial states of the quantum system for the statistical ensembles is given in terms of the eigenstates $\{|\phi_0(R_0)\rangle, |\phi_1(R_0)\rangle, \ldots\}$ of the electronic Hamiltonian $H_e(R_0)$ for the initial positions of the cores. Three different statistical ensembles are considered:

1. For the first statistical ensemble, the initial quantum state is taken as the first excited state of the electronic Hamiltonian:

$$|\psi_0\rangle = |\phi_1(R_0)\rangle. \tag{5.58}$$

The initial positions of the cores are taken as their equilibrium positions for this quantum state. These equilibrium positions are computed by performing numerical simulations with Octopus. These simulations show that the cores vibrates about the equilibrium positions; the oscillation amplitude depends on the initial distance to the equilibrium positions. By performing several simulations, it is possible to find initial conditions for which the amplitude of oscillation is negligible. These are taken as the the equilibrium positions of the cores; their values are

$$\mathbf{R}_{1,0} = (3.35 \text{ a.u.}, 0, 0), \quad \mathbf{R}_{2,0} = (-3.35 \text{ a.u.}, 0, 0). \tag{5.59}$$

The initial momenta of the cores have to be carefully chosen. Small momenta would yield almost static dynamics, while large momenta would cause dissociation of the molecule or, at least, unrealistic behaviour. Numerical computations show that momentum initial values up to $4 \cdot 10^{-5}$ a.u. produce reasonable dynamics, as seen in Figures 5.3a and 5.3b. Observe that oscillations occur, approximately, around the positions proposed in (5.59). The initial momenta of the cores are also chosen so that the centre of mass is static and the movement occurs. The following values have

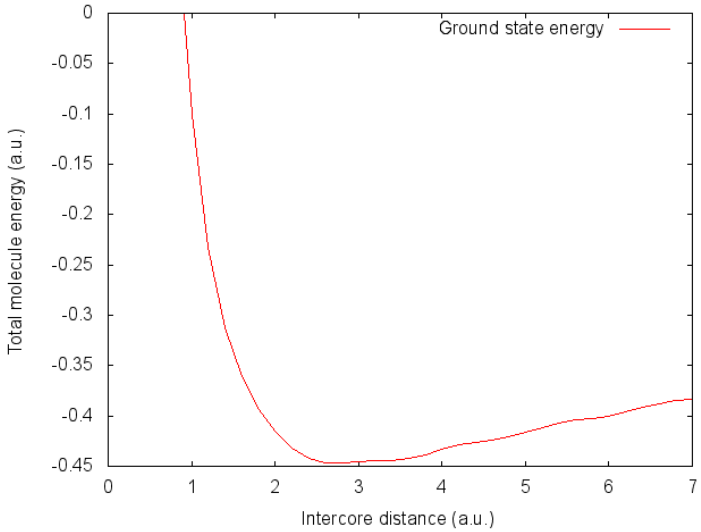


Figure 5.2: Total energy $E_T(R)$ of the diatomic molecule for $a = 0.40$ a.u. The minimum energy corresponds to an interatomic distance of 2.69554 a.u.

been chosen:

$$\begin{aligned}
&\mathbf{P}_{1,1} = (0.1 \cdot 10^{-4} \text{ a.u.}, 0, 0), \ \mathbf{P}_{2,1} = (-0.1 \cdot 10^{-4} \text{ a.u.}, 0, 0);\\
&\mathbf{P}_{1,2} = (0.3 \cdot 10^{-4} \text{ a.u.}, 0, 0), \ \mathbf{P}_{2,2} = (-0.3 \cdot 10^{-4} \text{ a.u.}, 0, 0);\\
&\ldots;\\
&\mathbf{P}_{1,20} = (3.9 \cdot 10^{-4} \text{ a.u.}, 0, 0), \ \mathbf{P}_{2,20} = (-3.9 \cdot 10^{-4} \text{ a.u.}, 0, 0);\\
&\mathbf{P}_{1,21} = (-0.1 \cdot 10^{-4} \text{ a.u.}, 0, 0), \ \mathbf{P}_{2,21} = (0.1 \cdot 10^{-4} \text{ a.u.}, 0, 0);\\
&\mathbf{P}_{1,22} = (-0.3 \cdot 10^{-4} \text{ a.u.}, 0, 0), \ \mathbf{P}_{2,22} = (0.3 \cdot 10^{-4} \text{ a.u.}, 0, 0);\\
&\ldots;\\
&\mathbf{P}_{1,40} = (-3.9 \cdot 10^{-4} \text{ a.u.}, 0, 0), \ \mathbf{P}_{2,40} = (3.9 \cdot 10^{-4} \text{ a.u.}, 0, 0).
\end{aligned} \tag{5.60}$$

2. The initial quantum state for the second statistical ensemble is taken as a linear combination of the ground state and the excited state of the electronic Hamiltonian:

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}(|\phi_0(R_0) + |\phi_1(R_0))\rangle. \tag{5.61}$$

The initial positions of the cores are again taken as their equilibrium positions for this state of the quantum subsystem. Their values are found to be:

$$\mathbf{R}_{1,0} = (2.70 \text{ a.u.}, 0, 0), \quad \mathbf{R}_{2,0} = (-2.70 \text{ a.u.}, 0, 0). \tag{5.62}$$

Initial momenta of the cores are again given by (5.60). Figures 5.3c and 5.3d show oscillations for some of these values, which again occur around the proposed positions for the cores.

3. For the third statistical ensemble, the initial quantum state is taken as a linear combination of the three first eigenvectors of the electronic Hamiltonian:

$$|\psi_0\rangle = \frac{1}{\sqrt{3}}(|\phi_0(R_0) + |\phi_1(R_0) + |\phi_2(R_0))\rangle. \tag{5.63}$$

The initial positions of the cores are taken as the equilibrium positions of the cores, whose values are

$$\mathbf{R}_{1,0} = (2.70 \text{ a.u.}, 0, 0), \quad \mathbf{R}_{2,0} = (-2.70 \text{ a.u.}, 0, 0). \tag{5.64}$$

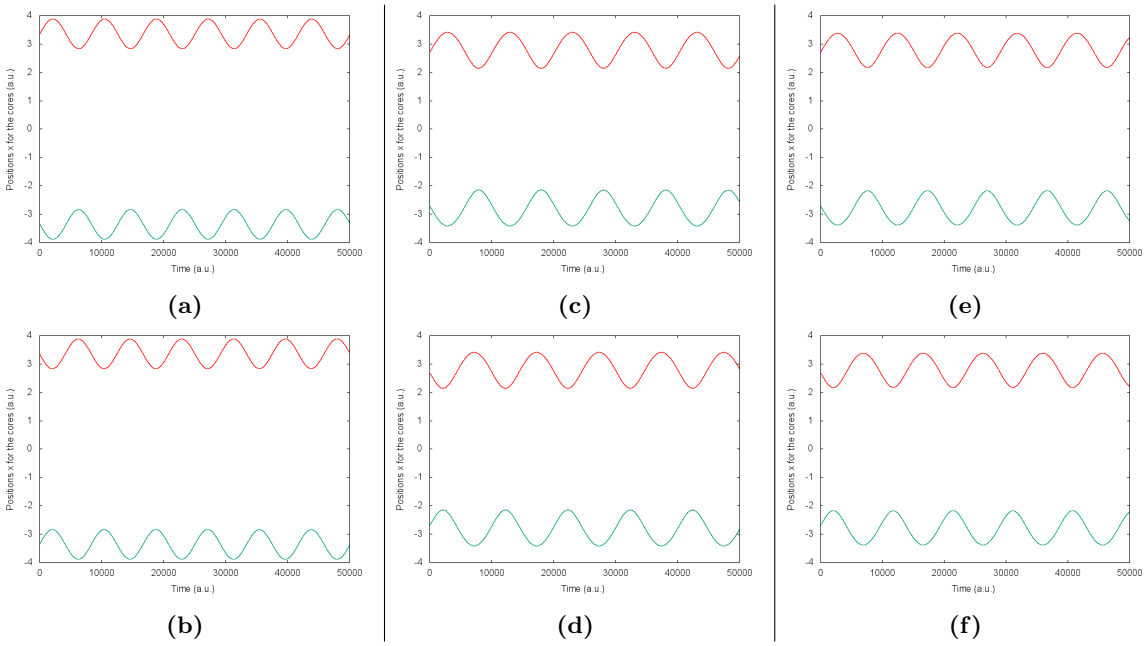


Figure 5.3: Oscillations of the cores along the x-axis for the proposed initial conditions, with the maximum values of the momenta proposed in (5.60), i.e. values $\mathbf{P}_{1,20}, \mathbf{P}_{2,20}$ and $\mathbf{P}_{1,40}, \mathbf{P}_{2,40}$, with module $3.9 \cdot 10^{-4}$ a.u.. Each pair of graphisc corresponds to a different statistical ensamble. Graphics (a) and (b) are obtained by taken as initial conditions the ones proposed for the first statistical ensemble in (5.58) and (5.59). Graphics (c) and (d) correspond to the second statistical ensemble, with initial conditions (5.61) and (5.62). Graphics (e) and (f) represent oscillations for the initial conditions proposed for the third statistical ensemble in (5.63) and (5.64).

Initial momenta of the cores are taken by (5.60), as in the previous cases. Figures 5.3e and 5.3f show oscillations for some these values.

Numerical simulations for each set of initial conditions have been performed. Each simulation computes the molecular dynamics for a time of $50,000$ a.u., which corresponds roughly to 5 oscillations of the molecule, as in the graphics in Figure 5.3. With the chosen parameters, the molecular system is stable for this simulation time. The time step used in the simulations is 0.1 a.u., having thus simulated 500,000 time steps for a total of 120 trajectories.

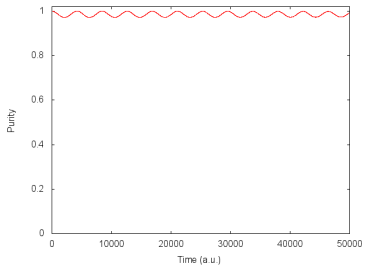
As a result of the simulations, trajectories $(\xi(t), [\psi(t)])$ on M_{QC} are obtained. They define the time-dependent distribution $F_{QC}(\xi, [\psi]; t)$, given by (5.50):

$$F_{QC}(\xi, [\psi]; t) = \frac{1}{N} \sum_{k=1}^{N} \delta(\xi - \xi_k(t)) \delta([\psi] - [\psi_k(t)]), \quad t \geq 0. \tag{5.65}$$

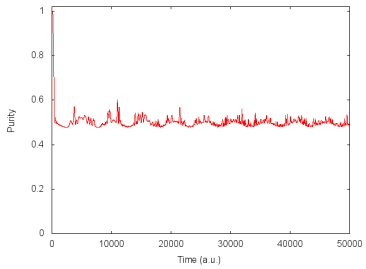
The aim of the simulations is the study of the properties of the quantum subsystem in each statistical ensemble. These properties can be computed by means of the density matrix of the quantum subsystem, whose value is given by (5.51):

$$\widehat{\rho}(t) = \int_{M_{QC}} \mathrm{d}\mu_{QC} \; F_{QC}(\xi, [\psi]; t) \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} = \frac{1}{N} \sum_{k=1}^{N} \frac{|\psi_k(t)\rangle\langle\psi_k(t)|}{\langle\psi_k(t)|\psi_k(t)\rangle}. \tag{5.66}$$

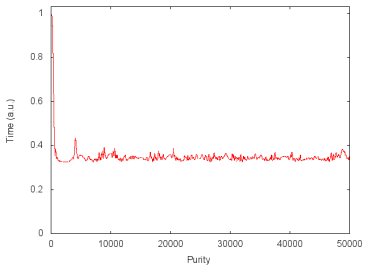
Thus, once that the computations have been performed, it is immediate to compute $\widehat{\rho}(t)$, thus characterising the system.



(a) Purity for the ensemble *1.*



(b) Purity for the ensemble *2.*



(c) Purity for the ensemble *3.*

Figure 5.4: Purity of the quantum subsystem for the three statistical ensembles. In all cases, purity approximately stabilises around the value $1/n$, with n the number of eigenstates of the electronic Hamiltonian that form the initial state of the ensemble.

5.4.5 Numerical results: decoherence-like effects

Recall that the purity of a quantum state represented by a density matrix $\widehat{\rho}$ is a scalar with value

$$P(\widehat{\rho}) = \mathrm{Tr}(\widehat{\rho}^2). \tag{5.67}$$

The purity of a pure state is 1, while mixed states have lower purity. For a system with n possible states, the lowest value of the purity is $\frac{1}{n}$; it corresponds to the maximally entangled state of the system.

Purity can be computed for the simulated statistical ensembles. The value of purity for the whole simulation time and for each of the three statistical ensembles appears in Figure 5.4. A qualitative difference appears between the different ensembles. The first ensemble shows that the purity of the subsystem is constant and equal to 1. Thus, the quantum state is always pure. This result proves that the eigenstates of the electronic Hamiltonian are very stable along evolution (similar results have been obtained for other initial states).

The other ensembles show completely different behaviours. The purity greatly decreases in the first part of the simulation, and after that it only suffers small variations. Several conclusions can be deduced from this graphics:

- The lower value of the purity is related with the number of eigenvectors of $H_e(R_0)$ considered in the initial state of the system. Graphic 5.4b resembles the decoherence of a 2-level system, which would have a minimum for the purity of 0.5. Similarly, graphic 5.4c could represent the behaviour of a 3-level system, with $\frac{1}{3}$ being the minimum of the purity. The actual purity has in fact smaller values. This may be due to the fact that the basis of the electronic Hamiltonian changes with the positions of the cores, and more than 2 or 3 eigenvectors have to be considered to fully describe the state of the electron. Anyway, this result proves that the asymptotic value of purity does not correspond to a distribution of random projectors as it happened in the toy model considered in [14]. Instead, the purity reflects the emergence of relevant projectors of $\widehat{\rho}(t)$, related with the eigenvectors of $H_e(R_0)$ considered in the initial states.

- Consider the ensembles in which decoherence-like effects, in particular changes in purity, appears. These effects are in direct relation with the number of trajectories considered in the sample. Figure 5.5 represents the value of the purity for values of the number N of total simulations between 2 and 40, for ensemble number *2.* (whose purity is represented in Figure 5.4b). For low numbers of N, purity shows a periodical behaviour that disappears when more trajectories are considered. This graphic shows that the relative maxima in the purity presented in Figure 5.4b are remininscences of this periodic behaviour. In the limit $N \to \infty$, it is expectable for these small variations to dissapear. Thus, the statistical Ehrenfest model correctly predicts the behaviour of purity in systems subject to the decoherence phenomenon.

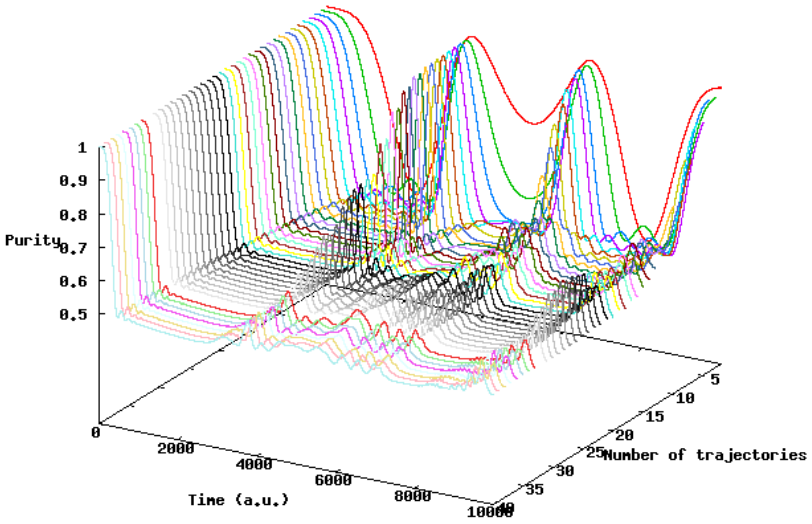


Figure 5.5: Purity of the ensemble number *2.*, with initial conditions given by (5.60), (5.61) and (5.62). The purity is computed for different numbers N of trajectories, between 2 and 40. The purity for $N = 40$ coincides with the graph in Figure 5.4b. While the purity for low numbers of N presents a periodic behaviour (specially for $N = 2, 3$), the decoherence-like behaviour is clear for large values of N. The decoherence time stabilises and the oscillations in the value of the purity become smaller, thus proving the appearance of decoherence-like properties in the statistical description of the Ehrenfest model.

- Observe that small periodic oscillations appear in 5.4b, and also slightly in 5.4c. This corresponds precisely with the oscillations of the cores, as seen in 5.3. Again, the positions of the cores determine the electronic Hamiltonian $H_e(R)$ and its spectrum. As oscillations of the cores are approximately harmonic, all of them pass through the equilibrium position at similar times. When this occurs, the resemblance with 2-level and 3-levels systems is more accurate, and the relative minimum of the purity goes to $\frac{1}{2}$ or $\frac{1}{3}$, respectively.

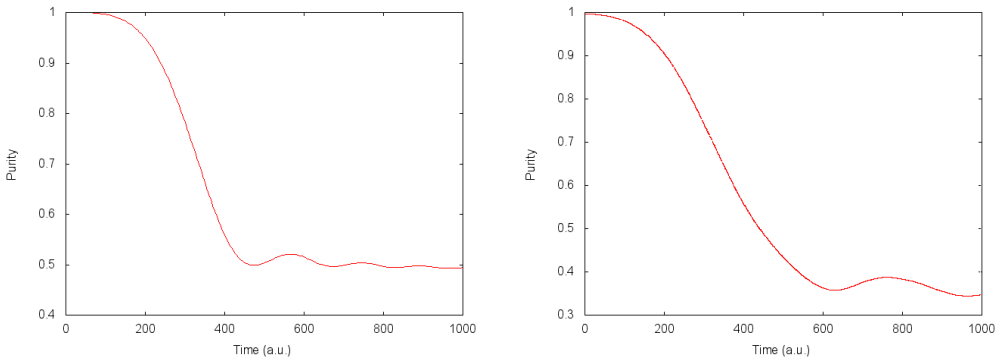
- Decoherence time can be estimated as the time in which the purity of the system reaches values near its minimum. Figure 5.6 offers the value of the purity for the first part of the simulation. Estimated values for the decoherence time are 450 a.u. for the second statistical ensemble and 650 a.u. for the third statistical ensemble. Observe also in 5.5 that decoherence time depends on the number N of considered trajectories, and stabilises for large values.

An analogous characterisation can be carried in terms of the von Neumann entropy of the quantum subsystem. Its value for a density matrix $\widehat{\rho}$ is

$$S_N(\widehat{\rho}) = -\widehat{\rho}\ \ln(\widehat{\rho}) = -\sum_{\lambda \in \mathrm{spec}(\widehat{\rho})} \lambda \ln(\lambda). \tag{5.68}$$

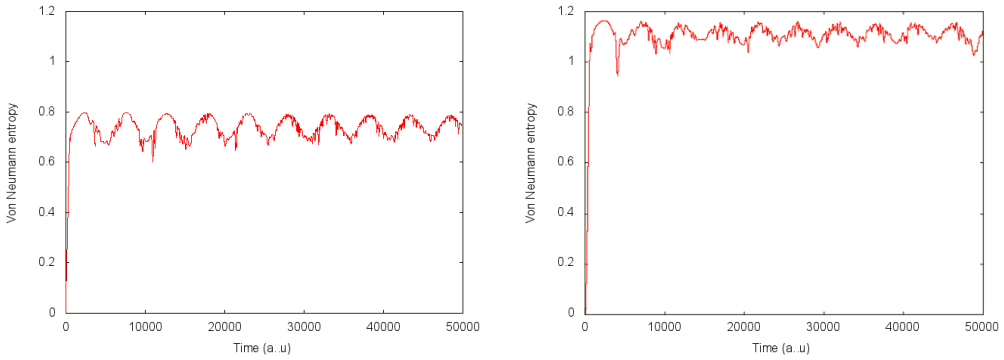
The von Neumann entropy is shown in Figure 5.7. As seen, the results are in accordance to those obtained for the purity.

Observe that the behaviour of both purity and von Neumann entropy is similar to the evolution of bipartite systems with entanglement between their parts. The Hamiltonian evolution of a system preserves coherence; however if one part of the system is traced out and there exists entanglemente, the remaining subsystem does not evolve in general in a coherent way. Formally, the same situation



(a) **(b)**

Figure 5.6: Enlargement of the first part of graphics 5.4b and 5.4c, respectively.



(a) **(b)**

Figure 5.7: Von Neumann entropy of the quantum subsystem for the statistical ensembles given by **(a)** initial state (5.61) and **(b)** initial state (5.63).

occurs in the description of the statistical Ehrenfest model. The description of the quantum subsystem in terms of density matrices is equivalent to the concept of partial trace in bipartite systems. While no true entanglement can occur between classical and quantum subsystems, as discussed in Section 5.2.1, statistical ensembles act on a similar way, as it is no longer possible to consider separately both subsystems.

Summarising, it can be concluded that the use of a statistical model based on Ehrenfest dynamics does provide a framework to describe non-coherent evolutions of molecular systems. It allows to take into account, to some extent, the correlation of the nuclear and electronic degrees of freedom via the uncertainty transfer capabilities of the hybrid quantum-classical statistical framework.

5.5 The hybrid canonical ensemble for the Ehrenfest model

5.5.1 Hybrid microcanonical and canonical ensembles

The statistical description of the Ehrenfest model can be applied to relevant physical examples. In [10], both the microcanonical and the canonical ensembles were considered. Their definitions are simple, once that the geometric formalism has unified the description of the classical and quantum subsystems. The microcanical ensemble is defined as the probability distribution on M_{QC} where all points with energy E

are equally probable:

$$F^E_{Hm}(\xi,[\psi]) := \frac{1}{V_E}\delta(E-\epsilon_H(\xi,[\psi])), \quad V_E := \int_{M_{QC}} \mathrm{d}\mu_{QC}\ \delta\big(E-\epsilon_H(\xi,[\psi])\big), \quad (\xi,[\psi])\in M_{QC}, \quad (5.69)$$

that is, V_E is the volume of the subset $\epsilon_H^{-1}(E)\subset M_{QC}$. Observe that this is analogous to the microcanonical ensemble for pure quantum systems introduced by Brody and Hughston [62].

The hybrid microcanonical ensemble determined by F^E_{Hm} resembles the classical case because of the geometric characterisation of hybrid quantum-classical systems. Thus, tools of Statistical Mechanics are useful in this setting. The hybrid canonical ensemble can be directly defined by the following probability distribution:

$$F_{HC}(\xi,[\psi]) := \frac{1}{Z_{HC}} e^{-\beta\epsilon_H(\xi,[\psi])}, \quad (\xi,[\psi])\in M_{QC}, \quad (5.70)$$

where $\beta=(k_BT)^{-1}$ is the usual parameter of the canonical ensemble and H is the energy observable of the hybrid quantum-classical system. The partition function Z_{HC} is defined as expected:

$$Z_{HC} := \int_{M_{QC}} \mathrm{d}\mu_{QC}\ e^{-\beta\epsilon_H(\xi,[\psi])}. \quad (5.71)$$

Particularising to the case of molecular systems, the energy function ϵ_H is given by (5.25). It is thus possible to perform some computations on the partition function. Recall that the volume form is defined by (5.29). Thus, the integral in (5.71) can be separated as

$$Z_{HC} = \int_{M_C} \mathrm{d}\mu_C\ e^{-\beta\sum_J \frac{\mathbf{P}_J^2}{2M_J}} \int_{\mathcal{P}} \mathrm{d}\mu_{\mathcal{P}}\ e^{-\beta\epsilon_{H_e(R)}([\psi])}. \quad (5.72)$$

As $M_C=\mathbb{R}^{6m}$, positions and momenta of classical particles can be further separated. The integral in momenta is a simple Gaussian integral, which yields the following result:

$$Z_{HC} = \left(\frac{2\pi M_C}{\beta}\right)^{\frac{3m}{2}} \int_{\mathbb{R}^{3m}} \mathrm{d}R \int_{\mathcal{P}} \mathrm{d}\mu_{\mathcal{P}}\ e^{-\beta\epsilon_{H_e(R)}([\psi])}, \quad M_C := \left(\prod_{J=1}^m M_J\right)^{\frac{1}{m}}.$$

It is interesting to compute the ξ-dependent density matrix, defined in (5.36) for the general case. Its value in the hybrid canonical ensemble is

$$\widehat{\rho}_{HC}(\xi) = \int_{\mathcal{P}} \mathrm{d}\mu_Q F_{HC}(\xi,[\psi])\frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} = \frac{1}{Z_{HC}} e^{-\beta\sum_J \frac{\mathbf{P}_J^2}{2M_J}} \int_{\mathcal{P}} d\mu_{\mathcal{P}}\ e^{-\beta\epsilon_{H_e(R)}([\psi])}\frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}. \quad (5.73)$$

The formulas presented here are the starting point in the analysis of statistical distribution of molecular systems described by the Ehrenfest model.

Extensivity of molecular magnitudes is not a general property. Observe that the partition function (5.71) is not factorisable even for non-interacting Hamiltonians [9]. Thus, magnitudes such as the entropy or the internal energy of the system, which are derived from Z_{HC} are not in general extensive. Interestingly, extensivity is recovered for some magnitudes in the thermodynamic limit, as proved in [15] and reproduced below.

5.5.2 Numerical simulations for the hybrid canonical ensemble

The hybrid canonical ensemble can be incorporated into the statistical description of the Ehrenfest model previously discussed. In this way, it is possible to consider the validity of the formalism in a more realistic setting. Consider therefore a hybrid classical-quantum system an its associated symplectic manifold M_{QC}, as in Proposition 5.2. Let H be the Hamiltonian of the system and ϵ_H its expectation value function on M_{QC}. In the Ehrenfest model, Theorem 5.3 proves that the dynamics of the system is governed by

the Hamiltonian vector field X_H^{QC} associated with ϵ_H. As a consequence, the evolution of a probability density function F on M_{QC} obeys the Liouville equation (5.46):

$$\frac{\mathrm{d}}{\mathrm{d}t}F(t) = \{\epsilon_H, F(t)\}_{QC}, \tag{5.74}$$

Proposition 5.5. *The probability distribution function F_{HC} of the hybrid canonical ensemble, introduced in (5.70), is invariant under the dynamics described by the Ehrenfest model.*

Proof. Probability distribution function F_{HC} is defined only in terms of the expectation value function ϵ_H. Therefore, the Poisson bracket between both functions is zero, and by Liouville equation F_{HC} is constant in time. □

As a consequence, all quantities derived from F_{HC} are time independent. This is the case of the different objects describing the statistical ensemble. Consider in particular the marginal probability density function $F_{HC,C}$ for the classical subsystem:

$$F_{HC,C}(\xi) = \int_{\mathcal{P}} \mathrm{d}\mu_{\mathcal{P}} F_{HC}(\xi, [\psi]) = \mathrm{Tr}(\rho_{HC}(\xi)), \quad \forall \xi \in M_C, \tag{5.75}$$

Proposition 5.6. *Consider a molecular system with probability density described by the hybrid canonical ensemble. The marginal probability density function $F_{HC,C}$ for the classical subsystem takes the form*

$$F_{HC,C}(\xi) = \frac{1}{Z_{QC}} \exp\left(-\beta \sum_J \frac{\mathbf{P}_J^2}{2M_J} - \beta\, V_{eff}(R)\right), \tag{5.76}$$

where the effective potential V_{eff} is defined as

$$V_{eff}(R) := -\frac{1}{\beta} \ln\left[\int_{\mathcal{P}} \mathrm{d}\mu_{\mathcal{P}}\ e^{-\beta \epsilon_{H_e(R)}([\psi])}\right]. \tag{5.77}$$

Proof. Due to the particular expression of the Hamiltonian expectation value function ϵ_H, it is possible to separate the exponentials in R and P in expression (5.70) for F_{HC}. As a consequence, integration over the quantum degrees of freedom yields the proposed result. □

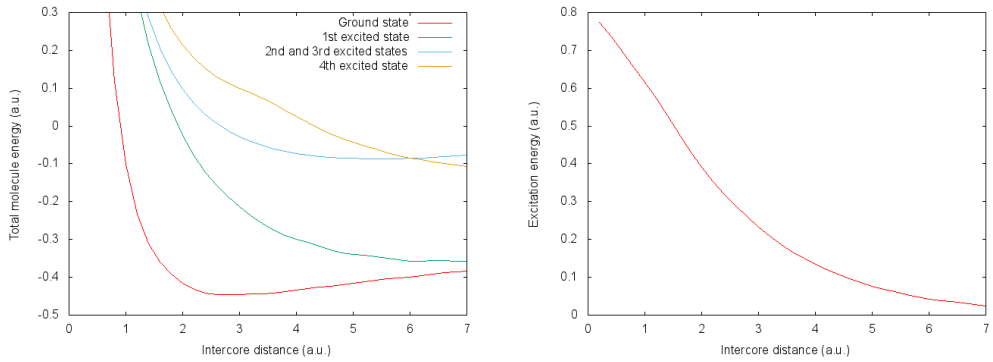
This proposition provides a useful characterisation of the probability density describing the classical subsystem. Indeed, it is identical to the one obtained for a canonical ensemble of the classical subsystem under potential V_{eff}. The interaction between the quantum and classical subsystems is thus incorporated in this effective potential, a powerful tool in the description of molecular dynamics. Observe also that the effective potential depends on the parameter β, hence the behaviour of classical particles, mainly oscillations, is expected to change with the temperature of the system.

Observe that it is always possible to write the effective potential as

$$V_{eff}(R) = E_0(R) - \frac{1}{\beta} \ln\left[\int_{\mathcal{P}} \mathrm{d}\mu_{\mathcal{P}}\ \exp\left(-\beta \frac{\langle\psi|H_e(R) - E_0(R)I|\psi\rangle}{\langle\psi|\psi\rangle}\right)\right]. \tag{5.78}$$

where $E_0(R)$ is the ground state energy for the electronic Hamiltonian $H_e(R)$. As the exponents in the integrand are always non-positive, it can be deduced that $V_{eff}(R) \leq E_0(R)$ for every positions R of the cores (see [11, 12]). Observe that the difference between the effective potential and the ground state energy depends on the temperature and the energy levels of the Hamiltonian.

In order to confirm the validity of this description of the hybrid canonical ensemble, numerical simulations have been performed. The chosen model is again an ionised diatomic molecule, as in simulations presented in Section 5.4. The molecule is assumed to evolve by the Ehrenfest model. Probabilities for



(a) **(b)**

Figure 5.8: **(a)** Eigenvalues of the electronic Hamiltonian $H_e(R)$ in (5.81), corresponding to the ground state and the 4 first excited states. **(b)** Difference between the ground state energy and the energy of the first excited state of $H_e(R)$.

each initial condition are computed from (5.70) with different values for β. Thus, the hybrid canonical ensemble for the Ehrenfest model is effectively represented by the following probability density function:

$$F'_{HC}(\xi,[\psi]) = \frac{1}{\zeta_{HC}} \sum_{j=1}^{N} \lambda(\xi_{0,j},[\psi_{0,j}])\, \delta(\xi-\xi_{0,j})\, \delta([\psi]-[\psi_{0,j}]), \quad (\xi,[\psi]) \in M_{QC}, \tag{5.79}$$

where $(\xi_{0,1},[\psi_{0,1}]),\dots,(\xi_{0,N},[\psi_{0,N}])$ are the initial conditions for the N simulations, and with the following definitions:

$$\lambda(\xi_{0,j},[\psi_{0,j}]) := e^{-\beta\epsilon_H(\xi_{0,j},[\psi_{0,j}])}, \quad j=1,2,\dots,N; \qquad \zeta_{HC} := \sum_{j=1}^{N} \lambda(\xi_j,[\psi_j]). \tag{5.80}$$

Recall that the value of ϵ_H is the total energy of the system (including kinetic, potential and electronic terms), as given in (5.25):

$$\epsilon_H(\xi,[\psi]) = \frac{1}{2M} \sum_{J=1}^{2} \mathbf{P}_J^2 + \frac{\langle\psi|H_e(R)|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{5.81}$$

The R-dependent eigenvalues of $H_e(R)$ are represented in Figure 5.8. In order to understand the relevance in the proposed statistical ensemble of each energy level, the difference between the two lowest eigenvalues $E_0(R)$ and $E_1(R)$ is also represented. From this graph the following lower bound can deduced:

$$E_1(R) - E_0(R) > 0.01 \text{ a.u.}, \tag{5.82}$$

for the relevant positions R in the simulation. From this bound, it can be deduced for which temperatures the contribution of the two lowest energy levels are comparable:

$$\frac{0.01 \text{ a.u.}}{k_B T} = 1 \Rightarrow T = 3,157\,\text{K}, \tag{5.83}$$

with the value $k_B = 3.1668 \cdot 10^{-6}$ a.u./K for the Boltzmann constant. Thus, for ambient temperatures, the most relevant contribution corresponds to the ground state. This implies, for example, that the effective potential is not very different from the ground state energy if temperatures are much lower than 3,000 K. Nevertheless, in order to minimise numerical errors, several energy levels will be considered in the computations below, and in particular in the computation of quantities represented in Figures 5.9 and 5.10.

For $j = 1, 2, \ldots, N$, the evolution $(\xi_j(t), [\psi_j(t)])$ of the diatomic molecule with initial conditions $(\xi_{0,j}, [\psi_{0,j}])$ is simulated by Octopus. The parameters for the simulations are identical to those presented in Section 5.4.2. The result is a time-dependent probability density function with expression

$$F'_{HC}(\xi, [\psi], t) = \frac{1}{\zeta_{HC}} \sum_{j=1}^{N} \lambda(\xi_{0,j}, [\psi_{0,j}])\, \delta(\xi - \xi_j(t))\, \delta([\psi] - [\psi_j(t)]), \quad (\xi, [\psi]) \in M_{QC}. \tag{5.84}$$

Observe that the probability of each particular trajectory does not change in time. The hybrid canonical ensemble gives a initial probability distribution over the manifold M_{QC} of the hybrid system. Probability is assigned only to the initial conditions, which henceforth evolve according to the Ehrenfest model. Proposition 5.5 ensures that, for any posterior time t, function $F'_{HC}(\xi, [\psi], t)$ obtained by (5.84) is again (up to the possibilities of the discretisation procedure) the probability distribution function of the hybrid canonical ensemble.

The accuracy of this statement can be checked computationally. Simulations have been performed with the following initial condition for the molecules:

$$\begin{gathered} \mathbf{R}_{01,j} = -\mathbf{R}_{02,j}, \quad \|\mathbf{R}_{01,j} - \mathbf{R}_{02,j}\| \in \{5 \text{ a.u.}, 6.5 \text{ a.u.}, 8 \text{ a.u.}\}, \\ \mathbf{P}_{01,j} = -\mathbf{P}_{02,j}, \quad \|\mathbf{P}_{01,j}\| = \|\mathbf{P}_{02,j}\| \in \{0, 2 \cdot 10^{-4} M \text{ a.u.}\}, \\ |\psi_{0,j}\rangle \in \{|\phi_0(R_{0,j})\rangle, |\phi_1(R_{0,j})\rangle, |\phi_2(R_{0,j})\rangle, |\phi_3(R_{0,j})\rangle, |\phi_4(R_{0,j})\rangle, |\phi_5(R_{0,j})\rangle\}, \end{gathered} \tag{5.85}$$

with $\xi_{0,j} = (R_{0,j}, P_{0,j}) = (\mathbf{R}_{01,j}, \mathbf{R}_{02,j}, \mathbf{P}_{01,j}, \mathbf{P}_{01,j}) \in M_C$ the initial position and momenta of the cores, and $M = 23$ u.m.a. The possible initial states of the electron depend on the positions of the cores, as they are taken to be the eigenstates of the R-dependent electronic Hamiltonian of the Ehrenfest model. Initial positions and momenta of the cores are taken scattered on the manifold, satisfying conditions in (5.85). As a result, a small sample of trajectories is obtained. A much detailed analysis of the hybrid canonical ensemble in the Ehrenfest model can be carried out by considering a larger number of initial conditions. Such a comprehensive study, however, lays beyond the scope of this dissertation. The computed simulations are indeed enough to check the qualitative validity of the proposed description of the hybrid canonical ensemble of the Ehrenfest model.

Proposition 5.6 can be adapted to the analysis of the described sample of trajectories. If the probability density function of the hybrid system is given by (5.84), then the marginal classical probability density function is

$$F'_{HC,C}(\xi, t) = \frac{1}{\zeta_{HC}} \sum_{j=1}^{N} \lambda(\xi_{0,j}, [\psi_{0,j}])\, \delta(\xi - \xi_j(t)), \quad (\xi) \in M_C. \tag{5.86}$$

Following Proposition 5.6, the behaviour of classical particles can be modelled by an effective potential $V'_{eff}(R, t)$. In order to properly define this effective potential, for every positions $R = (\mathbf{R}_1, \mathbf{R}_2) \in \mathbb{R}^6$ of the cores, consider a neighbourhood $U(R)$ of R. Then, for each time $t \geq 0$, define the set of trajectories $I(R, t) = \{j_1, j_2, \ldots\}$ as those for which the positions of the cores at t are in $U(R)$, i.e. $R_{j1}(t), R_{j2}(t), \ldots \in U(R)$. With this definitions, the effective potential can be computed with the following expression

$$V'_{eff}(R, t) = -\frac{1}{\beta} \ln \left[\sum_{j \in I(R,t)} \exp\left(-\frac{\beta}{2M} \sum_{J=1}^{2} (\mathbf{P}_{J,j}(t))^2 \right) \lambda(\xi_{0,j}, [\psi_{0,j}]) \right], \tag{5.87}$$

The sum thus incorporates all simulated trajectories for which the cores at t are in positions close to R.

Figure 5.9 presents, for different values of the temperature, the time average values of the effective potential, defined as usual:

$$V'_{eff}(R) = \frac{1}{\tau} \int_0^{\tau} V'_{eff}(R, t)\, \mathrm{d}t. \tag{5.88}$$

The reason for this time-average is the need for a largee sampling of points on the configuration space of the cores, so that expression (5.87) gives valid results. The values presented in Figure 5.9 are thus computed

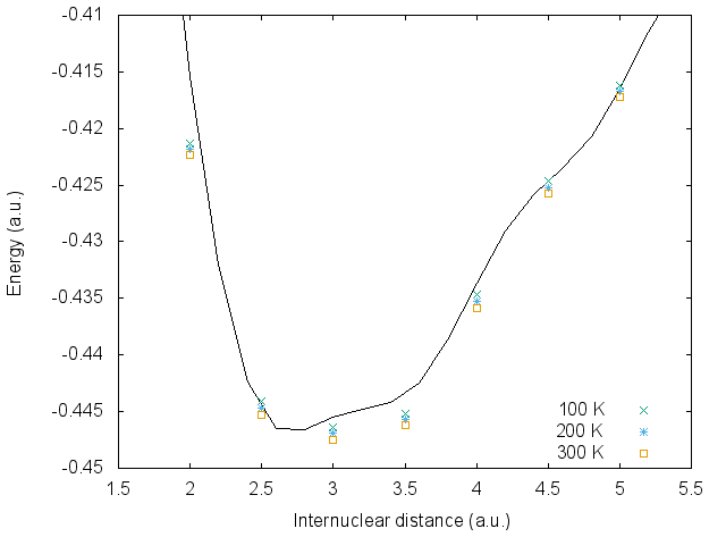


Figure 5.9: Time-average effective potential V'_{eff} for the computed simulations, in terms of the distance between the cores. The solid line represents the ground state energy $E_0(R)$ of the electronic Hamiltonian. As expected from (5.78) and [12], the values of the effective potential are below the ground state energy. This difference depends on the values of the temperature, thus reproducing the results in the aforementioned work.

by the simulated trajectories of the diatomic molecule. Lower temperatures are characterised by effective potentials closer to the ground state energy $E_0(R)$. In agreement with (5.78), the effective potential is lower when the temperature increases. These computations are in perfect agreement with the results presented in [12], and support the validity of the proposed description of the hybrid canonical ensemble. Thus, the proposed model has applications in the computation of statistical molecular ensembles and potential energy surfaces, not only of diatomic molecules, but hopefully of more complex systems.

Other relevant magnitude in the analysis of molecular systems is the internuclear distance D. Its expectation value can be computed for the proposed hybrid statistical ensemble as

$$\langle D\rangle(t) = \int_{M_C} \mathrm{d}\mu_C \|\mathbf{R}_1 - \mathbf{R}_2\| F'_{HC,C}(\xi, t). \tag{5.89}$$

Figure (5.10) presents, for different temperatures, the value of the time-average expectation value of the internuclear distance:

$$\langle D\rangle = \frac{1}{\tau}\int_0^\tau \langle D\rangle(t)\mathrm{d}t. \tag{5.90}$$

The internuclear distance increases with the temperature, as larger molecular vibrations are statistically relevant. This increment, however, is small compared with the value of the internuclear distance. This graph can be compared with the results presented by Alonso and co-workers [11]. In their work, the authors obtain a similar graph for a manganese diatomic molecule. The increment in the internuclear distance computed by them, however, was at least 20 times higher than the one presented in Figure 5.10. Two possible explanations exist for this discrepance. Firstly, the molecules considered are not equal, and their energy levels may present different behaviours. Furthermore, the diatomic molecule here presented is ionised, which also has relevance in the description of the energy levels of the molecule. And secondly, the statistical ensemble presented in (5.85) is probably not large enough for a cuantitative description of the molecular properties. As a consequence, mor re precise computations may be carried out in order to confirm the validity of the presented results.

It can thus be concluded that the offered description of the hybrid canonical ensemble of the Ehrenfest model describes a realistic behaviour of molecular systems. The model is able to describe in an

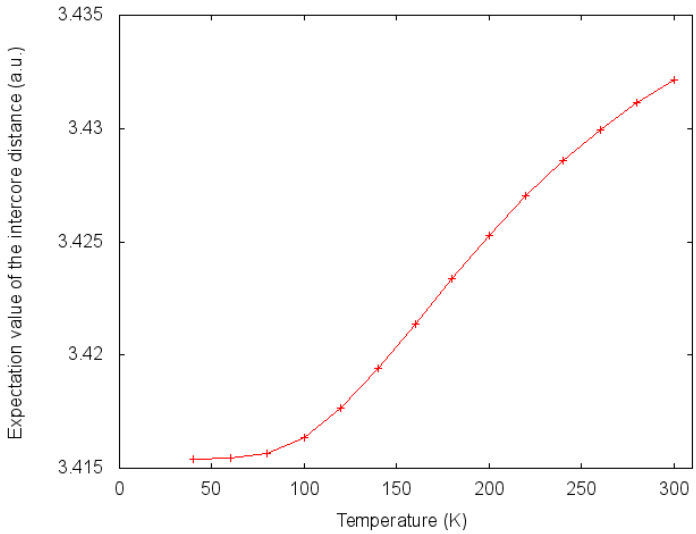


Figure 5.10: Intercore distance for different temperatures, in the described hybrid canonical ensemble. The observed increments in the intercore distance is small, in comparison with the value of the distance. Nevertheless, this is in agreement with the equilibrium positions for the cores that can be estimated from Figure 5.9 as the minima of the effective potential, and which are approximately equal to the expectation values of the intercore distance.

accurate way the behaviour of nuclei in the molecule, and characterises the changes in this behaviour for different temperatures. Also, this proposal incorporates in a natural way the decoherence effects that are expectable in these systems, therefore providing an adequate characterisation of the actual dynamics of molecules.

5.5.3 Extensivity of the hybrid canonical ensemble in the thermodynamic limit

The description of a thermodynamic limit for a hybrid classical-quantum system is not immediate. In order to clearly identify the problem, consider first the case of Classical Statistical Mechanics. The thermodynamic limit of a classical ensemble is defined in terms of a family of systems with an increasing number of components, but with a given constraint. Namely, that the number of components by volume element is constant. This volume is obviously defined in terms of the positions of the components of the system.

When considering finite dimensional quantum systems, it is precisely this definition of volume that has to be carefully considered. It is not so clear what three-dimensional volume means in terms of the quantum projective manifold $\mathcal{P}$, whose points represent the states of the quantum system. In other words, without a notion of volume it is not possible to define a density that has to be kept constant when reaching the thermodynamic limit. For this reason, finite dimensional quantum statistical ensembles are hard to describe in this limit.

Hybrid classical-quantum ensembles, however, do not have this problem. It is possible to determine a volume associated to the classical subsystem. Because of this, it makes sense to consider the thermodynamics limit in the description of molecular systems in terms of hybrid models.

In order to describe this limit, consider an ensemble of N hybrid quantum-classical systems, each one with n quantum particles and m classical particles, as before. The ensemble is modelled on a differentiable manifold

$$M_{QC}(N) = M_C(N) \times \mathcal{P}(N), \tag{5.91}$$

where the classical part is simply the Cartesian product of the classical manifolds of each component:

$$M_C(N) = \overbrace{M_C \times \cdots \times M_C}^{N}. \tag{5.92}$$

The quantum manifold, however, has to be carefully defined. The entanglement between the quantum subsystems has to be considered. Therefore, if $\mathcal{P}$ is the projective manifold of a Hilbert space $\mathcal{H}$, then $\mathcal{P}(N)$ is the projective manifold of

$$\mathcal{H}(N) = \overbrace{\mathcal{H} \otimes \cdots \otimes \mathcal{H}}^{N}. \tag{5.93}$$

Observables on the ensemble of N systems are written as A_N. In particular, the volume of the ensemble is V_N. The density of the ensembles is thus defined as

$$d_N = \frac{N}{V_N}. \tag{5.94}$$

Thus, for any observable A_N, its thermodynamic limit A_∞ is defined as

$$A_\infty = \lim_{N\to\infty} A_N, \tag{5.95}$$

while keeping d_N constant.

Any one-system observable can be extended to the whole ensemble by adding their contributions to each system. This can be directly done at the level of observables on the quantum subsystem. Let A be a hybrid one-system observable, which defines a family of quantum Hermitian operators $A(\xi)$ depending on the classical parameters. Consider an ensemble of N systems. The contributions to all of the systems defines a quantum operator

$$A_N(\xi) = \sum_{k=1}^{N} \overbrace{I \otimes \cdots \otimes I}^{k-1} \otimes A(\xi_k) \otimes \overbrace{I \otimes \cdots \otimes I}^{N-k}, \qquad \xi = (\xi_1, \xi_2, \ldots, \xi_N) \in M_C(N), \tag{5.96}$$

with I the identity operator on $\mathcal{H}$. Thus, the hybrid observable A_N is represented by a smooth function $\epsilon_A^N : M_{QC}(N) \to \mathbb{R}$ defined as

$$\epsilon_A^N(\xi, [\psi]) = \frac{\langle\psi|A_N(\xi)|\psi\rangle}{\langle\psi|\psi\rangle}, \quad (\xi, [\psi]) \in M_{QC}(N). \tag{5.97}$$

The probability density function for a hybrid canonical ensemble of N system is obtained as in (5.70). It is defined as

$$F_{HC}^N(\xi, [\psi]) = \frac{1}{Z_{HC}^N} e^{-\beta\epsilon_H^N(\xi,[\psi])}, \quad (\xi, [\psi]) \in M_{QC}(N), \tag{5.98}$$

where the partition function is

$$Z_{HC}^N = \int_{M_{QC}(N)} \mathrm{d}\mu_{QC}^N \; e^{-\beta\epsilon_H^N(\xi,[\psi])}, \tag{5.99}$$

with $\mathrm{d}\mu_{QC}^N$ the corresponding volume form. Observe that the molecular Hamiltonian H and the electronic Hamiltonian H_e are extended according to (5.96). As before, it is possible to separate variables in the definition of the partition function, which gives the following result:

$$Z_{HC}^N = \left(\frac{2\pi M_C}{\beta}\right)^{\frac{3Nm}{2}} \int_{\mathbb{R}^{3Nm}} \mathrm{d}R \int_{\mathcal{P}} \mathrm{d}\mu_{\mathcal{P}}^N \; e^{-\beta\epsilon_{H_e(R)}^N([\psi])}. \tag{5.100}$$

Statistical description of the thermodynamic limit

It is possible to compute from (5.100) the thermodynamic limit of the partition function, the operator $\rho(\xi)$ and other thermodynamic magnitudes [15]. The following results allow for a good characterisation of the properties of hybrid quantum-classical systems in the thermodynamic limit. The thermodynamic limit of the partition function and the matrix $\rho^N_{HC}(\xi)$ for the given ensemble are presented next. The proofs can be found in Appendix B.

Theorem 5.7. *In the thermodynamic limit, the partition function Z^N_{HC} of the hybrid canonical ensemble takes the value*

$$Z^N_{HC} = \frac{\pi^{d-1}}{(d-1)!}\left(\frac{2\pi M_C}{\beta}\right)^{\frac{3Nm}{2}} \int_{\mathbb{R}^{3Nm}} \mathrm{d}R \, \exp\left(-\beta \frac{\mathrm{Tr} H_{eN}(R)}{d}\right), \quad d := n^N. \tag{5.101}$$

Observe that the partition function does not factorise even for large values of N. Physically, this factor represents the volume of the quantum subsystem. Due to the presence of entanglement, the addition of components to the ensemble modifies the possible states of the quantum particles. It is useful to write (5.101) as

$$Z^N_{HC} = \gamma_d (Z^1)^N, \quad \gamma_d := \frac{\pi^{d-1}}{(d-1)!}, \quad Z^1 := \left(\frac{2\pi M_C}{\beta}\right)^{\frac{3m}{2}} \int_{\mathbb{R}^{3m}} \mathrm{d}R \, \exp\left(-\beta \frac{\mathrm{Tr}(H_e(R))}{n}\right). \tag{5.102}$$

Observe that Z^1 is the partition function for a probability distribution F^1 on M_{QC} on which all the quantum states are equally probable, while classical states follow the canonical ensemble distribution. Such a distribution is a particular case of F_{HC} obtained for a Hamiltonian proportional to the identity, $H_e(R) = f_e(R)I$, for every $R \in \mathbb{R}^{3m}$.

Theorem 5.8. *Consider the matrix $\rho^N_{HC}(\xi)$ describing the hybrid canonical ensemble of N systems:*

$$\widehat{\rho}^N_{HC}(\xi) = \int_{\mathcal{P}(N)} \mathrm{d}\mu_Q F^N_{HC}(\xi, [\psi]) \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} \tag{5.103}$$

The value of $\rho^N_{HC}(\xi)$ in the thermodynamics limit is

$$\begin{aligned} \rho^N_{HC}(\xi) =& \frac{1}{d(Z^1)^N} \exp\left(-\beta\left(\sum_{J=1}^{mN} \frac{\mathbf{P}_J^2}{2M_J} + \frac{\mathrm{Tr} H_{eN}(R)}{d}\right)\right) I_N \\ =& \bigotimes_{k=1}^{N} \frac{1}{nZ^1} \exp\left(-\beta\left(\sum_{J=1}^{m} \frac{\mathbf{P}_J^2}{2M_J} + \frac{\mathrm{Tr} H_e(R)}{n}\right)\right) I, \end{aligned} \tag{5.104}$$

with $d = n^N$ and I_N the identity observable in $\mathcal{H}(N)$.

The matrix $\rho^N_{HC}(\xi)$ can thus be written as a tensor product of one-system matrices. This proves that, in the thermodynamic limit, the matrix $\rho^N_{HC}(\xi)$ is factorisable, and the entanglement between different systems vanishes.

Thermodynamic magnitudes

Consider on the first place the internal energy U_N for an ensemble of N particles, given by

$$U_N = -\frac{\partial}{\partial \beta} \ln(Z^N_{HC}). \tag{5.105}$$

The following result presents the behaviour of the internal energy in the thermodynamic limit.

Proposition 5.9. *The internal energy for an ensemble with a large number N of particles can be approximated as*

$$U_N = Nu_1, \tag{5.106}$$

with u_1 being defined in terms of the Z^1 factor introduced in (5.102):

$$u_1 := -\frac{1}{Z^1}\frac{\partial Z^1}{\partial \beta} = \frac{3m}{2\beta} + (Z^1)^{-1}\left(\frac{2\pi M_C}{\beta}\right)^{\frac{3m}{2}} \int_{\mathbb{R}^{3Nm}} \mathrm{d}R\, \frac{\mathrm{Tr}(H_e(R))}{n} \exp\left(-\beta \frac{\mathrm{Tr}(H_e(R))}{n}\right). \tag{5.107}$$

Proof. For large values of N, the logarithm of Z^N_{HC} can be directly computed. Its value is

$$\ln(Z^N_{HC}) = \ln(\gamma_N) + N\ln(Z^1),$$

and thus, the internal energy for an ensemble with a large number of components is simply

$$U_N = -\frac{N}{Z^1}\frac{\partial Z^1}{\partial \beta} = Nu_1,$$

with u_1 the density of internal energy, or equivalently the internal energy associated to Z^1. Its value can be computed from the derivative with respect to β of (5.102):

$$\frac{\partial Z^1}{\partial \beta} = -\frac{3m}{2\beta}Z^1 - \left(\frac{2\pi M_C}{\beta}\right)^{\frac{3m}{2}} \int_{\mathbb{R}^{3Nm}} \mathrm{d}R\, \frac{\mathrm{Tr}(H_e(R))}{n} \exp\left(-\beta \frac{\mathrm{Tr}(H_e(R))}{n}\right),$$

thus obtained the proposed expression. □

The internal energy U_N is therefore an extensive magnitude in the thermodynamic limit. Observe that the non-extensivity for finite values of N is mainly due to the quantum nature of the model, in particular to the entanglement between the quantum subsystems of the components. While this effect cannot be totally neglected in the thermodynamic limit, as the partition function is not factorisable, it becomes a residual effect that does not affect the extensivity of magnitudes.

Other thermodynamic magnitudes can be analysed in a similar way. Again, extensivity is recovered in the thermodynamic limit. In particular, results in Theorems 5.7 and 5.8 allow to compute the thermodynamic limit of average values of quantum-like observables.

Proposition 5.10. *Consider an observable A giving rise to a ξ-dependent quantum observables $A(\xi)$, as in (5.38). The expectation value of the extended observable A_N to an ensemble of N systems, defined by (5.96), can be approximated for large values of N as*

$$\langle A_N\rangle = \frac{N}{Z^1}\int_{M_C} \mathrm{d}\mu_C \exp\left(-\beta\left(\sum_{J=1}^{m}\frac{\mathbf{P}_J^2}{2M_J} + \frac{\mathrm{Tr}(H_e(R))}{n}\right)\right)\frac{\mathrm{Tr}\left(A(\xi)\right)}{n}. \tag{5.108}$$

Proof. By definition, the expectation value of A_N is obtained as

$$\langle A_N\rangle = \int_{M_C(N)} \mathrm{d}\mu_C\, \mathrm{Tr}\left(\rho^N_{HC}(\xi)A_N(\xi)\right).$$

For large values of N, the matrix $\rho^N_{HC}(\xi)$ is approximated by (5.104). As a result, expectation value $\langle A_N\rangle$ can be approximated by

$$\begin{aligned}\langle A_N\rangle =& \frac{1}{d(Z^1)^N}\int_{M_C(N)} \mathrm{d}\mu_C \exp\left(-\beta\left(\sum_{J=1}^{mN}\frac{\mathbf{P}_J^2}{2M_J} + \frac{\mathrm{Tr}H_{eN}(R)}{d}\right)\right)\mathrm{Tr}\left(A_N(\xi)\right) = \\ =& \frac{1}{(Z^1)^N}\sum_{j=1}^{N}\int_{M_C(N)} \mathrm{d}\mu_C \exp\left(-\beta\left(\sum_{J=1}^{mN}\frac{\mathbf{P}_J^2}{2M_J} + \sum_{k=1}^{N}\frac{\mathrm{Tr}H_e(R_k)}{n}\right)\right)\frac{\mathrm{Tr}\left(A(\xi_j)\right)}{n},\end{aligned} \tag{5.109}$$

where (B.15) is used for both $H_{eN}(\xi)$ and $A_N(\xi)$. For each $j = 1, 2, \ldots, N$, it is possible to integrate every classical variable except ξ_j; by (5.102), these integrals are all equal to Z^1. The only remaining term is the integral in ξ_j, which is identical for every j, thus obtaining the proposed result. □

The expectation value computed in Proposition 5.10 is therefore extensive in the thermodynamic limit. In fact, it can be written as

$$\langle A_N\rangle = N\langle A\rangle^1, \quad \langle A\rangle^1 := \frac{1}{Z^1}\int_{M_C} \mathrm{d}\mu_C \exp\left(-\beta\left(\sum_{J=1}^{m}\frac{\mathbf{P}_J^2}{2M_J} + \frac{\mathrm{Tr}(H_e(R))}{n}\right)\right)\frac{\mathrm{Tr}\left(A(\xi)\right)}{n} \tag{5.110}$$

Observe that $\langle A\rangle^1$ is the expectation value of A for the same distribution F^1 defining the partition function Z^1 in (5.102). Observe that both purely classical and quantum observables are particular cases of the proposed ξ-dependent observables. Purely quantum observables are represented in this setting as constant observables with respect to ξ. On the other part, a purely classical observable A_C, represented by a smooth function f_C on the classical manifold M_C, can be extended to the hybrid quantum-classical system as

$$A_C(\xi) = f_C(\xi)\, I, \quad \xi \in M_C. \tag{5.111}$$

Consider the thermodynamic limit. It is immediate from (5.108) that the expectation value of the observable extended to an ensemble of N systems can be approximated, for large values of N, as

$$\langle (A_C)_N\rangle = N\langle A_C\rangle, \tag{5.112}$$

with $\langle A_C\rangle$ the expectation value of A_C for a single system. This expectation value can be computed with respect to both F_{QC} or, as in (5.110), with respect to a distribution F^1 for a Hamiltonian $H_e(R) = f_e(R)I$ proportional to the identity for every $R \in \mathbb{R}^{3m}$. Both distribution produce the same result, as they differ only on the quantum part and A_C is a purely classical observable.

Von Neumann entropy

Finally, the von Neumann entropy S_N of the system can also be analysed in the thermodynamic limit. Equation (3.38) gives the the expression for the von Neumann entropy of a purely quantum system. In order to extend this definition to a hybrid quantum-classical ensemble, it is very important to take into account the proper definition of its probabilistic nature. When considering the entropy of a system, the set of microstates considered must be chosen in such a way that each one of them defines a mutually exclusive event with respect to any other state. This is what von Neumann entropy does for purely quantum systems, where the spectral decomposition of the density matrix represents the mutually exclusive set of events. In the case of a hybrid system, two points of the phase space $(\xi_1, [\psi_1]), (\xi_2, [\psi_2]) \in M_{CQ}$ represent mutually exclusive events if and only if $\xi_1 \neq \xi_2$ and $[\psi_1], [\psi_2]$ represent orthogonal states. For each point $\xi \in M_C$, the representation of the probability of the corresponding quantum system is the matrix $\rho(\xi)$. Thus, the von Neumann entropy can be computed for each $\xi \in M_C$. As any two points in M_C are mutually exclusive, in order to consistently define the entropy of the hybrid system, this value has to be integrated over M_C. As a result, the von Neumann entropy of a hybrid quantum-classical system is defined (in natural units) as

$$S_N := -\int_{M_C} \mathrm{d}\mu_C\, \mathrm{Tr}\Big(\rho_{HC}(\xi)\ln\rho_{HC}(\xi)\Big). \tag{5.113}$$

Proposition 5.11. *In the thermodynamic limit, the von Neumann entropy $(S_N)_N$ of an ensemble of N systems can be approximated as*

$$\begin{aligned}(S_N)_N &:= -\int_{M_C} \mathrm{d}\mu_C\, \mathrm{Tr}\left(\rho_{HC}^N(\xi)\ln\rho_{HC}^N(\xi)\right)\\ &= -N\ln(nZ^1) - \frac{N\beta}{Z^1}\int \mathrm{d}\mu_C \exp\left[-\beta\left(\sum_{J=1}^{m}\frac{\mathbf{P}_J^2}{2M_J} + \frac{\mathrm{Tr}(H_e(R))}{n}\right)\right]\left(\sum_{J=1}^{m}\frac{\mathbf{P}_J^2}{2M_J} + \frac{\mathrm{Tr}(H_e(R))}{n}\right).\end{aligned} \tag{5.114}$$

Proof. This expression is directly computed by considering approximation (5.104) for the matrix $\rho^N_{HC}(\xi)$. □

The von Neumann entropy is therefore additive in the thermodynamic limit. This additivity is in direct connection with the factorisability of $\rho^N_{HC}(\xi)$, shown in (5.104). The entropy of a system computes the number of accessible states of an ensemble. If there is no entanglement between the different systems of the ensemble, then necessarily the entropy is an additive magnitude on these systems.

5.6 Outlook of the geometric Ehrenfest model

Quantum Mechanics is a theory with a broad range of applications. One of the main problems it presents, however, is the difficulty to find exact solutions for the Schrödinger equation. Approximations are mandatory in almost every problem. In the context of molecular systems, hybrid quantum-classical dynamics are a powerful tool in the description of the evolution of complex quantum systems [40, 184, 222, 255–257, 261–264, 276, 279].

The present chapter shows a relevant application of the geometric formalism developed along this dissertations. Molecular systems have to be divided in two constituent subsystems, namely electrons and nuclei. They are assumed to evolve accordingly to different theories, Quantum and Classical Mechanics, respectively. Thus, it is not easy, at first, to give a joint distribution of the constituent elements of the molecule. Nevertheless, the geometric formalism offers a solution to this problem, as shown. It is possible to describe both the classical and quantum part in geometric terms. The properties of differentiable manifolds allow for the definition of a product manifold that describes the states of the molecule as a whole [8, 10, 14]. Thus, a geometric formalism provides a suitable framework for the study of hybrid quantum-classical models.

This chapter focuses on the Ehrenfest model for hybrid quantum-classical systems. This is a deterministic model that, at first, do not incorporate the probabilistic properties that are inherent to quantum systems. However, the geometric description of molecular systems allows for the development of statistical distribution. After all, in the geometric setting, states of hybrid quantum-classical system are described by points on a Poisson manifold. There exists a symplectic volume (preserved by Hamiltonian evolution), which allows to consider time-dependent probability densities on the manifold. The relevant statistical objects have thus been computed. It is interesting to consider the termodynamical limit, in which some classical properties, in particular separability of thermodynamical magnitudes (but not of the partition function), are recovered.

In this geometric setting, Ehrenfest dynamics does incorporate decoherence-like properties [8, 14]. This has been deeply proved along the chapter, where numerical results are offered. A specific molecular system has been studied, namely a diatomic molecule with a single valence electron. Yet even this simple model is enough to prove the changes in the properties of quantum systems that are usually associated with the probabilistic nature of the measurement process. The purity of the system changes as expected, and so does the von Neumann entropy. Thus, it has been proved that is is enough to consider statistical distributions of molecular system in order to reproduce by the Ehrenfest model some aspects of the decoherence phenomenon.

The results presented here follow the path started by the collaborators of the author [10, 14]. It is thus expectable that more complex models will be studied in the future. The geometric formalism is a powerful tool in the study of molecular dynamics. It offers the possibility to analyse changes in the properties presented here, such as purity and von Neumann entropy, and even other phenomena, as the possible appearance of pointer states. All of this may help to understand the decoherence phenomenon of quantum systems and the probabilistic nature of Quantum Mechanics.

Appendix A

Properties of the 3-level system

This appendix deals with the description of the set of states of a 3-level system. Chosen a basis, the Hilbert space $\mathcal{H}$ of the system is isomorphic to $\mathbb{C}^3$, and the observables of the system are identified as $\mathcal{O} \cong \mathrm{Herm}(3)$, the set of 3×3 complex Hermitian matrices. A basis $\{\lambda_0, \lambda_1, \lambda_2, \ldots, \lambda_8\}$ for this space is given by the Gell-Mann matrices, together with the identity matrix:

$$\begin{aligned}
\lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
\lambda_4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \\
\lambda_7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, \quad \lambda_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I,
\end{aligned} \tag{A.1}$$

Gell-Mann matrices were introduced as an extension to Herm(3) of the Pauli matrices. They are traceless, orthogonal matrices, with respect to the inner product defined by the trace:

$$\mathrm{Tr}(\lambda_j) = 0, \quad \mathrm{Tr}(\lambda_j \lambda_k) = 2\delta_{jk}, \quad j, k = 1, 2, \ldots, 8. \tag{A.2}$$

As proved in the text, the observables of a quantum system form a Lie-Jordan algebra. The Lie bracket and the Jordan product are determined by the structure constants c_{jkl} and d_{jkl}, obtained by the product of the elements in the bases:

$$\begin{aligned}
[\![\lambda_j, \lambda_k]\!] &= -\mathrm{i}(\lambda_j \lambda_k - \lambda_k \lambda_j) = \sum_{l=0}^{8} c_{jkl} \lambda_l, \\
\lambda_j \odot \lambda_k &= \lambda_j \lambda_k + \lambda_k \lambda_j = \sum_{l=0}^{8} d_{jkl} \lambda_l,
\end{aligned} \qquad j, k = 0, 1, 2, \ldots, 8. \tag{A.3}$$

These structure constants can be directly computed. The Lie structure constants c_{jkl} are a set of totally antisymmetric numbers with respect to the indices, with values

$$c_{123} = 2, \quad c_{147} = c_{165} = c_{246} = c_{257} = c_{345} = c_{376} = 1, \quad c_{458} = c_{678} = \sqrt{3}. \tag{A.4}$$

The remaining elements are either zero or obtained by permutations of the indices. Similarly, the Jordan

structure constants d_{jkl} are totally symmetric with respect to the indices. The non-zero values are

$$\begin{gathered} d_{000} = 2., \quad d_{110} = d_{220} = d_{330} = d_{440} = d_{550} = d_{660} = d_{770} = d_{880} = \frac{4}{3}, \\ d_{118} = d_{228} = d_{338} = \frac{2}{\sqrt{3}}, \quad d_{146} = d_{157} = d_{256} = d_{344} = d_{355} = 1, \quad d_{247} = d_{366} = d_{377} = -1, \\ d_{448} = d_{558} = d_{668} = d_{778} = -\frac{1}{\sqrt{3}}, \quad d_{888} = -\frac{2}{\sqrt{3}}. \end{gathered} \tag{A.5}$$

and their permutations.

A dual basis $\{\lambda^j\}_{j=0,\dots,8}$ on the space $\mathcal{O}^*$ of $\mathbb{R}$-linear functionals on $\mathcal{O}$ is defined as

$$\lambda^j(\lambda_k) = \delta^j_k, \quad j,k = 0,1,2,\dots,8. \tag{A.6}$$

Due to the presence of an inner product on $\mathcal{O}$, defined by the trace of observables, there exists an isomorphism $\mathcal{O}^* \cong \mathcal{O} \cong \mathrm{Herm}(3)$. Thus, it is possible to identify the elements in the dual bases with the following complex matrices:

$$\lambda^j = \frac{1}{2}\lambda_j, \quad j = 1,2,\dots,8; \quad \lambda^0 = \frac{1}{3}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{A.7}$$

As presented in the main text, the set $\mathcal{S}$ of pure and mixed states is a subset of this dual space, defined as

$$\mathcal{S} = \{\rho \in \mathcal{O}^* \mid \rho(I) = 1;\, \rho(A^2) \geq 0,\, \forall A \in \mathcal{O}\}. \tag{A.8}$$

The normalisation condition can be directly implemented in the given basis by writting states as

$$\rho = \sum_{j=1}^{8} x_j \lambda^j + \lambda^0, \quad \mathbf{x} = (x_1, x_2, \dots, x_8) \in \mathbb{R}^3. \tag{A.9}$$

The positivity of states imposes conditions on the possible values of this coefficients. However, unlike in the case of a 2-level system, these conditions are of a huge complexity. A recent work by Goyal and co-workers [140] presents a detalied characterisation of states of a 3-level system. They show that the stratum $\mathcal{S}_1$ of pure states of the three-level system corresponds to imposing in (A.9) the following conditions:

$$\mathcal{S}_1 = \left\{ \rho \in \mathcal{O}^* \mid \rho(I) = 1,\, \mathbf{x} * \mathbf{x} = \frac{4}{3}\mathbf{x},\; \mathbf{x}\cdot\mathbf{x} = \frac{4}{3} \right\}, \tag{A.10}$$

where the $*$ product is defined in terms of the Jordan structure constants of the Lie-Jordan algebra of observables as

$$(\mathbf{x} * \mathbf{y})_l = \sum_{j,k=1}^{8} d_{jkl}\, x_j y_k, \quad \mathbf{x},\mathbf{y} \in \mathbb{R}^8, \quad l = 1,2,\dots,8. \tag{A.11}$$

Thus, pure states of the system are represented by points on a sphere. However, unlike in the case of the 2-level systemin, only a portion of this sphere is required for this description. Recall also that $\mathcal{S}_1$ is the image by the momentum map of the manifold $\mathcal{P}$ of pure states, which in this case is isomorphic to $\mathbb{C}\mathrm{P}^2$, hence 4-dimensional, the same as $\mathcal{S}_1$.

Another difference between 2-level and 3-level systems appears in the study of the boundary of the set $\mathcal{S}$ of pure and mixed states. In the present case, the boundary $\partial\mathcal{S}$ is composed of pure states, but also of rank-2 elements, thus $\partial\mathcal{S} = \mathcal{S}_1 \cup \mathcal{S}_2$. It was also proved by Goyal and co-workers [140] that this boundary can be described as

$$\partial\mathcal{S} = \left\{ \rho \in \mathcal{O}^* \mid \rho(I) = 1,\, 2\,\mathbf{x}\cdot\mathbf{x} - (\mathbf{x} * \mathbf{x})\cdot\mathbf{x} = \frac{8}{9},\; \mathbf{x}\cdot\mathbf{x} \leq \frac{4}{3} \right\}, \tag{A.12}$$

with relation (A.9) between ρ and $\mathbf{x}$. This boundary has a rich structure, and it is possible to consider pairs of points, evolution of von Neumann entropy and other characteristics of its points. Finally, the total set $\mathcal{S}$ is defined as

$$\mathcal{S} = \left\{ \rho \in \mathcal{O}^* \mid \rho(I) = 1,\, 2\,\mathbf{x}\cdot\mathbf{x} - (\mathbf{x} * \mathbf{x})\cdot\mathbf{x} \leq \frac{8}{9},\ \mathbf{x}\cdot\mathbf{x} \leq \frac{4}{3} \right\}, \tag{A.13}$$

The set $\mathcal{S}$ is therefore a manifold with boundary, embedded into the larger differentiable manifold $\widehat{\mathcal{S}} = \{\rho \in \mathcal{O}^* \mid \rho(I) = 1\}$. Thus, differentiable calculus can be carried out on $\mathcal{S}$ by considering this embedding. Coordinate functions are associated to the Gell-Mann matrices:

$$\epsilon_{\lambda_j}(\rho) = \mathrm{Tr}(\lambda_j \rho) = x_j, \quad j = 1, 2, \ldots, 8. \tag{A.14}$$

The contravariant tensor fields $\Lambda_{\mathcal{S}}$ and $\mathcal{R}_{\mathcal{S}}$ reproduce the algebraic properties of observables. In the given coordinate system, these tensor fields are

$$\begin{aligned} \Lambda_{\mathcal{S}} =& \frac{1}{2} \sum_{j,k,l=1}^{8} c_{jkl} x_l \frac{\partial}{\partial x_j} \wedge \frac{\partial}{\partial x_k}, \\ R_{\mathcal{S}} =& \sum_{j,k=1}^{8} \left(d_{jk0} + \sum_{l=1}^{8} d_{jkl} x_l \right) \frac{\partial}{\partial x_j} \otimes \frac{\partial}{\partial x_k} - 2 \sum_{j,k=1}^{8} x_j x_k \frac{\partial}{\partial x_j} \otimes \frac{\partial}{\partial x_k}, \end{aligned} \tag{A.15}$$

with the structure constants given by (A.4) and (A.5). It is thus possible to carry out computations similar to those implemented for 2-level systems. In particular, in the main text contractions of the corresponding Lie-Jordan algebras of expectation value functions are considered. These contractions are found by computing the Lie derivatives of $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ with respect to the vector fields determining the evolution. These lengthy computations can be carry out by means of mathematical software, such as Wolfram Mathematica or MATLAB. In this way, it is possible to devise a practical method for the study of higher dimensional quantum systems.

Appendix B

Thermodynamic limit for the hybrid canonical ensemble

B.1 Integrals on spherical surfaces

The computations for the thermodynamic limit of the hybrid quantum-classical canonical ensemble involve the computation of integrals to spherical surfaces. For this reason, the present section deals with some useful computations. Consider an even-dimensional Euclidean space $\mathbb{R}^{2q}$, with Cartesian coordinates $(x_1, x_2, \ldots, x_{2q})$. Spherical coordinates are introduced by means of a radial coordinate r and $2q-1$ angles $\theta_1, \theta_2, \ldots, \theta_{2q-2}$ and φ, as follows [151]:

$$\left.\begin{aligned} &x_1 = r\cos\theta_1, \\ &x_2 = r\sin\theta_1\cos\theta_2, \\ &\cdots \\ &x_{2q-1} = r\sin\theta_1\sin\theta_2\cdots\sin\theta_{2q-2}\cos\varphi, \\ &x_{2q} = r\sin\theta_1\sin\theta_2\cdots\sin\theta_{2q-2}\sin\varphi, \end{aligned}\right\} \quad \begin{aligned} &r \in (0,\infty), \\ &\theta_1, \theta_2, \ldots, \theta_{2q-2} \in (0,\pi), \\ &\varphi \in (0, 2\pi). \end{aligned} \tag{B.1}$$

The volume element $\mathrm{d}\mu_{\mathbb{R}}$ in spherical coordinates is immediately obtained as

$$\mathrm{d}\mu_{\mathbb{R}} = \mathrm{d}x_1\mathrm{d}x_2\cdots\mathrm{d}x_{2q} = r^{2q-1}\sin^{2q-2}\theta_1\sin^{2q-3}\theta_2\cdots\sin\theta_{2q-2}\,\mathrm{d}r\,\mathrm{d}\theta_1\mathrm{d}\theta_2\cdots\mathrm{d}\theta_{2q-2}\,\mathrm{d}\varphi. \tag{B.2}$$

Consider now the restriction to the unit sphere $S^{2q-1} \subset \mathbb{R}^q$. The volume element $\mathrm{d}\mu_S$ is simply obtained by considering constant radius $r = 1$:

$$\mathrm{d}\mu_S = \sin^{2q-2}\theta_1\sin^{2q-3}\theta_2\cdots\sin\theta_{2q-2}\,\mathrm{d}\theta_1\mathrm{d}\theta_2\cdots\mathrm{d}\theta_{2q-2}\,\mathrm{d}\varphi. \tag{B.3}$$

Integrals can easily computed in this coordinates. As a first example, consider the integral of the volume element, which gives the area A_S of S^{2q-1} considered as a hypersurface in $\mathbb{R}^{2q}$:

$$A_S := \int_{S^{2q-1}}\mathrm{d}\mu_S = \int_0^\pi \sin^{2q-2}\theta_1\mathrm{d}\theta_1\int_0^\pi\sin^{2q-3}\theta_2\mathrm{d}\theta_2\cdots\int_0^\pi\sin\theta_{2q-2}\,\mathrm{d}\theta_{2q-2}\int_0^{2\pi}\mathrm{d}\varphi. \tag{B.4}$$

Integrals of trigonometric functions are tabulated. Thus, given the following values,

$$\begin{aligned} I_{2j} &:= \int_0^\pi \sin^{2j}\theta\,\mathrm{d}\theta = \pi\,\frac{1\cdot 3\cdot\cdots\cdot(2j-1)}{2\cdot 4\cdot\cdots\cdot 2j}, \\ I_{2j+1} &:= \int_0^\pi \sin^{2j+1}\theta\,\mathrm{d}\theta = 2\,\frac{2\cdot 4\cdot\cdots\cdot 2j}{1\cdot 3\cdot\cdots\cdot(2j+1)}, \end{aligned} \qquad j = 1, 2, \ldots \tag{B.5}$$

the area A_S is given by the following expression:

$$A_S = 4\pi\ I_{2q-2}I_{2q-3}\cdots I_2 = 2\pi^2(I_3I_4)\cdots(I_{2q-3}I_{2q-2}) = \frac{2\pi^q}{(q-1)!}. \tag{B.6}$$

The integrals of powers of coordinate functions can also be computed. Odd powers are odd functions on S^{2n-1}, hence their integrals are zero. On the other side, consider for example the function x_1^2. By comparison with (B.4), its integral is obtained as follows:

$$\begin{aligned} A_S^{(2)} :=& \int_{S^{2q-1}} x_1^2\,\mathrm{d}\mu_S = \frac{A_S}{I_{2q-2}}\int_0^\pi \cos^2\theta_1 \sin^{2q-2}\theta_1 \mathrm{d}\theta_1 = \frac{A_S}{I_{2q-2}}\int_0^\pi (\sin^{2q-2} - \sin^{2q})\theta_1 \mathrm{d}\theta_1 \\ =& \frac{A_S}{I_{2q-2}}\,(I_{2q-2} - I_{2q}) = A_S\left(1 - \frac{2q-1}{2q}\right) = \frac{2\pi^q}{(q-1)!}\frac{1}{2q} = \frac{\pi^q}{q!} \end{aligned} \tag{B.7}$$

Because of symmetry, integrals of x_2^2, x_3^2, etc. are also equal to $A_S^{(2)}$. Higher order powers define a family of integrals that play a relevant role in the computation of partition functions. They will be denoted as

$$A_S^{(2j_1,2j_2,\ldots,2j_r)} := \int_{S^{2q-1}} x_{k_1}^{2j_1} x_{k_2}^{2j_2}\cdots x_{k_r}^{2j_r}\,\mathrm{d}\mu_S, \quad j_1, j_2, \ldots, j_r = 1, 2, \ldots, \quad r \le 2q, \tag{B.8}$$

and $k_1, k_2, \ldots, k_r = 1, 2, \ldots, 2q$, with $k_j \neq k_{j'}$ for any $j \neq j'$. Again, because of the symmetry of the space, the integrals are equal for any set of coordinate functions. The values of these integrals are computed in the same way as (B.7), i.e. by use of the expression (B.4) for the area and integrals defined in (B.5):

$$\begin{aligned} A_S^{(2,2)} =& \int_{S^{2q-1}} x_1^2 x_2^2\,\mathrm{d}\mu_S = \frac{A_S}{I_{2q-2}I_{2q-3}}\int_0^\pi \cos^2\theta_1 \sin^{2q}\theta_1 \mathrm{d}\theta_1 \int_0^\pi \cos^2\theta_2 \sin^{2q-3}\theta_2 \mathrm{d}\theta_2 \\ =& \frac{A_S}{I_{2q-2}I_{2q-3}}\int_0^\pi (\sin^{2q}\theta_1 - \sin^{2q+2}\theta_1)\mathrm{d}\theta_1 \int_0^\pi (\sin^{2q-3}\theta_2 - \sin^{2q-1})\theta_2 \mathrm{d}\theta_2 \\ =& \frac{A_S}{I_{2q-2}I_{2q-3}}(I_{2q} - I_{2q+2})(I_{2q-3} - I_{2q-1}) = A_S\left(\frac{2q-1}{2q} - \frac{(2q-1)(2q+1)}{2q(2q+2)}\right)\left(1 - \frac{2q-2}{2q-1}\right) \\ =& \frac{2\pi^q}{(q-1)!}\frac{2q-1}{2q}\frac{1}{2q+2}\frac{1}{2q-1} = \frac{\pi^q}{2(q+1)!}, \end{aligned} \tag{B.9}$$

$$\begin{aligned} A_S^{(4)} =& \int_{S^{2q-1}} x_1^4\,\mathrm{d}\mu_S = \frac{A_S}{I_{2q-2}}\int_0^\pi \cos^4\theta_1 \sin^{2q-2}\theta_1 \mathrm{d}\theta_1 \\ =& \frac{A_S}{I_{2q-2}}\int_0^\pi (\sin^{2q-2}\theta_1 - 2\sin^{2q}\theta_1 + \sin^{2q+2}\theta_1)\mathrm{d}\theta_1 = \frac{A_S}{I_{2q-2}}\,(I_{2q-2} - 2I_{2q} + I_{2q+2}) \\ =& A_S\left(1 - 2\frac{2q-1}{2q} + \frac{(2q-1)(2q+1)}{2q(2q+2)}\right) = \frac{2\pi^q}{(q-1)!}\frac{3}{2q(2q+2)} = \frac{3\pi^q}{2(q+1)!}, \end{aligned} \tag{B.10}$$

$$A_S^{(2,2,2)} = \int_{S^{2q-1}} x_1^2 x_2^2 x_3^2\,\mathrm{d}\mu_S = A_S\frac{(I_{2q+2} - I_{2q+4})(I_{2q+1} - I_{2q+1})(I_{2q-4} - I_{2q-2})}{I_{2q-2}I_{2q-3}I_{2q-4}} = \frac{\pi^q}{4(q+2)!}, \tag{B.11}$$

$$A_S^{(4,2)} = \int_{S^{2q-1}} x_1^4 x_2^2\,\mathrm{d}\mu_S = A_S\frac{(I_{2q} - 2I_{2q+2} + I_{2q+4})(I_{2q-3} - I_{2q-1})}{I_{2q-2}I_{2q-3}} = \frac{3\pi^q}{4(q+2)!}, \tag{B.12}$$

$$A_S^{(6)} = \int_{S^{2q-1}} x_1^6\,\mathrm{d}\mu_S = A_S\frac{I_{2q-2} - 3I_{2q} + 3I_{2q+2} - I_{2q+4})}{I_{2q-2}} = \frac{15\pi^q}{4(q+2)!}. \tag{B.13}$$

It is important to notice that the total value of the integral decrease with the increase of the powers of the coordinate function. The integral of a $2p$-grade polynomial is proportional to $\frac{1}{(q+p-1)!}$, which decreases rapidly for higher values of p.

B.2 Trace of observables in thermodynamic limit

Consider an ensemble of N molecules. Any one-molecule observable $A(\xi)$ can be extended to the whole ensemble by (5.96). Consider in particular the case of the electronic Hamiltonian H_e:

$$H_{eN}(\mathcal{R}) = \sum_{k=1}^{N} \overbrace{I \otimes \cdots \otimes I}^{k-1} \otimes H_e(R_k) \otimes \overbrace{I \otimes \cdots \otimes I}^{N-k}, \qquad R = (R_1, R_2, \ldots, R_N) \in \mathbb{R}^{3Nm}, \tag{B.14}$$

with I the identity operator on the n-dimensional complex Hilbert space $\mathcal{H}$ associated to a single molecule. The behaviour of the partition function in the thermodynamic limit depends on the trace of this operator:

$$\mathrm{Tr} H_{eN}(R) = \sum_{k=1}^{N} (\mathrm{Tr} I)^{N-1} \mathrm{Tr} H_e(R_k) = n^{N-1} \sum_{k=1}^{N} \mathrm{Tr} H_e(R_k) \tag{B.15}$$

As the different subsystems are identical, the integrals on the positions of the cores must coincide. In particular,

$$\int_{\mathbb{R}^{3Nm}} \mathrm{Tr} H_e(R_j) \mathrm{d}R = \int_{\mathbb{R}^{3Nm}} \mathrm{Tr} H_e(R_k) \mathrm{d}R, \tag{B.16}$$

for any pair of indexes $j, k = 1, 2, \ldots, N$. Computations of partition functions always involve integrals on the degrees of freedom. Thus, the trace of $H_{eN}(R)$ can be written

$$\mathrm{Tr} H_{eN}(R) \sim N n^{N-1} \mathrm{Tr} H_e(r) = \frac{Nd}{n} \mathrm{Tr} H_e(r), \quad R \in \mathbb{R}^{3Nm}, \quad r \in \mathbb{R}^{3m}, \tag{B.17}$$

with $d = n^N$, and where the symbol $\sim$ indicates that the integrals of both sides over the corresponding spaces are equal. A similar behaviour occurs for powers of $H_{eN}(R)$:

$$\mathrm{Tr}(H_{eN}(R)^p) \sim \frac{Nd}{n} \mathrm{Tr}(H_e(r)^p) + \binom{N}{2} \frac{d}{n^2} \mathrm{Tr}(H_e(r)^{p-1}) \mathrm{Tr} H_e(r) + \vartheta(n^{-3}). \tag{B.18}$$

B.3 Proof of Theorem 5.7

The results obtained above are useful for the computation of the thermodynamics limit of the partition function for a hybrid quantum-classical system. Consider first a simpler case, namely a canonical distribution for a (finite-dimensional) purely quantum system, described by the following partition function:

$$Z_Q = \int_{\mathcal{P}} e^{-\beta \epsilon_H([\psi])} \mathrm{d}\mu_{\mathcal{P}}, \tag{B.19}$$

with $H \in \mathcal{O}$ the Hamiltonian of the system. The manifold $\mathcal{P}$ of pure states is obtained by means of a foliation of the d-dimensional complex Hilbert space $\mathcal{H}$, or alternatively of the $2d$-dimensional real manifold M_Q. Section 1.3.2 describes the properties of this foliation. As a consequence, it is possible to write $\mathcal{P}$ as

$$\mathcal{P} = S^{2d-1}/S^1. \tag{B.20}$$

with S^{2d-1} the unit sphere in M_Q. It is therefore possible to replace the integral on $\mathcal{P}$ in (B.19) by an integral to S^{2d-1}, multiplied by the corresponding factor:

$$\begin{aligned} Z_Q &= \frac{1}{2\pi} \int_{S^{2d-1}} e^{-\beta \langle \psi | H | \psi \rangle} \mathrm{d}\mu_S = \frac{1}{2\pi} \sum_{j=0}^{\infty} \frac{(-\beta)^j}{j!} \int_{S^{2d-1}} \langle \psi | H | \psi \rangle^j \mathrm{d}\mu_S \\ &= \frac{1}{2\pi} \left(\int_{S^{2d-1}} \mathrm{d}\mu_S - \beta \int_{S^{2d-1}} \langle \psi | H | \psi \rangle \mathrm{d}\mu_S + \frac{\beta^2}{2} \int_{S^{2d-1}} \langle \psi | H | \psi \rangle^2 \mathrm{d}\mu_S - \frac{\beta^3}{6} \int_{S^{2d-1}} \langle \psi | H | \psi \rangle^3 \mathrm{d}\mu_S + \ldots \right). \end{aligned} \tag{B.21}$$

The value of each integral can be computed by the results presented in Section B.1. Consider a basis $\{|\phi_j\rangle\}$ for the Hilbert space $\mathcal{H}$, composed of eigenvectors of the Hamiltonian H, say

$$H|\phi_j\rangle = E_j|\phi_j\rangle, \quad j = 1, 2, \ldots, d. \tag{B.22}$$

Any vector $|\psi\rangle \in \mathcal{H}$ can thus be written in a unique way as a linear combination of these vectors, which gives the following expression for the expectation value of the Hamiltonian on S^{2d-1}:

$$|\psi\rangle = \sum_{j=1}^{d} z_j|\phi_j\rangle \;\Rightarrow\; \langle\psi|H|\psi\rangle = \sum_{j=1}^{d} E_j|z_j|^2. \tag{B.23}$$

By decomposing the complex coefficients in their real and imaginary parts, namely $z_j = a_j + \mathrm{i}b_j$ for $j = 1, 2, \ldots, d$, the integrals in (B.21) can be computed with the results given in Section B.1:

$$\int_{S^{2d-1}} \mathrm{d}\mu_S = A_S = \frac{2\pi^d}{(d-1)!}, \tag{B.24}$$

$$\int_{S^{2d-1}} \langle\psi|H|\psi\rangle \mathrm{d}\mu_S = \sum_{j=1}^{d} E_j \int_{S^{2d-1}} (a_j^2 + b_j^2)\mathrm{d}\mu_S = 2A_S^{(2)} \sum_{j=1}^{d} E_j = \frac{2\pi^d}{d!}\,\mathrm{Tr}H, \tag{B.25}$$

$$\begin{aligned}
\int_{S^{2d-1}} \langle\psi|H|\psi\rangle^2 \mathrm{d}\mu_S &= \sum_{j,k=1}^{d} E_j E_k \int_{S^{2d-1}} (a_j^2 + b_j^2)(a_k^2 + b_k^2)\mathrm{d}\mu_S \\
&= \sum_{j\neq k} E_j E_k \int_{S^{2d-1}} (a_j^2 a_k^2 + b_j^2 b_k^2)\mathrm{d}\mu_S + 2\sum_{j,k} E_j E_k \int_{S^{2d-1}} a_j^2 b_k^2 \mathrm{d}\mu_S + \sum_j E_j^2 \int_{S^{2d-1}} (a_j^4 + b_j^4)\mathrm{d}\mu_S \\
&= 2A_S^{(2,2)} \sum_{j\neq k} E_j E_k + 2A_S^{(2,2)} \sum_{j,k} E_j E_k + 2A_S^{(4)} \sum_j E_j^2 = 4A_S^{(2,2)} (\mathrm{Tr}H)^2 + 2(A_S^{(4)} - A_S^{(2,2)})\mathrm{Tr}(H^2) \\
&= \frac{2\pi^d}{(d+1)!}(\mathrm{Tr}H)^2 + 2\left(\frac{3\pi^d}{2(d+1)!} - \frac{\pi^d}{2(d+1)!}\right)\mathrm{Tr}(H^2) = \frac{2\pi^d}{(d+1)!}\left((\mathrm{Tr}H)^2 + \mathrm{Tr}(H^2)\right),
\end{aligned} \tag{B.26}$$

$$\begin{aligned}
\int_{S^{2d-1}} \langle\psi|H|\psi\rangle^3 \mathrm{d}\mu_S &= \sum_{j,k,l=1}^{d} E_j E_k E_l \int_{S^{2d-1}} (a_j^2 + b_j^2)(a_k^2 + b_k^2)(a_l^2 + b_l^2)\mathrm{d}\mu_S = 2A_S^{(2,2,2)} \sum_{j\neq k\neq l} E_j E_k E_l \\
&\quad + 6A_S^{(4,2)} \sum_{j\neq k} E_j^2 E_k + 2A_S^{(6)} \sum_j E_j^3 + 6A_S^{(2,2,2)} \sum_{j\neq k,l} E_j E_k E_l + 6A_S^{(4,2)} \sum_{j,l} E_j^2 E_k \\
&= 2A_S^{(2,2,2)} \left((\mathrm{Tr}H)^3 - 3\,\mathrm{Tr}H\,\mathrm{Tr}(H^2) + 2\,\mathrm{Tr}(H^3)\right) + 6A_S^{(4,2)} \left(\mathrm{Tr}H\,\mathrm{Tr}(H^2) - \mathrm{Tr}(H^3)\right) \\
&\quad + 2A_S^{(6)}\mathrm{Tr}(H^3) + 6A_S^{(2,2,2)} \left((\mathrm{Tr}H)^3 - \mathrm{Tr}H\,\mathrm{Tr}(H^2)\right) + 6A_S^{(4,2)}\mathrm{Tr}H\,\mathrm{Tr}(H^2) \\
&= \frac{2\pi^d}{(d+2)!}\left((\mathrm{Tr}H)^3 + 3\,\mathrm{Tr}H\,\mathrm{Tr}(H^2) + 2\,\mathrm{Tr}(H^3)\right).
\end{aligned} \tag{B.27}$$

Substituting in (B.21), the following expression for the quantum partition function A_Q is obtained:

$$\begin{aligned}
Z_Q = &\frac{\pi^{d-1}}{(d-1)!}\left(1 - \frac{\beta}{d}\,\mathrm{Tr}H + \frac{\beta^2}{2d(d+1)}\left((\mathrm{Tr}H)^2 + \mathrm{Tr}(H^2)\right) + \right. \\
&\left. - \frac{\beta^3}{6d(d+1)(d+2)}\left((\mathrm{Tr}H)^3 + 3\,\mathrm{Tr}H\,\mathrm{Tr}(H^2) + 2\,\mathrm{Tr}(H^3)\right) + \cdots\right).
\end{aligned} \tag{B.28}$$

This is the expression for the partition function of a quantum canonical ensemble associated to a system with Hamiltonian H and d-dimensional complex Hilbert space. It is immediate to extend this expression to hybrid quantum-classical systems, and also to ensembles with large numbers of particles.

Thus, partition function Z_{HC}^N, given in (5.100), can be written in a similar way to (B.28) as

$$Z_{HC}^N = \frac{\pi^{d-1}}{(d-1)!}\left(\frac{2\pi M_C}{\beta}\right)^{\frac{3Nm}{2}}\int_{\mathbb{R}^{3Nm}} \mathrm{d}R\left(1-\frac{\beta}{d}\operatorname{Tr}H_{eN}(R)+\frac{\beta^2}{2d(d+1)}\left((\operatorname{Tr}H_{eN}(R))^2+\operatorname{Tr}(H_{eN}(R)^2)\right)+\right.$$
$$\left.-\frac{\beta^3}{6d(d+1)(d+2)}\left((\operatorname{Tr}H_{eN}(R))^3+3\operatorname{Tr}H_{eN}(R)\operatorname{Tr}(H_{eN}(R)^2)+2\operatorname{Tr}(H_{eN}(R)^3)\right)+\cdots\right), \tag{B.29}$$

with $H_{eN}(R)$ the extension for N particles of the electronic Hamiltonian system, and $d=n^N$ the dimension of the total Hilbert space for N instances of n-level systems. In the thermodynamic limit, the number of systems N goes to infinity, and the dimension d of the total Hilbert space diverges much faster. It is thus simple to describe the behaviour in this limit of the different terms in (B.29). First, consider the following expression for the coefficients:

$$\frac{1}{d(d+1)\cdots(d+s-1)} = \frac{1}{d^s}\left(1-\frac{s(s-1)}{2d}+\vartheta\left(\frac{1}{d^2}\right)\right). \tag{B.30}$$

This is an alternating series, which allows to determine the following bounds for the coefficients in (B.29):

$$\frac{1}{d^s}\left(1-\frac{s(s-1)}{2d}\right) < \frac{1}{d(d+1)\cdots(d+s-1)} < \frac{1}{d^s}. \tag{B.31}$$

Each summand in (B.29) consists of a sum of terms with different combinations of powers and traces. The given bounds allow to determine the leading term for each summand by applying the results in Section B.2:

$$\frac{N^s}{n^s}(\operatorname{Tr}H_e(r))^s\left(1-\frac{s(s-1)}{2d}\right) \lesssim \frac{(\operatorname{Tr}H_{eN}(R))^s}{d(d+1)\cdots(d+s-1)} \lesssim \frac{N^s}{n^s}(\operatorname{Tr}H_e(r))^s, \tag{B.32}$$

$$\frac{N^{s-1}}{d\,n^{s+1}}(\operatorname{Tr}H_e(r))^{s-2}\operatorname{Tr}H_e(r)^2\left(1-\frac{s(s-1)}{2d}\right) \lesssim \frac{(\operatorname{Tr}H_{eN}(R))^{s-2}\operatorname{Tr}H_{eN}(R)^2}{d(d+1)\cdots(d+s-1)} \lesssim \frac{N^{s-1}}{d\,n^{s+1}}(\operatorname{Tr}H_e(r))^{s-2}\operatorname{Tr}H_e(r)^2, \tag{B.33}$$

etcetera. For large values of N, dimension $d=n^N$ diverges very fast. It is clear that the first term is the only relevant contribution, as all the remaining terms are negligible compared to it. Thus, the expression (B.29) for large values of N is

$$\begin{aligned} Z_{HC}^N &= \frac{\pi^{d-1}}{(d-1)!}\left(\frac{2\pi M_C}{\beta}\right)^{\frac{3Nm}{2}}\int_{\mathbb{R}^{3Nm}}\mathrm{d}R\left(1-\frac{\beta}{d}\operatorname{Tr}H_{eN}(R)+\frac{\beta^2}{2d^2}(\operatorname{Tr}H_{eN}(R))^2-\cdots\right) \\ &= \frac{\pi^{d-1}}{(d-1)!}\left(\frac{2\pi M_C}{\beta}\right)^{\frac{3Nm}{2}}\int_{\mathbb{R}^{3Nm}}\mathrm{d}R\,\exp\left(-\frac{\beta\operatorname{Tr}H_{eN}(R)}{d}\right). \end{aligned} \tag{B.34}$$

where relation $\operatorname{Tr}H_{eN}(R)\sim n^{N-1}N\operatorname{Tr}H_e(r)$ has been used.

B.4 Proof of Theorem 5.8

Consider a purely quantum canonical ensemble for a d-dimensional quantum system with Hamiltonian H:

$$F_Q([\psi]) = \frac{1}{Z_Q}e^{-\beta\epsilon_H([\psi])}, \quad Z_Q = \int_{\mathcal{P}} e^{-\beta\epsilon_H([\psi])}\mathrm{d}\mu_{\mathcal{P}}. \tag{B.35}$$

Distribution F_Q determines a density matrix ρ_Q, which gives a better description of the statistical ensemble. It is defined as

$$\rho_Q = \int_{\mathcal{P}}\mathrm{d}\mu_{\mathcal{P}}F_Q([\psi])\rho_\psi = \frac{1}{Z_Q}\int_{\mathcal{P}}\mathrm{d}\mu_{\mathcal{P}}e^{-\beta\epsilon_H([\psi])}\rho_\psi. \tag{B.36}$$

Consider a basis $\{|\phi_j\rangle\}$ for the Hilbert space $\mathcal{H}$, composed of eigenvectors of the Hamiltonian H, as in (B.22). It is then possible to compute the elements of ρ_Q as

$$\rho_{jk} = \langle\phi_j|\rho_Q|\phi_k\rangle = \frac{1}{Z_Q}\int_{\mathcal{P}} \mathrm{d}\mu_{\mathcal{P}} e^{-\beta\epsilon_H([\psi])} z_j z_k^* = \frac{1}{2\pi Z_Q}\sum_{l=0}^{\infty}\frac{(-\beta)^l}{l!}\int_{S^{2d-1}} \mathrm{d}\mu_S \,\langle\psi|H|\psi\rangle^l z_j z_k^*. \tag{B.37}$$

with the decomposition given in (B.23). Integrals are computed as in Section B.3. For $j \neq k$, integrals involve odd powers of coordinate functions on S^{2d-1}, hence

$$\rho_{jk} = 0, \quad j \neq k. \tag{B.38}$$

Density matrix is therefore diagonal on this basis. Its diagonal elements are

$$\begin{aligned}
\rho_{jj} =& \frac{1}{2\pi Z_Q}\left(\int_{S^{2n-1}} \mathrm{d}\mu_S\,|z_j|^2 - \beta\sum_{r=1}^{n} E_r \int_{S^{2n-1}} \mathrm{d}\mu_S\,|z_r|^2|z_j|^2 \right.\\
&\left. + \frac{\beta^2}{2}\sum_{r,s=1}^{n} E_r E_s \int_{S^{2n-1}} \mathrm{d}\mu_S\,|z_r|^2|z_s|^2|z_j|^2 + \dots\right)\\
=& \frac{1}{2\pi Z_Q}\left(2A_S^{(2)} - 4\beta A_S^{(2,2)}\mathrm{Tr}H + 4\beta^2 A_S^{(2,2,2)}(\mathrm{Tr}H)^2 + 2\beta^2(A_S^{(4,2)} - A_S^{(2,2,2)})\mathrm{Tr}H^2 + \dots\right)\\
&+ \frac{1}{2\pi Z_Q}\left(2\beta A_S^{(2,2)} - 2\beta A_S^{(4)} + 2\beta^2(A_S^{(4,2)} - 3A_S^{(2,2,2)})\mathrm{Tr}H + \cdots\right)E_j\\
&+ \frac{1}{2\pi Z_Q}\left(\beta^2 A_S^{(6)} - 3\beta^2 A_S^{(4,2)} + 2\beta^2 A_S^{(2,2,2)} + \cdots\right)E_j^2 + \cdots\\
=& \frac{\pi^{d-1}}{d!Z_Q}\left(1 - \frac{\beta}{d+1}\mathrm{Tr}H + \frac{\beta^2}{2(d+1)(d+2)}\left((\mathrm{Tr}H)^2 + \mathrm{Tr}H^2\right) + \dots\right)\\
&- \frac{\pi^{d-1}\beta}{(d+1)!Z_Q}E_j + \frac{\pi^{d-1}\beta^2}{(d+2)!Z_Q}E_j^2 + \cdots,
\end{aligned}$$

computed with the integrals presented in Section B.1. Finally, the expression for the density matrix of the given ensemble is

$$\begin{aligned}
\rho_Q =& \frac{\pi^{d-1}}{d!Z_Q}\left(1 - \frac{\beta}{d+1}\mathrm{Tr}H + \frac{\beta^2}{2(d+1)(d+2)}\left((\mathrm{Tr}H)^2 + \mathrm{Tr}H^2\right) + \dots\right)I\\
&- \frac{\pi^{d-1}\beta}{(d+1)!Z_Q}H + \frac{\pi^{d-1}\beta^2}{(d+2)!Z_Q}H^2 + \cdots
\end{aligned} \tag{B.39}$$

As in Section B.3, this result can be directly extended to the case of a hybrid quantum-classical ensemble of N molecules. Thus, a matrix $\rho^N(\xi)$ is obtained in terms of a partition function Z_{HC}^N and a Hamiltonian $H_{eN}(R)$ as

$$\begin{aligned}
\rho_{HC}^N(\xi) =& \frac{\pi^{d-1}e^{-\beta E_k}}{d!Z_{HC}^N}\left(1 - \frac{\beta}{d+1}\mathrm{Tr}H_{eN}(R) + \frac{\beta^2}{2(d+1)(d+2)}\left((\mathrm{Tr}H_{eN}(R))^2 + \mathrm{Tr}H_{eN}(R)^2\right) + \dots\right)I\\
&- \frac{\pi^{d-1}\beta e^{-\beta E_k}}{(d+1)!Z_{HC}^N}H_{eN}(R) + \frac{\pi^{d-1}\beta^2 e^{-\beta E_k}}{(d+2)!Z_{HC}^N}H_{eN}(R)^2 + \cdots,
\end{aligned} \tag{B.40}$$

with E_k the total kinetic energy of the cores and $d = n^N$. The coefficient of I is similar to the expression (B.29) for the partition function. Therefore, the same arguments of Section B.3 can be used here to simplify this coefficient in the thermodynamic limit. In the remaining terms, observe that the elements of the Hamiltonian for N molecules scale with N. Therefore, for large values of N, as d diverges much faster,

the terms proportional to $H_{eN}(R)$, $H_{eN}(R)^2$, etc., are negligible with respect to the term proportional to the identity I. Thus, in the thermodynamic limit,

$$\rho_{HC}^{N}(\xi) = \frac{\pi^{d-1} e^{-\beta E_k}}{d! Z_{HC}^{N}} \exp\left(-\frac{\beta \,\mathrm{Tr} H_{eN}(R)}{d}\right) I. \tag{B.41}$$

Conclusions

The present dissertation describes in detail geometrical properties, dynamics and statistical behaviour of open quantum systems. The geometric formalism had already been successfully developed for the Schrödinger picture. The dissertation presents an extension or generalisation of this formalism to the study of pure and mixed states of quantum systems. This is a necessary tool in order to fully describe the properties of open quantum systems. Applications of the formalism to different situations have also been discussed. The dynamics of open quantum systems, in particular the Markovian evolution induced by the Kossakowski-Lindblad contributions, has been analysed. Applications in the field of Molecular Dynamics include the study of hybrid quantum-classical systems from a geometric perspective. Dynamics and also statistics of these systems are studied, obtaining interesting results in the description of molecular systems. The main conclusions that can be drawn from the dissertation are the following:

- The geometric formalism of the the Schrödinger picture of Quantum Mechanics identifies the complex Hilbert space $\mathcal{H}$ of the system with a Kähler manifold M_Q. The Hermitian product on $\mathcal{H}$ is represented by a pair of contravariant tensor fields Ω and G on M_Q. Quantum observables are identified with smooth functions on this manifold. A similar construction allows to describe geometrically the projective Hilbert space $\mathcal{P}$, whose elements represent the pure states of the quantum system. The main contribution of the dissertation in this topic is the precise description of the reduction procedure that relates geometric structures on M_Q and on $\mathcal{P}$. As a result, tensor fields $\Omega_{\mathcal{P}}$ and $G_{\mathcal{P}}$, which encode the Lie bracket and Jordan products of observables respectively, are obtained on $\mathcal{P}$.

- A geometric formulation of Quantum Mechanics allows to use geometric tools in the analysis of different problems. The dissertation deals with the description of the Schrödinger equation in terms of Lie-Kähler systems. Due to the existing geometric structures on M_Q, it is possible to define in a rigorous way a superposition rule for this equation. This is a non-linear superposition rule (except for a 2-level system). It presents advantges over typical linear superposition rules for linear systems, as it depends on less particular solution. Furthermore, the described method can be easily applied to other manifolds, such as $\mathcal{P}$. Thus, the analysis of the Schrödinger picture in terms of Lie-Kähler systems makes possible to obtain a superposition rule directly on the manifold $\mathcal{P}$ of pure states of the system.

- In order to provide a better characterisation of open quantum systems, a description of Lie-Jordan algebras is offered. The dissertation proves that the Lie structure of a Lie-Jordan algebra can be described in terms of only the inner derivations of the Jordan product. This offers the possibility for a classification of Lie-Jordan algebras, which physically amounts for a characterisation of the different algebras of observables that can be found in quantum systems. From a physical point of view, the connection between Lie and Jordan structures proves that both are relevant in the description of Quantum Mechanics, as they encode the unitary dynamics and the probabilistic nature of the theory.

- The main contribution of the dissertation to the study of Quantum Mechanics is the geometric description of the manifold $\mathcal{S}$ of pure and mixed states of a quantum system. The Heisenberg picture describes the states of a system as linear, positive functionals on the Lie-Jordan algebra $\mathcal{O}$

of observables on the system. Thus the set $\mathcal{S}$ is a convex subset of the dual space $\mathcal{O}^*$ to the algebra $\mathcal{O}$. By means of a reduction procedure, similar and indeed related to the one performed on the Schrödinger picture, it is possible to describe the tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ on $\mathcal{S}$ that reproduce the algebraic structure of $\mathcal{O}$. Following the results proved in the characterisation of Lie-Jordan algebras, these new tensor fields codify the quantum nature of the system. While $\Lambda_{\mathcal{S}}$ is a Poisson tensor field governing unitary dynamics of the system, the tensor field $R_{\mathcal{S}}$ describes the probabilistic nature of Quantum Mechanics, as it determines the standard derivation of an observable A as

$$R_{\mathcal{S}}(\mathrm{d}\epsilon_A, \mathrm{d}\epsilon_A)(\rho) = 2\epsilon_{A^2}(\rho) - 2(\epsilon_A(\rho))^2 = 2(\Delta_\rho A)^2, \quad \forall \rho \in \mathcal{S}.$$

The manifold of states $\mathcal{S}$ has a rich structure, that can be analysed by the foliation induced by gradient and Hamiltonian vector fields. It can thus be concluded that a geometric description of quantum systems allows for a better characterisation of the manifold $\mathcal{S}$ of pure and mixed states of the system. Also, it offers new tools for the study of dynamics and properties of quantum systems.

- The dissertation presents a geometric description of Markovian evolution of open quantum systems. The geometric formalism makes possible to describe the Kossakowski-Lindblad equation in terms of a vector field on the manifold $\mathcal{S}$ of the form

$$Z_L = X_H + Y_V + Z_K,$$

i.e. as a sum of a Hamiltonian vector field, a gradient vector field, and a vector field determined by a Kraus operator. This decomposition allows for a better characterisation of the properties of Markovian dynamics.

- One of the properties of Markovian evolution of open quantum systems is the contraction of its associated algebra of observables. The dissertations offers a description of these contractions by means of the geometric formalism, which presents some advantages over the usual algebraic approach. Given the tensor fields $\Lambda_{\mathcal{S}}$ and $R_{\mathcal{S}}$ on the manifold $\mathcal{S}$, the Markovian evolution determined by the Kossakowski-Lindblad vector field Z_L defines the following families of tensor fields on $\mathcal{S}$:

$$\begin{aligned} \Lambda_{\mathcal{S},t} =& e^{-t\mathcal{L}_{Z_L}}\Lambda_{\mathcal{S}} = \Lambda_{\mathcal{S}} - t\mathcal{L}_{Z_L}\Lambda_{\mathcal{S}} + \frac{t^2}{2!}(\mathcal{L}_{Z_L})^2\Lambda_{\mathcal{S}} - \cdots, \\ R_{\mathcal{S},t} =& e^{-t\mathcal{L}_{Z_L}}R_{\mathcal{S}} = R_{\mathcal{S}} - t\mathcal{L}_{Z_L}R_{\mathcal{S}} + \frac{t^2}{2!}(\mathcal{L}_{Z_L})^2R_{\mathcal{S}} - \cdots, \end{aligned} \qquad t \geq 0,$$

If the limits of these families for $t \to \infty$ exist, they define a contraction of the Lie-Jordan algebra of observables on the system. Physically, the limit of the Markovian evolution defines a new quantum system, with an algebra of observables which is different from the initial one.

- Evolution of open quantum systems and contractions of algebras benefit from an appropriate description of the limit manifolds of the evolution. In the case of Markovian evolution, limit manifolds can be studied in terms of affine structures. The dissertation presents a set of results that connects the properties of these limit manifold with the contraction of algebras. It has been shown that the restriction to limit manifolds always produces a contraction of the algebras of observables. In physical terms, the limit of a quantum system always can be described as a quantum system, although usually with differences from the initial one. The obtained result also present the conditions under which this contraction can be extended to the whole manifold of states $\mathcal{S}$.

- Control problems of open quantum systems are investigated. In the geometric formalism, it is possible to apply the results of geometric control theory in order to classify open quantum systems with respect to their controllability properties, as it is detailed in the dissertation. Thus, the geometric formalism offers new tools for the design of control strategies of open quantum systems.

- Lastly, properties open quantum systems are analysed in the context of Molecular Dynamics. Hybrid quantum-classical models are common in the description of molecular systems A geometric characterisation of the models presentes advantages in the study of these systems. The dissertation presents particular case of the Ehrenfest model, for which the geometric formalism makes possible to consider an extension of the model to statistical ensembles. In this way, it is possible to describe the decoherence-like effects, observed in molecular systems, and which are not present in the standard Ehrenfest model. Other aspects of the model, such as the hybrid canonical ensemble and its thermodynamic limit, are also investigated. Numerical simulation have been performed in order to support the validity of the proposed statistical Ehrenfest model.

Future research on the properties and dynamics of open quantum systems will take profit of the results of this dissertation. Some of the many possible topic that will be covered in future works are the following:

- The description of Lie systems in Quantum Mechanics has been restricted to the Schrödinger picture. However, the existing geometric structures on the manifold $\mathcal{S}$ of pure and mixed states makes relevant the analysis of Lie systems also in this setting. It is thus expectable that similar or more general results will be obtained. This offers the possibility to study superposition rules not only for unitary evolution, but also for more general dynamics of open quantum systems.

- Control theory of open quantum systems has applications in a broad range of fields, from Molecular Dynamic to Quantum Optics. For this reason, a deep characterisation of control problems in Quantum Mechanics is a relevant problem. The described geometric formalism offers the possibility to analyse these problems from a new point of view, which may offer new solutions and application to many different situations.

- The geometric description of hybrid quantum-classical systems allows to describe the different components of the systems in similar terms. This provides a better characterisation of the systems and their dynamics. The proposed description of the Ehrenfest model will be further analysed and extended. Also, it remains open the possibility to describe geometrically other hybrid models in Molecular Dynamics.

Conclusiones

La presente tesis describe de forma detallada las propiedades geométricas, la dinámica y el comportamiento estadístico de los sistemas cuánticos abiertos. Basándose en el formalismo geométrico para la imagen de Schrödinger desarrollado con anterioridad, la tesis presenta una extensión o generalización al estudio de estados puros y mezcla de sistemas cuánticos, necesarios para una completa descripción de las propiedades de los sistemas cuánticos abiertos. A su vez, se han enunciado diversas aplicaciones del formalismo a distintas situaciones. Se ha analizado la dinámica de sistemas cuánticos abiertos, en particular la evolución markoviana inducida por la ecuación de Kossakowski-Lindblad. Otras aplicaciones, esta vez en el campo de la Dinámica Molecular, incluyen el estudio de sistemas híbridos clásico-cuánticos desde una perspectiva geométrica. Las principales conclusiones extraídas de la tesis doctoral son las siguientes:

- El formalismo geométrico de la imagen de Schrödinger de la Mecánica Cuántica permite identificar el espacio de Hilbert complejo $\mathcal{H}$ del sistema con una variedad Kähler M_Q. El producto hermítico en $\mathcal{H}$ se representa mediante un par de campos tensoriales contravariantes Ω y G en M_Q, mientras que los observables del sistema cuántico se identifican con funciones diferenciables en la variedad. Una construcción similar permite describir de forma geométrica el espacio projectivo de Hilbert $\mathcal{P}$, cuyos elementos representan los estados puros del sistema cuántico. La principal contribución de la tesis a esta descripción es la caracterización del proceso de reducción que relaciona las estructuras geométricas en las variedades diferenciables M_Q y $\mathcal{P}$. Como resultado de esta reducción, se obtienen los campos tensoriales $\Omega_{\mathcal{P}}$ and $G_{\mathcal{P}}$ en $\mathcal{P}$ que describen el paréntesis de Lie y el producto de Jordan de observables, respectivamente.

- La formulación geométrica de la Mecánica Cuántica permite el uso de herramientas geométricas en el análisis de diversos problemas. La tesis trata en particular la descripción de la ecuación de Schrödinger como un sistema de Lie-Kähler. Gracias a las estructuras geométricas existentes en M_Q, es posible definir de manera rigurosa una regla de superposición para esta ecuación, la cual es no lineal, excepto en el caso de sistemas de 2 niveles. Ésta presenta ventajas frente a la regla de superposición lineal típica de sistemas lineales, ya que depende de menos soluciones particulares. Además, el método descrito puede aplicarse fácilmente a otras variedades, como es el caso de $\mathcal{P}$. De esta forma, el análisis de la ecuación de Schrödinger mediante sistemas de Lie-Kähler hace posible la obtención de una regla de superposición directamente en la variedad $\mathcal{P}$ de estados puros del sistema.

- En el contexto de la caracterización de sistemas cuánticos abiertos, la tesis presenta una descripción de las álgebras de Lie-Jordan. Se ha demostrado que la estructura de Lie en estas álgebras puede describirse mediante el análisis de las derivaciones internas del producto de Jordan. Esto ofrece la posibilidad de realizar una clasificación de álgebras de Lie-Jordan, lo que puede interpretarse físicamente como una caracterización de las disversas álgebras de observables que pueden encontrarse en los sistemas cuánticos. Desde un punto de vista físico, la relación entre las estructuras de Lie y Jordan demuestra que ambas son relevantes en la descripción de la Mecánica Cuántica, dado que son necesarios para la descripción de la evolución unitaria y la naturaleza probabilística de la teoría.

- La principal contribución de la tesis al estudio de la Mecánica Cuántica es la descripción geométrica de la variedad $\mathcal{S}$ de estados puros y mezcla del sistema cuántico. La imagen de Heisenberg escribe los estados de un sistema como funcionales lineales y positivos en el álgebra de Lie-Jordan de observables $\mathcal{O}$ del sistema. Como resultado, el conjunto $\mathcal{S}$ es un subconjunto convexo del espacio dual $\mathcal{O}^*$ del álgebra $\mathcal{O}$. Mediante un proceso de reducción, similar y de hecho relacionado con el presentado en la imagen de Schrödinger, es posible describir los campos tensoriales $\Lambda_{\mathcal{S}}$ y $R_{\mathcal{S}}$ en $\mathcal{S}$ que reproducen la estructura algebraica en $\mathcal{O}$. De acuerdo con los resultados obtenidos en la caracterización de las álgebras de Lie-Jordan, estos nuevos campos tensoriales describen la naturaleza cuántica del sistema. El campo tensorial $\Lambda_{\mathcal{S}}$ es de tipo Poisson, y determina la evolución unitaria del sistema. Por su partte, el campo tensorial $R_{\mathcal{S}}$ describe la naturaleza probabilística de la Mecánica Cuántica, dado que determina la desviación estandar de un observable A mediante la siguiente relación:

$$R_{\mathcal{S}}(\mathrm{d}\epsilon_A, \mathrm{d}\epsilon_A)(\rho) = 2\epsilon_{A^2}(\rho) - 2(\epsilon_A(\rho))^2 = 2(\Delta_\rho A)^2, \quad \forall \rho \in \mathcal{S}.$$

  La variedad de estados $\mathcal{S}$ tiene una estructura muy rica, la cual puede analizarse mediante la foliación inducida por los campos vectoriales gradientes y hamiltonianos. Por tanto, se concluye que una descripción geométrica de los sistemas cuánticos permite una mejor caracterización de la variedad $\mathcal{S}$ de estados puros y mixtos del sistema, además de ofrecer nuevas herramientas para el estudio de la dinámica y las propiedades de los sistemas cuánticos.

- La tesis presenta una descripción geométrica de la evolución markoviana de sistemas cuánticos abiertos. El formalismo geométrico permite describir la evolución de Kossakowski-Lindblad mediante un campo vectorial en la variedad $\mathcal{S}$ dado por

$$Z_L = X_H + Y_V + Z_K,$$

  es decir, como una suma de un campo vectorial hamiltoniano, un campo vectorial gradiente y un tercer campo vectorial determinado por un operador de Kraus. Esta descomposición permite una mejor descripción de las propiedades de la dinámica markoviana.

- Una de las propiedades de la evolución markoviana de un sistemas abierto es la contracción de su álgebra de observables asociada. La tesis estudia estas contracciones mediante el formalismo geométrico, lo que presenta ventajas frente al análisis algebraico usual. Dados los campos tensorials $\Lambda_{\mathcal{S}}$ y $R_{\mathcal{S}}$ en la variedad $\mathcal{S}$, la evolución markoviana determinada por el campo vectorial de Kossakowski-Lindblad Z_L define las siguientes familias de tensores en $\mathcal{S}$:

$$\begin{aligned} \Lambda_{\mathcal{S},t} =& e^{-t\mathcal{L}_{Z_L}}\Lambda_{\mathcal{S}} = \Lambda_{\mathcal{S}} - t\mathcal{L}_{Z_L}\Lambda_{\mathcal{S}} + \frac{t^2}{2!}(\mathcal{L}_{Z_L})^2\Lambda_{\mathcal{S}} - \cdots, \\ R_{\mathcal{S},t} =& e^{-t\mathcal{L}_{Z_L}}R_{\mathcal{S}} = R_{\mathcal{S}} - t\mathcal{L}_{Z_L}R_{\mathcal{S}} + \frac{t^2}{2!}(\mathcal{L}_{Z_L})^2R_{\mathcal{S}} - \cdots, \end{aligned} \qquad t \geq 0,$$

  Si existen los límites de estas familias cuando $t \to \infty$, se obtiene una contracción del álgebra de observables del sistema. Desde un punto de vista físico, el límite de la evolución markoviana define un nuevo sistema cuántico, con un álgebra de observables distinta a la inicial.

- Los análisis de la evolución de sistemas cuánticos abiertos y de las contracciones de álgebras se benefician de una correcta descripción de las variedades límite para la evolución. En el caso de evolución markoviana, las variedades límite presentan una estructura afin. La tesis expone un conjunto de resultados que relacionan las propiedades de estas variedades límite con las contracciones de álgebras. Se ha demostrado que la restricción de la dinámica a las variedades límite siempre produce una contracción del álgebra de observables. Físicamente, este hecho implica que el límite de un sistema cuántico siempre puede interpretarse como otro sistema cuántico, normalmente con importantes diferencias con el inicial. La tesis presenta también las condiciones bajo las cuales esta contracción puede extenderse al total de la variedad $\mathcal{S}$ de estados puros y mezcla.

- Se han analizado problemas de control de sistemas cuánticos abiertos. En el formalismo geométrico, es posible aplicar los resultados de la teoría de control geométrico para realizar una clasificacion de sistemas cuánticos abiertos de acuerdo a criterios de controlabilidad, como se explica en la tesis. De esta forma, el formalismo geométrico ofrece nuevas herramientas para el diseño de estrategias de control de sistemas cuánticos abiertos.

- Por último, se han estudiado las propiedades de los sistemas cuánticos abiertos en el contexto de la Dinámica Molecular. Es común utilizar modelos híbridos clásico-cuánticos en el análisis de sistemas moleculares. Una descripción geométrica de estos modelos presenta ventajas en el estudio de estos sistemas. La tesis presenta el caso particular del modelo de Ehrenfest, para el cual el formalismo geométrico hace posible considerar una extensión del modelo a distribuciones estadísticas. De esta forma, se logran describir efectos de decoherencia observados en sistemas moleculares, y que no son predichos por el modelo de Ehrenfest estándar. Se han analizado otros aspectos del modelo, como la distribución canónica híbrida y su límite termodinámico. Además, se han realizado simulaciones numéricas que respaldan la validez del modelo de Ehrenfest estadístico propuesto.

Los resultados presentados en esta tesis serán de utilidad en futuras investigacione en torno a las propiedades y dinámica de los sistemas cuánticos abiertos. Algunos de los muchos posibles temas de investigación que serán tratados en próximos trabajos son los siguientes:

- La descripción de sistemas de Lie en Mecánica Cuántica se ha restringido a la imagen de Schrödinger. Sin embargo, las estructuras geométricas presentes en la variedad $\mathcal{S}$ de estados puros y mezcla pone de relevancia el análisis de sistemas de Lie en este contexto. Se espera por tanto obtener resultados similares a los presentados, o incluso más generales. Esto ofrece la posibilidad de estudiar reglas de superposición, no solo para evoluciones unitarias, sino también para dinámicas de sistemas cuánticos abiertos más generales.

- La teoría de control de sistemas cuánticos abiertos tiene aplicaciones en un muchos campos, desde Dinámica Molecular hasta Óptica Cuántica. Por este motivo, es importante llevar a cabo una descripción detallada de problemas de control de sistemas cuánticos. El formalismo geométrico aquí descrito ofrece la posilidad de analizar estos problemas desde una nueva perspectiva, lo que puede ofrecer nuevas soluciones y aplicaciones a situaciones muy diversas.

- La descripción geométrica de sistemas híbridos clásico-cuánticos permite describir los distintos componentes del sistema de manera similar. Esto permite una mejor caracterización de los sistemas y de su dinámica. La descripción del modelo de Ehrenfest propuesta será analizada en detalle y extendida. Además, queda abierta la posibilidad de describir geométricamente otros modelos híbridos de Dinámica Molecular.

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