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On the controllability of the quantum dynamics of closed and open systems

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Title: On the controllability of the quantum dynamics of closed and open systems
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Abstract: We investigate the controllability of quantum systems in two different settings: the standard "closed" setting, in which a quantum system is seen as isolated and the control problem is formulated on the Schrödinger equation; the open setting that describes a quantum system in interaction with a larger one, of which just qualitative parameters are known, by means of the Lindblad equation on states.

In the context of closed systems we focus our attention to an interesting class of models, namely the spin-boson models. The latter describe the interaction between a 2-level quantum system and finitely many distinguished modes of a bosonic field. We discuss two prototypical examples, the Rabi model and the Jaynes-Cummings model, which despite their age are still very popular in several fields of quantum physics. Notably, in the context of cavity Quantum Electro Dynamics (C-QED) they provide an approximate yet accurate description of the dynamics of a 2-level atom in a resonant microwave cavity, as in recent experiments of S. Haroche. We investigate the controllability properties of these models, analyzing two different types of control operators acting on the bosonic part, corresponding -in the application to cavity QED- to an external electric and magnetic field, respectively. We review some recent results and prove the approximate controllability of the Jaynes-Cummings model with these controls. This result is based on a spectral analysis exploiting the non-resonances of the spectrum. As far as the relation between the Rabi and the Jaynes-Cummings Hamiltonians concerns, we treat the so called rotating wave approximation in a rigorous framework. We formulate the problem as an adiabatic limit in which the detuning frequency and the interaction strength parameter goes to zero, known as the weak-coupling regime. We prove that, under certain hypothesis on the ratio between the detuning and the coupling, the Jaynes-Cumming and the Rabi dynamics exhibit the same behaviour, more precisely the evolution operators they generate are close in norm.

In the framework of open quantum systems we investigate the controllability of the Lindblad equation. We consider a control acting adiabatically on the internal part of the system, which we see as a degree of freedom that can be used to contrast the action of the environment. The adiabatic action of the control is chosen to produce a robust transition. We prove, in the prototype case of a two-level system, that the system approach a set of equilibrium points determined by the environment, i.e. the parameters that specify the Lindblad operator. On that set the system can be adiabatically steered choosing a suitable control. The analysis is based on the application of geometrical singular perturbation methods.

Titre: Sur la contrôlabilité de la dynamique quantique des systèmes fermés et ouverts

Mots clés: Systèmes Quantiques Ouverts, équation de Lindblad, Méthods Adiabatiques, Côntrole Géométrique.

Résumé: on étudie la contrôlabilité des systèmes quantiques dans deux contextes différents: le cadre standard fermé, ou un système quantique est considéré comme isolé et le problème de contrôle est formulé sur l'équation de Schrödinger ; le cadre ouvert qui décrit un système quantique en interaction avec un plus grand, dont seuls les paramètres qualitatifs sont connus, au moyen de l'équation de Lindblad sur les états.

Dans le contexte des systèmes fermés on se focalise sur la classe intéressante des systèmes spin-boson, qui décrivent l'interaction entre un système quantique à deux niveaux et un nombre fini de modes distingués d'un champ bosonique. On considére deux exemples prototypiques, le modèle de Rabi et le modèle de Jaynes-Cummings, qui sont encore très populaires dans plusieurs domaines de la physique quantique. Notamment, dans le context de la Cavity Quantum Electro Dynamics (C-QED), ils fournissent une description précise de la dynamique d'un atome à deux niveaux dans une cavité micro-onde en résonance, comme dans les expériences récentes de S. Haroche. Nous étudions les propriétés de contrôlabilité de ces modèles avec deux types différents d'opérateurs de contrôle agissant sur la partie bosonique, correspondant respectivement – dans l'application à la C-QED – à un champ électrique et magnétique externe. On passe en revue quelques résultats récents et prouvons la contrôlabilité approximative du modèle de Jaynes-Cummings avec ces contrôles. Ce résultat est basé sur une analyse spectrale exploitant les non-résonances du spectre. En ce qui concerne la relation entre l'Hamiltonien de Rabi et Jaynes-Cummings nous traitons dans un cadre rigoureux l'approximation appeleé d'onde tournante. On formule le problème comme une limite adiabatique dans lequel la fréquence de detuning et le paramètre de force d'interaction tombent à zero, ce cas est connu sous le nom de régime de weak-coupling. On prouve que, sous certaines hypothèses sur le rapport entre le detuning et le couplage, la dynamique de Jaynes-Cumming et Rabi montrent le même comportement, plus précisément les opérateurs d'évolution qu'ils génèrent sont proches à la norme.

Dans le cadre des systèmes quantiques ouverts nous étudions la contrôlabilité de l'équation de Lindblad. Nous considérons un contrôle agissant adiabatiquement sur la partie interne du système, que nous voyons comme un degré de liberté qui peut être utilisé pour contraster l'action de l'environnement. L'action adiabatique du contrôle est choisie pour produire une transition robuste. On prouve, dans le cas prototype d'un système à deux niveaux, que le système approche un ensemble de points d'équilibre déterminés par l'environnement, plus précisément les paramètres qui spécifient l'opérateur de Lindblad. Sur cet ensemble, le système peut être piloté adiabatiquement en choisissant un contrôle approprié. L'analyse est fondée sur l'application de méthodes de perturbation géométrique singulière.

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Contents

Chapter 1

Introduction

Quantum mechanics deeply changed our understanding of physical phenomena at atomic scales. The first quantum revolution introduced a theoretical, and mathematically rich, framework that still produces interesting results and new insights in a lot of physic's fields.

Nowadays, with the advancement of research and new technologies, quantum mechanics is revolutionizing (or is about to) our daily lives. As the effective capabilities of manipulating matter and light at atomic scales is steadily growing, in a lot of experimental contexts new technological tools allow to manipulate the state of a quantum system during its evolution with great precision. Therefore, a large number of possibilities are available for daylife applications.

This led to the analysis of quantum systems from a new point of view: the controllability. In this regard, the interest is to develop techniques, both experimental and theoretical, to efficiently drive the evolution of a quantum system. In the last decade this approach produced a large number of practical applications, e.g. laser-driven molecular reactions, pulse sequences design in nuclear magnetic resonance, stabilization of optical systems, Josephson-junctions, ion traps, etc.

For the purpose of controllability quantum systems are usually considered closed. This means that the description of a quantum system is given by a self-adjoint operator on a Hilbert space and its evolution is governed by the Schrödinger equation. Theoretically, numerous approaches were developed to control the Schrödinger dynamics. We remark in particular: abstract controllability criteria of geometric control theory, Lyapunov-based techniques, optimal control methods, spectral analysis of resonances, adiabatic control techniques.

Newer perspectives of application for quantum systems are related to the theory of information. The goal is to understand if it is possible to build a new generation of computers based on quantum phenomena. To achieve this task we must possess the ability of employing quantum systems to store, manipulate and retrieve information, and this requires an unprecedented degree of control and stability. Therefore the actual challenge in quantum control are open systems.

Open quantum systems allow to describe a wide variety of phenomena related to stability. The environment in this approach can be seen as the ensemble of factors that interacting with a system cause the loss of its unitary behaviour. Find strategies to avoid this process is indispensable to ensure usability of quantum systems in information theory.

In this thesis we make some contributions in the control of both closed and open systems.

In Chapter 2 we review the basic geometric control theory and its application to quantum control. A detailed explanation of the various controllability notions for quantum system is presented, underlining the problems related to the infinite dimension of spaces that are used in quantum mechanics.

In Chapter 5 and 6 we treat an interesting class of closed systems, namely the spin-boson models. These type of systems are of great interest because they describe the interaction between matter and light. In Chapter 5 our analysis is dedicated to show the controllability of a fundamental spin-boson model, the Jaynes-Cummings model. This result is based on a spectral analysis exploiting the non resonances of the spectrum. In Chapter 6 we present a partial derivation of the Jaynes-Cummings model from the Rabi model with adiabatic techniques. This is a preliminary result that we count to improve. Although this might seem not related to control theory, the approximation leading from the Rabi to the Jaynes-Cummings model, commonly known as rotating wave approximation, is widely used in the control community for a large number of models. The difficulty here is that we are in an infinite dimensional context, where this type of approximations have not a rigorous mathematical justification.

In Chapter 3 we review a formalism that describes the evolution of open quantum systems, namely the Lindblad equation and the classification of quantum dynamical semigroups. This is the framework that we will use in Chapter 4 to study the possibility of adiabatically control finite dimensional open systems. In particular we will treat the case of a two-level open system. Inspired by the adiabatic control methods for closed systems, we will show that we can still recover some features of these results but on a smaller subset of the state space.

Chapter 2

Controllability of dynamical systems

This chapter wants to be a brief introduction to standard control theory for dynamical systems, as well as a review of recent applications of control theory to quantum systems, which are the objects of our study. For an extended exposition one can consult the monographs [Jur],[D'Al], which will be our main references.

In particular in the first sections we will introduce basic concepts and recall some classic results about controllability of generic nonlinear systems. A special attention will be given to affine systems, which are often of great interest in the quantum framework.

When we introduce quantum system we will be forced to consider state spaces of infinite dimension. In this settings controllability concepts must be redefined, mainly due the impossibility of having strong forms of control. We will define the notion of approximate controllability and present a spectral criterion to determine controllability.

The last part of the chapter will be devoted to adiabatic control methods for quantum systems.

2.1 Standard geometric control theory

2.1.1 General framework

Consider the system

$$\dot{x} = F(x, u), \qquad x \in \mathbb{R}^n, \qquad u \in U \subset \mathbb{R}^m \tag{2.1}$$

where F is assumed to be a smooth function of its arguments. The variable u is called *control* and its domain U is called *control set*. The *family of vector fields generated by* F is

$$\mathcal{F} = \{F(\cdot, u) \mid u \in U\}. \tag{2.2}$$

Here and thereafter we assumed that every element X of $\mathcal{F}$ is a *complete* vector field, *i. e.* X generates a one-parameter family of diffeomorphism $\{\exp tX \mid t \in \mathbb{R}\}$.

Remark 2.1. In this discussion we consider systems on $\mathbb{R}^n$. However, one can assume to deal with a generic smooth manifold M and a smooth field $F : M \times U \to TM$. All statements of theorems that we will illustrate can be reformulated in this more general framework. ⌟

A continuous curve $x : [0, T] \to \mathbb{R}^n$ is called an *integral curve of* $\mathcal{F}$ if there exist a partition $0 = t_0 < t_1 < \cdots < t_m = T$ and a vector fields $X_1, ..., X_m$ in $\mathcal{F}$ such that $u(t) = u_i$, $x(t)$ is differentiable and $\frac{dx}{dt}(t) = X_i(x(t)) = F(x(t), u_i)$ for all $t \in [t_{i-1}, t_i]$, for each $i = 1, ..., m$. Hence $x(t)$ is the solution of (2.1) where $F(x, u(t))$ is a time-varying vector field given by the piecewise-constant control function $u(t)$.

A basic question in control problems is the following: given a finite time $T > 0$, an initial state $x_0 \in \mathbb{R}^n$ and final state $x_f \in \mathbb{R}^n$ find a control function $u : [0, T] \to \mathbb{R}^m$ such that $x(t; u(\cdot))$ the solution of (2.1) with input control $u(t)$ satisfies $x(0; u(\cdot)) = x_0$ and $x(T; u(\cdot)) = x_f$.

Definition 2.2.

(i) *For each* $T > 0$ *and each* $x_0 \in \mathbb{R}^n$*, the* **set of points reachable from** x_0 **at time** T*, denoted by* $\mathcal{A}(x_0, T)$*, is equal to the set of the terminal points* $x(T)$ *of integral curves of* $\mathcal{F}$ *that originates at* x_0.

(ii) *The union*

$$\mathcal{A}(x_0, \leq T) = \cup_{t \in [0,T]} \mathcal{A}(x_0, t) \tag{2.3}$$

is called **set reachable from** x_0 **in time** T.

(iii) *The union*

$$\mathcal{A}(x_0) = \cup_{t \in [0,\infty)} \mathcal{A}(x_0, t) \tag{2.4}$$

is called **set reachable from** x_0.

There is no particular a priori reason to restrict the class of control function to piecewise-constant functions. However, such a class is rich enough to characterize controllability properties of system (2.1) through the vector field family $\mathcal{F}$. Consider the group of diffeomorphism

$$G(\mathcal{F}) := \{\Phi = e^{t_k X_x} e^{t_{k-1} X_{k-1}} \cdots e^{t_1 X_1} \mid k \in \mathbb{N},\ t_1, ..., t_k \in \mathbb{R},\ X_1, ..., X_k \in \mathcal{F}\}. \tag{2.5}$$

The action of G on $\mathbb{R}^n$ partitions it into orbits. For each $x_0 \in \mathbb{R}^n$ the sets of reachable point of Def.2.2 are obtained by the action of a particular subgroup or subset of $G(\mathcal{F})$ on x_0:

$$\mathcal{A}(x_0) = G_+(\mathcal{F}).x_0 = \{e^{t_k X_x} \cdots e^{t_1 X_1} x_0 \mid k \in \mathbb{N},\ t_1, ..., t_k \geq 0,\ X_1, ..., X_k \in \mathcal{F}\};$$

$$\mathcal{A}(x_0, T) = G_T(\mathcal{F}).x_0 = \{e^{t_k X_x} \cdots e^{t_1 X_1} x_0 \mid k \in \mathbb{N},\ t_1, ..., t_k \geq 0,\ \sum_1^k t_i = T,\ X_1, ..., X_k \in \mathcal{F}\};$$

while we will refer to $G(\mathcal{F}).x_0$ as the *orbit of* x_0. Whenever we want to emphasize the dependence of $\mathcal{A}(x_0, \leq T), \mathcal{A}(x_0), \mathcal{A}(x_0, T)$ from $\mathcal{F}$ we will denote them adding the pedix $\cdot_{\mathcal{F}}$, respectively with $\mathcal{A}_{\mathcal{F}}(x_0, \leq T), \mathcal{A}_{\mathcal{F}}(x_0), \mathcal{A}_{\mathcal{F}}(x_0, T)$.

Given this basic formulation, one can define the notions of controllability as follow:

Definition 2.3.

(i) *The system* (2.1) *is said to be* **small time locally controllable at** x_0 *if* x_0 *belongs to the interior of* $\mathcal{A}(x_0, \leq T)$ *for every* $T > 0$.

(ii) *The system* (2.1) *is said to be* **completely controllable** *if* $\mathcal{A}(x_0) = \mathbb{R}^n$ *for every* $x_0 \in \mathbb{R}^n$.

(iii) *The system* (2.1) *is said to be* **strongly controllable** *if* $\mathcal{A}(x_0, \leq T) = \mathbb{R}^n$ *for every* $x_0 \in \mathbb{R}^n$ *and* $T > 0$.

We shall proceed to analyse these different types of controllability in order of strength.

The small times local controllability (STLC) is at first sight a condition on the dimension of sets $\mathcal{A}(x_0, \leq T)$ as subsets of $\mathbb{R}^n$ but, if analysed in detail, gives a lot of information about local properties of the trajectories realizable by means of controls. Roughly speaking STLC at a point x_0 guarantees the possibility of steering the system in any direction starting from x_0, with a velocity that generally depends on the direction as well as the initial point x_0. We will not discuss sufficient or necessary conditions for STLC but we will treat a weaker condition that is *accessibility*. For an extended discussion one can consult [Sus] and reference therein.

2.1.2 Orbits and accessibility

The first step to obtain sufficient conditions that guarantee controllability of system (2.1) is to study topological properties of its orbits. In particular, our main goal is to show that local orbit structure is determined by local properties of the family $\mathcal{F}$. The results in this section descend from the so called *orbit theorem* and the Frobenius theorem, however a complete explanation of those topics is beyond the scope of our discussion and we refer to [Jur, Chap. 2] for a detailed exposition.

The crucial object in the study of the controllability of (2.1) is the Lie algebra generated by its family of vector fields $\mathcal{F}$.

Denote by $F^\infty(\mathbb{R}^n)$ the space of smooth vector fields on $\mathbb{R}^n$. $F^\infty(\mathbb{R}^n)$ is obviously a vector space on $\mathbb{R}$ under the pointwise addiction of vectors. For any smooth vector fields X, Y on $\mathbb{R}^n$, their Lie bracket is defined by

$$[X, Y](x) = DY(x)X(x) - DX(x)Y(x) \tag{2.6}$$

where $DX(x) = [(\partial X_i/\partial x_j)(x)]_{i,j=1}^n$. Notice that $[\cdot,\cdot]$ is linear in each variable, antisymmetric *i. e.* $[X,Y] = -[Y,X]$, and satisfies the Jacobi identity

$$[X,[Y,Z]] + [Y,[Z,X]] + [Z,[X,Y]] = 0.$$

The vector space $F^\infty(\mathbb{R}^n)$ is an algebra with the product given by the bracket (2.6). Moreover since the bracket is bilinear, antisymmetric and satisfies the Jacobi identity is a Lie algebra.

Definition 2.4. *For any family of vector fields $\mathcal{F} \subset F^\infty(\mathbb{R}^n)$ we denote $Lie(\mathcal{F})$ the* **Lie algebra generated by** *$\mathcal{F}$, the smallest vector subspace S of $F^\infty(\mathbb{R}^n)$ that also satisfies $[X,S] \subset S$ for any $X \in \mathcal{F}$.*

Remark 2.5. $Lie(\mathcal{F})$ introduced in the latter definition could be shown to be equivalent to

$$Lie(\mathcal{F}) = \operatorname{span}\Big\{[X_1,[X_2,[...,[X_{k-2},[X_{k-1},X_k]]...]]] \;\Big|\; k \in \mathbb{N},\ X_1,...,X_k \in \mathcal{F}\Big\}.$$

⌟

As vector space $Lie_x(\mathcal{F}) := \{X(x) \mid X \in Lie(\mathcal{F})\}$, where $x \in \mathbb{R}^n$, has a dimension.

Definition 2.6. *We say that the family $\mathcal{F}$ is* **bracket-generating at point** *x if the dimension of $Lie_x(\mathcal{F})$ is equal to n. We say that the family $\mathcal{F}$ is* **bracket-generating** *if this condition is verified for every $x \in \mathbb{R}^n$.*

The following results state that $\dim Lie_x(\mathcal{F})$ determines the dimension of orbits of (2.1) as submanifolds of $\mathbb{R}^n$.

Theorem 2.7 ([Jur, Thm.2.3] **).** *Suppose that $\mathcal{F}$ is bracket-generating at point $x \in \mathbb{R}^n$. Then the orbit $G(\mathcal{F}).x$ is open in $\mathbb{R}^n$. In addition if $\mathcal{F}$ is bracket-generating, then there exists only one orbit of $\mathcal{F}$ equal to $\mathbb{R}^n$.*

Theorem 2.8 (the orbit theorem, [Jur, Corollary of Thm.2.5] **).** *Let $\mathcal{F}$ be a family of smooth vector fields such that the dimension of each vector space $Lie_x(\mathcal{F})$ is constant as x varies in $\mathbb{R}^n$. Then for each $x \in \mathbb{R}^n$, the tangent space at x of orbit $G(\mathcal{F}).x$ coincide with $Lie_x(\mathcal{F})$. Consequently, each orbit of $\mathcal{F}$ is a k-dimensional submanifold of $\mathbb{R}^n$.*

Remark 2.9. Previous theorems hold for families of smooth vector fields on a general smooth manifold M. Extensions also hold if the manifold and the vector families are analytic and for Lie groups (see [Jur, Sect.2.3]). ⌟

Theorems 2.7,2.8 imply that to have the controllability of $\mathcal{F}$, the condition to be bracket-generating is necessary under the assumption that $Lie_x(\mathcal{F})$ is constant as x varies in $\mathbb{R}^n$. However this is not enough, as we will see from topological properties of reachable sets. We will denote $\operatorname{cl}(\cdot)$ and $\operatorname{int}(\cdot)$ the topological closure and interior of a set.

Theorem 2.10. *Suppose that $\mathcal{F}$ is a smooth family of vector fields on $\mathbb{R}^n$ and $\mathcal{F}$ is bracket-generating at $x \in \mathbb{R}^n$. Then for each $T > 0$ and $\varepsilon > 0$,*

(a) *$\mathcal{A}(x, \leq T)$ contains non-empty open sets of $\mathbb{R}^n$,*

(b) *$\mathcal{A}(x, \leq T) \subset \mathrm{cl}(\mathrm{int}\mathcal{A}(x, \leq T))$,*

(c) *$\mathrm{int}(\mathrm{cl}\,\mathcal{A}(x, \leq T)) \subset \mathrm{int}\mathcal{A}(x, \leq T + \varepsilon)$,*

(d) *$\mathrm{int}(\mathrm{cl}\,\mathcal{A}(x)) = \mathrm{int}\mathcal{A}(x)$.*

Property (a) in Theorem 2.10 is called *accessibility.* It means that the trajectories starting from a point can reach (in an arbitrarily small time) a set having non-empty interior. While accessibility guarantees the existence of open reachable sets from any x initial point, it does not say anything on x belonging to it.

The previous result is crucial for a characterization of orbits that derives from it. Notice that we can regard a reachable set of type $\mathcal{A}_{\mathcal{F}}(x)$ or $\mathcal{A}_{\mathcal{F}}(x, \leq T)$, as a set with a topology inherited from $\mathbb{R}^n$ (the entire space), or inherited by the submanifold of the orbit $G(\mathcal{F}).x$, at least under hypothesis of Theorem 2.8. This motivates next definition.

Definition 2.11. *A smooth family of vector fields $\mathcal{F}$ is* **Lie-determined** *if the tangent space of each point x in an orbit of $\mathcal{F}$ coincides with $Lie_x(\mathcal{F})$.*

Obviously, bracket-generating systems are Lie-determined and, by Theorem 2.8, every system $\mathcal{F}$ such that $Lie_x(\mathcal{F})$ has constant dimension for every $x \in \mathbb{R}^n$ is Lie-determined.

Corollary 2.12. *For Lie-determined systems, the reachable sets $\mathcal{A}_{\mathcal{F}}(x)$ cannot be dense in an orbit of $\mathcal{F}$ without being equal to the entire orbit.*

For such systems, each reachable set $\mathcal{A}(x, \leq T)$ has a non-void interior in the topology of the orbit manifold, and the set of interior points grows regularly with T. This is equivalent to saying that the system is accessible in each of its orbits.

Thus, the essential property of a Lie-determined system is the one we claimed at the beginning of the section, its orbit structure is determined by the local properties of the elements of $\mathcal{F}$ and their Lie derivatives.

Moreover, this suggest that different families of vector fields could generate the same orbits if they differ by 'inessential' directions. More precisely, the closure of reachable sets could be taken as invariant to classify families of vector fields that generate the same orbits.

2.1.3 Compatible vector fields and completions

Definition 2.13. *A vector field Y is said to be* **compatible with the family** *$\mathcal{F}$ if defining $\mathcal{F}' = \mathcal{F} \cup \{Y\}$ we have the following. For every x_0, the reachable set $A_{\mathcal{F}'}(x_0) \subset \mathrm{cl}\,\mathcal{A}_{\mathcal{F}}(x_0)$.*

Clearly this defines an equivalence relation between family of vector fields: $\mathcal{F}$,$\mathcal{F}'$ are equivalent if

$$A_{\mathcal{F}\cup\mathcal{F}'}(x_0) \subset \operatorname{cl}\mathcal{A}_{\mathcal{F}}(x_0), \quad A_{\mathcal{F}\cup\mathcal{F}'}(x_0) \subset \operatorname{cl}\mathcal{A}_{\mathcal{F}'}(x_0),$$

for all $x_0 \in \mathbb{R}^n$. A simple reformulation of Corollary 2.12 states that compatible fields does not change the orbits of systems.

Proposition 2.14. *If $\mathcal{F}$ is a bracket-generating family of vector fields, Y is compatible with $\mathcal{F}$ and $\mathcal{F} \cup \{Y\}$ is controllable, then $\mathcal{F}$ is controllable as well.*

Therefore, it is interesting to understand under which operation on a family $\mathcal{F}$, the closure of reachable sets remains invariant. Natural candidates are topological operation on $\mathcal{F}$ as subset of the vector space $F^\infty(\mathbb{R}^n)$. Denote as $\operatorname{cl}(\mathcal{F})$ the topological closure of the set $\mathcal{F}$ in $F^\infty(\mathbb{R}^n)$. Define also $\operatorname{co}(\mathcal{F})$, the *convex hull of* $\mathcal{F}$, as the set

$$\operatorname{co}(\mathcal{F}) := \{\sum_{i=1}^{m} \lambda_i X_i \mid m \in \mathbb{N},\ \lambda_1, ..., \lambda_m \geq 0,\ \sum \lambda_i = 1,\ X_1, ..., X_n \in \mathcal{F}\}. \tag{2.7}$$

Notice that the zero vector field is always compatible with any family $\mathcal{F}$. Hence one can consider also $\operatorname{co}(\mathcal{F} \cup \{0\})$, the positive convex 'semi-cone' through $\operatorname{co}(\mathcal{F})$ and the *positive convex cone*

$$\operatorname{cone}(\mathcal{F}) := \{\sum_{i=1}^{m} \lambda_i X_i \mid m \in \mathbb{N},\ \lambda_1, ..., \lambda_m \geq 0,\ X_1, ..., X_n \in \mathcal{F}\}. \tag{2.8}$$

Theorem 2.15. *Let $\mathcal{F}$ be a family of smooth vector fields on $\mathbb{R}^n$. For any $x \in \mathbb{R}^n$ and $T > 0$*

(a) $\mathcal{A}_{\operatorname{cl}(\mathcal{F})}(x, T) \subset \operatorname{cl}(\mathcal{A}_{\mathcal{F}}(x, T))$,

(b) $\operatorname{cl}(\mathcal{A}_{\mathcal{F}}(x, T)) \subset \operatorname{cl}(\mathcal{A}_{\operatorname{co}(\mathcal{F})}(x, T))$,

(c) $\mathcal{A}_{\operatorname{co}(\mathcal{F}\cup\{0\})}(x, \leq T) \subset \operatorname{cl}(\mathcal{A}_{\mathcal{F}}(x, \leq T))$,

(d) $\mathcal{A}_{\operatorname{cone}(\mathcal{F})}(x) \subset \operatorname{cl}(\mathcal{A}_{\mathcal{F}}(x))$.

Given the equivalence relation defined in Definition 2.13 and the completion operations of the latter theorem, each family of smooth vector field $\mathcal{F}$ has a largest extension which is represented by the maximal element of its equivalent class.

Definition 2.16. *Let $\mathcal{F}$ be a Lie-determined family of vector fields.*

(i) *The* **strong Lie saturate of** $\mathcal{F}$*, denoted $\mathcal{LS}_s(\mathcal{F})$, is the largest subset $\hat{\mathcal{F}}$ of $Lie(\mathcal{F})$ such that*

$$\operatorname{cl}(\mathcal{A}_{\hat{\mathcal{F}}}(x, \leq T)) = \operatorname{cl}(\mathcal{A}_{\mathcal{F}}(x, \leq T))$$

for each $x \in \mathbb{R}^n$ and $T > 0$.

(ii) *The* **Lie saturate of** $\mathcal{F}$, *denoted* $\mathcal{LS}(\mathcal{F})$, *is the largest subset* $\hat{\mathcal{F}}$ *of* $Lie(\mathcal{F})$ *such that*

$$\mathrm{cl}(\mathcal{A}_{\hat{\mathcal{F}}}(x)) = \mathrm{cl}(\mathcal{A}_{\mathcal{F}}(x))$$

for each $x \in \mathbb{R}^n$.

For such a families it is possible to state an abstract criterion of controllability

Theorem 2.17 ([Jur, Thm.2.12]). *Suppose that* $\mathcal{F}$ *is a Lie-determined family of vectors fields. Then* $\mathcal{F}$ *is strongly controllable if and only if* $\mathcal{LS}_s(\mathcal{F}) = Lie(\mathcal{F})$ *and* $Lie(\mathcal{F})$ *is bracket-generating.* $\mathcal{F}$ *is controllable if and only if* $\mathcal{LS}(\mathcal{F}) = Lie(\mathcal{F})$ *and* $Lie(\mathcal{F})$ *is bracket-generating.*

As elegant as the latter criterion is, its applicability is nevertheless restricted to situations in which there are further symmetries that allow for explicit calculations of the Lie saturate. For that reason we will illustrate an application of this theorem in the next subsection, where our objects will be affine systems.

A notable case in which symmetries of the systems implies controllability is pointed out in the following theorem.

Theorem 2.18 (Chow). *Suppose that* $\mathcal{F}$ *is bracket-generating and for each* $X \in \mathcal{F}$ *then* $-X \in \mathcal{F}$. *Then* $\mathcal{A}(x_0) = \mathbb{R}^n$ *for every* $x_0 \in \mathbb{R}^n$.

2.1.4 Affine systems

An affine system is a differential system on $\mathbb{R}^n$ of the form

$$\dot{x} = f_0(x) + \sum_{i=1}^{m} u_i f_i(x), \qquad x \in \mathbb{R}^n, \quad u = (u_1, ..., u_m) \in U \subset \mathbb{R}^m \tag{2.9}$$

with $f_0, ..., f_m$ smooth vector fields on $\mathbb{R}^n$, and functions $u_1, ..., u_m$ that are the controls. The vector field f_0 is called *the drift*, and the remaining vector fields $f_1, ..., f_m$ are called *controlled vector fields*. A control affine system (2.9) defines the family of vector fields

$$\mathcal{F}(U) = \{f_0 + \sum_{i=1}^{m} u_i f_i \mid u = (u_1, ..., u_m) \in U\}. \tag{2.10}$$

It will be convenient to consider only the constraint subsets U of $\mathbb{R}^m$ that contain m linearly independent points of $\mathbb{R}^m$, in that case the Lie algebra generated by $\mathcal{F}(U)$ is independent of U and is generated by the vector fields $f_0, ..., f_m$, *i. e.*

$$Lie(\mathcal{F}(U)) = Lie\{f_0, ..., f_m\}.$$

Classification of control affine systems is based on properties of the drift.

Definition 2.19. *A control affine system is called* **driftless** *if* $f_0 = 0$.

Driftless systems are immediately treated with the theory developed in the previous section.

Theorem 2.20. *Assume that the system* (2.9) *is driftless and bracket-generating, i. e.* $\dim Lie_x\{f_1, ..., f_m\} = n$ *for all* $x \in \mathbb{R}^n$. *Then,*

(a) *whenever there are no restrictions on the size of controls the corresponding control affine system is strongly controllable,*

(b) *in the presence of constraints* $U \subset \mathbb{R}^m$, (2.9) *remains controllable (but not necessarily strongly controllable) if* $\mathrm{int}(\mathrm{co}(U)) \subset \mathbb{R}^m$ *contains the origin.*

Close to driftless systems are those systems in which the drift generates a dynamics that have almost closed orbits.

Definition 2.21. *A complete vector field* f *on* $\mathbb{R}^n$ *is said to be* **recurrent** *if for every point* $x_0 \in \mathbb{R}^n$, *every neighborhood* V *of* x_0 *and every time* $t > 0$ *there exists* $t^* > t$ *such that* $e^{t^* f}(x_0) \in V$.

Notice that every field f that generates periodic trajectories is recurrent. The following lemma is the key to investigate controllability of affine systems with recurrent drift.

Lemma 2.22. *If* f *is recurrent and compatible with* $\mathcal{F}$, *then* $-f$ *is also compatible with* $\mathcal{F}$.

This leads to the following

Theorem 2.23. *Assume that the system* (2.9) *has recurrent drift, is bracket-generating and* $\mathrm{int}(\mathrm{co}(U))$ *contains the origin of* $\mathbb{R}^m$. *Then the system is controllable.*

When the drift has no particular properties, it is in general an obstacle to controllability. In that case the control field should be strong enough to contrast the effect of the drift and steer the system in every direction.

Theorem 2.24. *Assume that the system* (2.9) *has unbounded controls, i. e.* $U = \mathbb{R}^m$. *If* $\mathcal{G} = \{f_1, ..., f_m\}$ *is bracket-generating then the system is controllable.*

2.2 Controllability of quantum systems

Let $\mathcal{H}$ be an Hilbert space. A *quantum system* on $\mathcal{H}$ is given by a self-adjoint operator H_0 which governs its dynamics, namely the evolution of the wavefunctions $\psi \in \mathcal{H}$, by means of the Schrödinger equation

$$i\hbar \frac{d}{dt}\psi = H_0\psi, \qquad \psi \in \mathcal{H}. \tag{2.11}$$

Let $H_1, ..., H_m$ be linear operators on $\mathcal{H}$, we will call them *control operators*, and $u_1, ..., u_m$ piecewise-constant control functions with the constraint $u = (u_1, ..., u_m) \in$

$U \subset \mathbb{R}^m$. A *bilinear Schrödinger equation* (sometimes called bilinear systems) is an affine control system of the form (2.9) that reads

$$i\hbar \frac{d}{dt}\psi = H(u)\psi = \left(H_0 + \sum_{k=1}^{m} u_k H_k \right) \psi, \qquad \psi \in \mathcal{H},\ u \in U \tag{2.12}$$

Remark 2.25. For the moment we will not assume anything on operators $H_1, ..., H_m$ but we recall that the operator $H_0+\sum u_k H_k$ must be a self-adjoint operator to represent the Hamiltonian of a quantum system. To ensure this, different assumptions are needed depending whether the dimension of $\mathcal{H}$ is finite or infinite. In the following discussion we will clarify these hypothesis. ⌟

2.2.1 Finite dimensional quantum systems

Suppose that $\dim_{\mathbb{C}} \mathcal{H} = N < \infty$, then $H_0, ..., H_m$ belongs to the set of linear bounded operators on $\mathcal{H}$, denoted $\mathcal{B}(\mathcal{H})$. Assume moreover that $H_0, ..., H_m$ are Hermitian operators, *i.e.* $H_k^\dagger = H_k$, $k = 0, ..., m$, hence every real linear combination of them is Hermitian. Therefore, for every $u_1, ..., u_m$ piecewise-constant control functions (assume them right-continuous) the solution of (2.12) with initial datum ψ_0 reads

$$U_u(t)\psi_0$$

with

$$U_u(t) := e^{-i(t-\sum_{i=1}^{j} t_i)(H_0+\sum u_k(t_j)H_k)/\hbar}\, e^{-it_j(H_0+\sum u_k(t_{j-1})H_k)/\hbar} \cdots e^{-it_1(H_0+\sum u_k(0)H_k)/\hbar} \tag{2.13}$$

where $t \in [t_j, t_{j+1}]$ and the sequence of times $0 = t_0 < t_1 < \cdots < t_n < \cdots$ is taken such that $u_k(t)$ is constant on $[t_j, t_{j+1}]$ for all $k = 1, ..., m$ and $n \in \mathbb{N}$.

Identifying the Hilbert space $\mathcal{H}$ with $\mathbb{R}^{2N}$, the whole theory on controlled affine systems developed in the previous section can be applied in this case. However this approach is deceitful from a physical viewpoint. In fact, a (pure) state of a quantum system $\mathcal{H}$ is an equivalent class in the complex projective space on $\mathcal{H}$ (see Sect.3.3). So, if two vectors $\psi_1, \psi_2 \in \mathcal{H}$ differ by a non zero complex number, namely $\psi_1 = z\psi_2$, $z \in \mathbb{C}^*$, they represent the same state. Moreover, being $-iH_0 - i\sum u_k H_k$ skew-adjoint, the propagator $U_u(t)$ defined in (2.13) is a unitary operator (see Stone theorem [RS$_1$]), hence the norm of vectors $\psi \in \mathcal{H}$ is preserved during the evolution.

For those reasons it is useful to state a notion of controllability specific for quantum systems

Definition 2.26. (Equivalent State Controllability)
The quantum system (2.12) *is* **equivalent state controllable** *if for every pair* $\psi_0, \psi_1 \in \mathcal{H}$ *with* $\|\psi_0\| = \|\psi_1\| = 1$*, there exists* $T > 0$ *and piecewise-constant functions* $u_k : [0, T] \to \mathbb{R}^m$ $k = 1, ..., m$ *such that the solution* $\psi(t)$ *of* (2.12) *satisfies* $\psi(0) = \psi_0$ *and* $\psi(T) = e^{i\theta}\psi_1$ *for some* $\theta \in [0, 2\pi)$.

Nevertheless, we can exploit in a useful way the control theory of affine systems considering system (2.12) at the propagator level, *i.e.* as an equation for $U_u(t)$. Set $A_k = -iH_k/\hbar$, $k = 0, ..., m$, then matrices A_k are skew-Hermitian, *i.e.* $A_k^\dagger = -A_k$. The set of skew-Hermitian $N \times N$ matrices, denoted $\mathfrak{u}(N)$, is a Lie algebra of dimension N^2 with respect to the usual bracket $[A, B] = AB - BA$. The subset of skew-Hermitian $N \times N$ matrices with zero trace, denoted $\mathfrak{su}(n)$, is a Lie subalgebra of $\mathfrak{u}(n)$ of dimension $n^2 - 1$. With those notations the equation for U reads

$$\begin{aligned} \frac{d}{dt}U &= \left(A_0 + \sum_{k=1}^{m} u_k(t) A_k\right) U, \qquad (2.14) \\ U(0) &= \mathbb{1}. \end{aligned}$$

This system is an affine control system on the Lie group of unitary matrix $N \times N$, denoted $\mathbb{U}(N)$, or if $\operatorname{tr} A_k = 0$ for all $k = 0, ..., m$, then U has determinant 1 and belong to the Lie subgroup $\mathbb{SU}(N)$.

Definition 2.27. (Operator controllability)
The quantum system (2.12) *is* **operator controllable** *if* $\mathcal{A}_\mathcal{G}(\mathbb{1}) = \mathbb{U}(N)$ *where* $\mathcal{G} = \{A_0, A_1, ..., A_m\}$*. In case* $\operatorname{tr} A_k = 0$ *for every* $k = 0, ..., m$ *is* **operator controllable** *if* $\mathcal{A}_\mathcal{G}(\mathbb{1}) = \mathbb{SU}(N)$*.*

Criteria of controllability for affine systems on compact Lie groups are in some sense analogs to the ones we stated for $\mathbb{R}^n$. In particular, the hypothesis of being bracket-generating must be reformulated accordingly to the characterization of tangent space of a Lie group, for a complete treatment see [D'Al]. However, the controllability of the system (2.14) still relies on the fact that $\mathcal{G}$ must generate the whole tangent space.

Theorem 2.28 (Lie algebra rank condition **).** *The system* (2.12) *is operator controllable if and only if Lie*$\{A_0, ..., A_m\}$ *is equal to* $\mathfrak{u}(n)$ *or, respectively,* $\mathfrak{su}(n)$ *in case that* $\operatorname{tr} A_k = 0$ *for every* $k = 0, ..., m$*.*

Remark 2.29. In the special case of system (2.14) the bracket-generating condition is also known as the Lie algebra rank condition, the theorem rephrase this condition for affine systems on $\mathbb{U}(N)$ or $\mathbb{SU}(N)$. The crucial point in the proof of the latter theorem is that there exists a one-to-one correspondence between Lie subalgebras of $\mathfrak{u}(n)$ and connected Lie subgroups of $\mathbb{U}(n)$. The theorem is based on the fact that $\mathcal{A}_\mathcal{G}(\mathbb{1})$ is the Lie group corresponding to the subalgebra *Lie*$\{A_0, ..., A_m\}$. ⌟

Remark 2.30. The notion of operator controllabilty is obviously stronger than the notion of equivalent state controllability. Results on compact and effective Lie groups acting transitively on $S_\mathbb{C}^{N-1}$, the unit sphere of $\mathbb{C}^N$ and also the projective complex space, allow to characterize the equivalent state controllability in terms of *Lie*$(\mathcal{G})$ [AD'A]. ⌟

We conclude this section with an explicit example.

Example 2.31. Consider the Lie algebra $\mathfrak{su}(2)$ with basis $\{i\sigma_1, i\sigma_2, i\sigma_3\}$ where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.15}$$

are the *Pauli matrices*. A natural choice for the (uncontrolled) Hamiltonian of a two-level quantum system is

$$H_0 = \frac{\omega_{eg}}{2}\sigma_3. \tag{2.16}$$

Consider the control operator $H_1 = \sigma_1$, then (2.12) reads

$$i\hbar\frac{d}{dt}\psi = \left(\frac{\omega_{eg}}{2}\sigma_3 + \frac{u(t)}{2}\sigma_1\right)\psi$$

where $\psi \in \mathbb{C}^2$. If $\omega_{eg} \neq 0$ one immediately obtains

$$[i\sigma_3, i\sigma_1] = -2i\sigma_2$$

then $Lie(i\sigma_3, i\sigma_1) = \mathfrak{su}(2)$ and by Theorem 2.28 the system is controllable. ⌟

2.2.2 Infinite dimensional quantum systems

We now introduce the controllability problem for an affine system in a general infinite dimensional setting. Let $\mathcal{H}$ be a separable Hilbert space endowed with an Hermitian product $\langle \cdot\,, \cdot \rangle$, let $\Phi_{\mathcal{I}}$ be an Hilbert basis for $\mathcal{H}$ and consider the equation

$$\frac{d}{dt}\psi = (A + uB)\psi, \quad \psi \in \mathcal{H} \tag{2.17}$$

where A, B are skew-adjoint linear operator on $\mathcal{H}$ with domain $\mathcal{D}(A)$ and $\mathcal{D}(B)$ respectively, u is a time depending function with values in $U \subset \mathbb{R}$.

Assumption 2.32. *The system $(A, B, U, \Phi_{\mathcal{I}})$ is such that:*

(A_1) $\Phi_{\mathcal{I}} = \{\phi_k\}_{k\in\mathcal{I}}$ *is a Hilbert basis of eigenvectors for A associated to the eigenvalues $\{i\lambda_k\}_{k\in\mathcal{I}}$;*

(A_2) $\phi_k \in \mathcal{D}(B)$ *for every $k \in \mathcal{I}$;*

(A_3) $A + wB : \mathrm{Span}_{k\in\mathcal{I}}\{\phi_k\} \to \mathcal{H}$ *is essentially skew-adjoint*[1] *for every $w \in U$;*

(A_4) *if $j \neq k$ and $\lambda_j = \lambda_k$, then $\langle \phi_j\,, B\phi_k \rangle = 0$.*

[1] A skew-symmetric operator X on $\mathcal{D}(X)$ is essentially skew-adjoint if iX admits a unique self-adjoint extension [RS_2, Chap.X]

Under these assumptions $A + wB$ generates a unitary group $t \mapsto e^{(A+wB)t}$ for every constant $w \in U$. Hence we can define for every piecewise constant function $u(t) = \sum_{i=1} u_i \chi_{[t_{i-1},t_i]}(t)$ with $0 = t_0 < t_1 < ... < t_n < ..$, the propagator

$$\Upsilon_u(t) := e^{(t-t_j)(A+u_{j+1}B)} \circ e^{(t_j-t_{j-1})(A+u_jB)} \circ \cdots \circ e^{t_1(A+u_1B)} \quad \text{for} \quad t_j < t \leq t_{j+1}. \tag{2.18}$$

The solution of (2.17) with initial datum $\psi(0) = \psi_0 \in \mathcal{H}$ is $\psi(t) = \Upsilon_u(t)(\psi_0)$.

Although in this framework it is possible to define a notion of operator controllability, since we already saw that the progator of the dynamics is well defined under Assumption 2.32, this type of controllability is in general too strong for bilinear infinite dimensional systems. This issue about the infinite dimension case is well known and studied in a more general context in a series of paper of Ball, Marsden e Slemrod [BMS]. Applications of this result to quantum system was given in [Tur], and reviewed in [ILT],[BCS].

Proposition 2.33 ([Tur, Theorem 1] **).** *Let $(A, B, U, \Phi_{\mathcal{I}})$ satisfy Assumption 2.32 and let B bounded. Then for every $r > 1$ and for all $\psi_0 \in \mathcal{D}(A)$, the set of reachable states from ψ_0 with control functions in L^r, $\{\Upsilon_u(t)\psi_0 \,|\, u \in L^r(\mathbb{R}, \mathbb{R})\}$ is a countable union of closes sets with empty interior in $\mathcal{D}(A)$. In particular this attainable set has empty interior in $\mathcal{D}(A)$.*

Remark 2.34. The proposition implies that, under its hypothesis, the set of attainable states can't be the whole domain $\mathcal{D}(A)$, therefore we can't have equivalent state controllability or operator controllability for the system $(A, B, U, \Phi_{\mathcal{I}})$. This does not mean that we can't recover strong forms of controllability under different hypothesis but clearly a general equivalent state controllability criteria for systems of type $(A, B, U, \Phi_{\mathcal{I}})$ cannot exist under Assumption 2.32. ⌟

Example 2.35. A notable non-controllable quantum system is the harmonic oscillator. In [MiRo], Mirrahimi e Rouchon proved the non-controllability of system

$$i\hbar \frac{d}{dt}\psi = \frac{1}{2}(P^2 + X^2)\psi - u(t)X\psi, \qquad \psi \in L^2(\mathbb{R}) \tag{2.19}$$

where the *position operator* $X : \mathcal{D}(X) \subset L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is defined

$$(X\psi)(x) := x\psi(x) \tag{2.20}$$

on the domain

$$\mathcal{D}(X) = \left\{ \psi \in \mathcal{H} \;\middle|\; \int_{\mathbb{R}} \|x\psi(x)\|^2 \, dx < \infty \right\}, \tag{2.21}$$

and the *pulse operator* $P : \mathcal{D}(P) \subset L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is the derivative

$$(P\psi)(x) := -i\frac{\partial}{\partial x}\psi(x) \tag{2.22}$$

with domain $\mathcal{D}(P) = H^1(\mathbb{R})$. The main idea is the following. System (2.19) can be decomposed in two parts, one of dimension two which is controllable, and the other infinite dimensional and uncontrollable. From Ehrenfest theorem (see [Mor, 12.2.2]) we obtain equations for average position and pulse

$$\langle X \rangle_t := \langle \psi(t)\,,\, X\psi(t) \rangle\,, \quad \langle P \rangle_t := \langle \psi(t)\,,\, P\psi(t) \rangle\,,$$

where $\psi(t)$ is the solution to (2.19). The equations are

$$\frac{d}{dt}\langle X \rangle_t = \langle P \rangle_t \qquad \frac{d}{dt}\langle P \rangle_t = -\langle X \rangle_t + u \tag{2.23}$$

and this bidimensional system is controllable.

Performing the change of coordinates $\psi(t,x) = e^{i\langle P \rangle z}\phi(t,z)$ with $(t,x) \mapsto (t, z = x - \langle X \rangle_t)$, the Schrödinger equation becomes

$$i\hbar\frac{d}{dt}\phi = \frac{1}{2}(\tilde{P}^2 + Z^2)\phi + \frac{1}{2}(\langle X \rangle^2 - \langle P \rangle^2 - 2u\langle X \rangle)\phi$$

where Z is the multiplication operator by z and $\tilde{P} = \partial/\partial z$. Applying another unitary transformation

$$\phi(t,z) = e^{-i\int_0^t (\langle X \rangle^2 - \langle P \rangle^2 - 2u\langle X \rangle)}\varphi(t,z)$$

one obtains

$$i\hbar\frac{d}{dt}\varphi = \frac{1}{2}(\tilde{P}^2 + Z^2)\varphi. \tag{2.24}$$

From equation (2.24) together with (2.23) one sees that (2.19) decomposes in two independent parts. One part is controllable while the other one is not because it does not depend on the control function u. Therefore the quantum harmonic oscillator is non-controllable. ⌟

As explained before, we need to introduce a weaker notion of controllability for infinite dimensional quantum systems. The natural way to proceed is to ask that reachable sets must be dense subsets of the state space.

Definition 2.36. *Let $(A, B, U, \Phi_{\mathcal{I}})$ satisfy Assumption 2.32. We say that (2.17) is* ***approximately controllable*** *if for every $\psi_0, \psi_1 \in \mathcal{H}$ with $\|\psi_0\| = \|\psi_1\| = 1$ and for every $\varepsilon > 0$ there exist a finite $T_\varepsilon > 0$ and a piecewise constant control function $u : [0, T_\varepsilon] \to U$ such that*

$$\|\psi_1 - \Upsilon_u(T_\varepsilon)(\psi_0)\| < \varepsilon.$$

Remark 2.37. The definition says that to have approximate controllability the set of attainable state from ψ_0, namely $\mathcal{A}(\psi_0) = \{\Upsilon_u(t)\psi_0 \mid u \text{ piecewice-const. function}\}$ must be dense in the unit sphere of $\mathcal{H}$ for every $\psi_0 \in \mathcal{H}$. ⌟

The notion of approximate controllability is clearly weaker that the exact controllability but one may search conditions under which the two coincides. We recall that an analogous result holds on orbits of Lie-determined systems (see Corollary 2.12), where reachable sets cannot be dense in an orbit without being equal to the entire orbit. For finite dimensional systems the two notions coincides.

Theorem 2.38 ([BGRS, Theorem 17] **).** *Suppose* $\dim \mathcal{H} = N < \infty$. *System* (2.12) *is approximately controllable if and only if is exactly controllable.*

Notable works on approximately controllable quantum systems concern spin-boson systems. In particular we mention the paper of Puel [ErPu], inspired to the work of Eberly and Law [EbLa].

An alternative to the introduction of a weak notion of controllability as in Definition (2.36) is to investigate controllability of infinite dimensional systems on smaller functional spaces. More precisely, consider a system $(A, B, U, \Phi_{\mathcal{I}})$ satisfying Assumption 2.32. The idea is to choose a functional space $\mathcal{S}$ contained in $\mathcal{D}(A)$ such that B is unbounded on $\mathcal{S}$ and prove exact controllability on this space. That method is carried out in [Be],[BeC],[BeL].

2.2.3 A spectral condition for controllability

In this section we present a criterion for approximate controllability which will be useful later in this thesis. This general result gives a sufficient condition for approximate controllability based on the spectrum of A and the action of the control operator B. More precisely, if $\sigma(A)$ has a sufficiently large number of non-resonant transitions, *i.e.* pairs of levels (i, j) such that their energy difference $|\lambda_i - \lambda_j|$ is not replicated by any other pair, and B is able to activate these transitions, then the system is approximately controllable.

This idea is made precise in the following definition

Definition 2.39. *Let* $(A, B, U, \Phi_{\mathcal{I}})$ *satisfy Assumption 2.32. A subset* S *of* $\mathcal{I}^2$ ***connects a pair*** $(j, k) \in \mathcal{I}^2$, *if there exists a finite sequence* $s_0, ..., s_p$ *such that*

(i) $s_0 = j$ *and* $s_p = k$;

(ii) $(s_i, s_{i+1}) \in S$ *for every* $0 \le i \le p-1$;

(iii) $\langle \phi_{s_i}, B\phi_{s_{i+1}} \rangle \neq 0$ *for every* $0 \le i \le p-1$.

S *is called a* ***chain of connectedness*** *for* $(A, B, U, \Phi_{\mathcal{I}})$ *if it connects every pair in* $\mathcal{I}^2$.

A ***chain of connectedness*** *is called* ***non-resonant*** *if for every* $(s_1, s_2) \in S$ *it holds*

$$|\lambda_{s_1} - \lambda_{s_2}| \neq |\lambda_{t_1} - \lambda_{t_2}|$$

for every $(t_1, t_2) \in \mathcal{I}^2 \setminus \{(s_1, s_2), (s_2, s_1)\}$ *such that* $\langle \phi_{t_1}, B\phi_{t_2} \rangle \neq 0$

Intuitively, if two levels of the spectrum are non-resonant and the control operator B couples them, one can tune the control function u in such a way to arrange arbitrarily the wavefunction's components on these levels, without modifying any other component. Therefore, having a non-resonant connectedness chain allow us to reach the target state by sequentially modifying the wavefunction. This idea is crucial to the proof of the following criterion by Boscain et al.

Theorem 2.40. [BCCS, Theorem 2.6] *Let $c > 0$ and let $(A, B, [0, c], \Phi_{\mathcal{I}})$ satisfy Assumption 2.32. If there exists a non-resonant chain of connectedness for $(A, B, [0, c], \Phi_{\mathcal{I}})$ then the system (2.17) is approximately controllable.*

Theorem 2.40 gives also an estimate on the norm of control functions.

Proposition 2.41. [BCCS, Proposition 2.8] *Let $c > 0$. Let $(A, B, [0, c], \Phi_{\mathcal{I}})$ satisfy Assumption 2.32 and S be a non-resonant chain of connectedness. Then for every $\varepsilon > 0$ and $(j, k) \in S$ there exists a piecewice-constant control function $u : [0, T_u] \mapsto [0, \delta]$ and $\theta \in \mathbb{R}$ such that $\left\|\Upsilon_u(T_u)\phi_j - e^{i\theta}\phi_k\right\| < \varepsilon$ and*

$$\|u\|_{L^1} \leq \frac{5\pi}{4\,\|\langle\phi_k\,,\,B\phi_j\rangle\|}.$$

2.2.4 Adiabatic control of quantum systems

Our previous analysis of controllability of quantum systems is entirely non constructive, in the sense that we studied criteria to determine abstractly the controllability of the system without producing control functions. In this section we will present a constructive method that relies on adiabatic theory. Consider the general Schrödinger equation

$$i\hbar\frac{d}{dt}\psi = H(u(t))\psi, \qquad \psi \in \mathcal{H}, \tag{2.25}$$

where $u : [0, T] \to U \subset \mathbb{R}^m$. The starting point is a spectral analysis of the operator family $H(u)$.

Assumption 2.42. *Assume that $\{H(u) \mid u \in U\}$ is a family of compact resolvent operators and that eigenfunctions and eigenvalues of the family are analytic functions of the variable u.*

Assumption 2.42 holds for a wide range of quantum systems, *e.g.* bilinear systems (2.12) on a finite dimensional Hilbert space, bilinear system on $L^2(\mathbb{R}^n)$ with $H_0 = -\Delta$ and $H_i = V_i$ with $V_i \in L^2 + L^\infty$ or any system $(A, B, U, \Phi_{\mathcal{I}})$ satisfying Assumption 2.32.

For the sake of clarity we will consider from here throughout the section a bilinear system (2.12) on $\mathcal{H}$ with two controls

$$i\hbar\frac{d}{dt}\psi = H(u(t))\psi = (H_0 + u_1(t)H_1 + u_2(t)H_2)\,\psi \tag{2.26}$$

where $u = (u_1, u_2) \in U \subset \mathbb{R}^2$ and U is assumed connected. However, what we explain can be generalized to the case $U \subset \mathbb{R}^m$ $m \geq 2$.

Assumption 2.43. *Suppose that $\Sigma(u) = \{\lambda_1(u), ..., \lambda_n(u)\}$ with $\lambda_1(u) \leq \lambda_2(u) \leq ... \leq \lambda_n(u)$ is a portion of the spectrum of $H(u)$ isolated from the rest, i. e. there exists $C > 0$ such that*

$$\inf_{u \in U} \inf_{\lambda \in \sigma(H(u) \backslash \Sigma(u))} dist(\lambda, \Sigma(u)) > C. \tag{2.27}$$

Moreover, suppose that λ_i are non degenerate and $\Phi(u) = \{\phi_1(u), ..., \phi_n(u)\}$ are the corrisponding eigenvectors.

Definition 2.44. *We will call $\bar{u} \in U$ a* **conical intersection** *between the eigenvalues λ_j and λ_{j+1} if $\lambda_j(\bar{u}) = \lambda_{j+1}(\bar{u})$ has multiplicity two and there exists $c > 0$ such that*

$$\lambda_j(\bar{u} + tv) - \lambda_{j+1}(\bar{u} + tv) > ct$$

We will say that $\Sigma(u)$ is **conically connected** *if for every $j = 1, ..., n-1$ there exists $\bar{u}_j$ conical intersection between λ_j and λ_{j+1}.*

Remark 2.45. Under Assumption 2.42 the intersections between the eigenvalues of $H(u)$ are generically conical if $m = 2, 3$ [BGRS]. ⌟

In this framework the adiabatic theorem gives a lot of qualitative informations about the dynamics of the system:

a) Suppose that $u = (u_1, u_2) : [0, 1] \to U$ is a path such that $\lambda_j(u(t))$ is simple for every $t \in [0, 1]$. For every $\varepsilon > 0$ let us consider the reparametrization $u^\varepsilon = (u_1^\varepsilon, u_2^\varepsilon) : [0, 1/\varepsilon] \to U$ defined as $(u_1^\varepsilon(t), u_2^\varepsilon(t)) := (u_1(\varepsilon t), u_2(\varepsilon t))$. Then, the solution ψ^ε of the equation

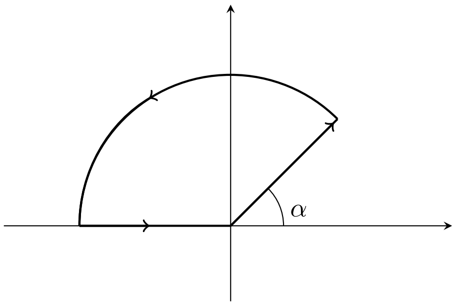
$$i\hbar \frac{d}{dt}\psi = H(u^\varepsilon(t))\psi = (H_0 + u_1^\varepsilon(t)H_1 + u_2^\varepsilon(t)H_2)\,\psi \tag{2.28}$$

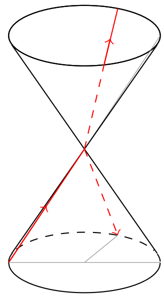
with initial state $\psi^\varepsilon(0) = \phi_j(u(0))$ satisfies

$$\left\| \psi^\varepsilon(1/\varepsilon) - e^{i\theta}\phi_j(u(1/\varepsilon)) \right\| < C_j \varepsilon.$$

So, if the control u is slowly varying, the system follows the eigenvector $\phi_j(u)$ of eigenvalue $\lambda_j(u)$ with an error of order ε. This is a classical result in quantum mechanics that goes back to Kato [Ka][Teu]. The constant C_j depends on the distance between λ_j and the closest of the remaining eigenvalues.

b) Now suppose to design a path $u = (u_1, u_2) : [0, 1] \to U$ passing once through a conical intersection $\bar{u}_j = u(t^*)$. The qualitative behavior of the system undergoing this dynamics is the following: starting from the eigenspace of eigenvalue λ_j and treading adiabatically the path, the system follows the eigenstate $\phi_j(u)$ until time t^*. During the passage through the conical intersection there is a non zero probability that the system jumps in the eigenspace of eiganvalue λ_{j+1}, *i. e.* a population transfer between two energy level of the system is realized. So, conical intersections could be used as "stairs" to move population between energy level of the spectrum. In particular the population transferred on the higher level depends on the angle between the ingoing and outgoing velocity vector of the path in the point of conical intersection [BCMS].





Passing through the intersection with zero angle cause a complete transfer of population at the higher level, *i. e.* if $u \in \mathcal{C}^1$ for every $\varepsilon > 0$ the solution ψ^ε of the equation (2.28) with initial state $\psi^\varepsilon(0) = \phi_j(u(0))$ satisfies

$$\left\| \psi^\varepsilon(1/\varepsilon) - e^{i\theta}\phi_{j+1}(u(1/\varepsilon)) \right\| < C_j\sqrt{\varepsilon}.$$

Choosing special paths we can improve the latter estimate obtaining an error estimate of higher order, $C_j\varepsilon$.

Combining together these different behaviours we are able to steer the state of a conically connected closed quantum system from an eigenstate of eigenvalue λ_0 to an eigenstate of eigenvalue λ_n with an error of order ε. More generally, we are able to steer the dynamics from an eigenstate of eigenvalue λ_j to an arbitrary superposition of eigenstates. The main theorem is the following.

Theorem 2.46 ([BCMS]). *Let $\Sigma(u) = \{\lambda_1(u), ..., \lambda_n(u)\}$ be an isolated portion of the spectrum of $H(u)$. For every $j = 1, ..., n-1$ let $u_j \in U$ be a conical intersection between λ_j and λ_{j+1} and assume $\lambda_j(u)$ simple for $u \neq \bar{u}_{j-1}, \bar{u}_j$. Given $u_0, u_1 \in U$ such that $\Sigma(u_0), \Sigma(u_1)$ are non degenerates, $\psi_0 \in \Phi(u_0)$ and $\psi_1 = \sum^n p_i\phi_j(u_1)$ with $\|\psi_1\| = 1$, then there exist $C > 0$ and a continuous path $\gamma : [0,1] \to U$ with $\gamma(0) = u_0, \gamma(1) = u_1$ such that for every $\varepsilon > 0$*

$$\left\| \psi^\varepsilon(1/\varepsilon) - \sum^n p_j e^{i\theta_j}\phi_j(u_1) \right\| < C\varepsilon$$

where ψ^ε is the solution of (2.28) with $u^\varepsilon(t) = \gamma(\varepsilon t)$ and initial state $\psi^\varepsilon(0) = \psi_0$.

The latter results implies exact controllability in case of a finite dimensional Hilbert space and approximate controllability otherwise (see Lemma 9,14 [BGRS]).

Chapter 3

General theory of open quantum systems

This Chapter is an introduction to the formalism that describes the evolution of open quantum systems. The crucial point is to view the dynamics at the level of states, which are a particular class of observables. After a brief review of the Heisenberg picture of quantum mechanics, we will discuss the fundamental properties of maps between state spaces. This will led finally to the definition of quantum dynamical semigroup, whose generator are the object that we will use to treat open quantum systems.

3.1 One-parameter groups on Hilbert spaces

The Schrödinger equation (2.11), as we have seen in the previous chapter, determines the evolution of the wavefunctions $\psi \in \mathcal{H}$. The operator valued function $U : t \to e^{iHt/\hbar}$ is a strongly continuous one-parameter group of unitary transformation accordingly to the following definition.

Definition 3.1. *If $\mathcal{B}$ is a Banach space a* **one-parameter group** *on $\mathcal{B}$ is a family $\{T_t\}_{t\in\mathbb{R}}$ of bounded linear operators on $\mathcal{B}$ satisfying $T_0 = \mathbb{1}$ and $T_t T_s = T_{t+s}$ for every $t, s \in \mathbb{R}$. The group is called* **strongly continuous** *if*

$$\lim_{t\to 0} \|T_t\phi - \phi\| = 0, \qquad \forall \phi \in \mathcal{D}$$

with $\mathcal{D}$ dense linear subspace in $\mathcal{B}$.

Given a strongly continuous group T_t the generator of the group is defined as

$$A\psi = \lim_{t\to 0} t^{-1}(T_t\psi - \psi) \tag{3.1}$$

and the domain $\mathcal{D}(A)$ of A is the set of all $\psi \in \mathcal{B}$ such that the above limit exists. The strongly continuous property implies that A is a densely defined closed linear operator.

In Hilbert spaces there exists a correspondence between self-adjoint operators and strongly continuous one-parameter unitary group. This correspondence is given by the functional calculus and the Stone's theorem [RS_1, Chap.VIII]. Let us recall briefly the main results.

Theorem 3.2 ([RS_1] Thm VIII.7 **).** *Let H be a self-adjoint operator on $\mathcal{H}$ and define $U(t) = e^{itH}$ by means of the functional calculus* [RS_1, Thm.VIII.5]. *Then $U(t)$ is a strongly continuous one-parameter unitary group. Moreover,*

a) For $\psi \in \mathcal{D}(H)$, $t^{-1}(U(t)\psi - \psi) \to iH$ as $t \to 0$.

b) If $\lim_{t\to 0} t^{-1}(U(t)\psi - \psi)$ exists then $\psi \in \mathcal{D}(H)$.

The converse result is the following.

Theorem 3.3 ([RS_1] Thm VIII.8 **).** *Let $U(t)$ be a strongly continuous one-parameter unitary group on a Hilbert space $\mathcal{H}$. Then, there is a self-adjoint operator H on $\mathcal{H}$ so that $U(t) = e^{itH}$.*

3.2 Observables and Heisenberg picture

Let A be a self-adjoint operator on an Hilbert space $\mathcal{H}$ endowed with an Hermitian product $\langle \cdot\,, \cdot \rangle$. We will refer to such an operator as an *observable*. The spectrum $\sigma(A)$ represents the values that the operator can assume. Given an Hamiltonian H on $\mathcal{H}$ (also an operator itself) and the evolution generated by the Schrödinger equation, the *expected values of the observable A at time $t \in \mathbb{R}$* is defined as the real value

$$\langle A \rangle_t = \langle \psi(t)\,, A\psi(t) \rangle = \left\langle e^{-itH/\hbar}\psi_0\,, Ae^{-itH/\hbar}\psi_0 \right\rangle, \tag{3.2}$$

where ψ_0 is the initial datum. Consider now a family of self-adjoint operators $A(t)$, $t \in \mathbb{R}$ (to avoid technicalities we refer to [Ka] for the minimal assumptions that one should assume on an operator valued function $A : t \in A_t$). Let us define the operator

$$A_H(t) := e^{itH/\hbar} A(t) e^{-itH/\hbar} \tag{3.3}$$

to which we will refer as *Heisenberg representation of A at time t*. It immediately follows that

$$\langle A(t) \rangle_t = \langle A_H(t) \rangle_0.$$

This suggests that instead of considering the evolution of wavefunctions one can alternatively consider the evolution of operators. In fact, at least formally, the operator $A_H(t)$ satisfies

$$\frac{d}{dt} A_H(t) = \left(\frac{\partial A}{\partial t} \right)_H + \frac{1}{i\hbar} [A_H(t), H_H(t)]. \tag{3.4}$$

known as *Heisenberg equation* [Co$_2$][Hall]. Observe that if the operator A does not depend on t, the previous eq.(3.4) reads

$$\frac{d}{dt}A = \frac{1}{i\hbar}[A, H]. \tag{3.5}$$

It is easy to verify that the solution to the previous equation is

$$A(t) = e^{itH/\hbar} A e^{-itH/\hbar}. \tag{3.6}$$

3.3 States

A special class of observables is of particular importance. Let us recall some preliminary definitions in order to introduce this class.

Let A be a positive linear operator on a separable Hilbert space $\mathcal{H}$. We define $\mathrm{tr}(A)$ as the possibly infinite series

$$\mathrm{tr}(A) := \sum_{n\in\mathbb{N}} \langle \psi_n \,,\, A\psi_n \rangle \tag{3.7}$$

where $\{\psi_n\}_{n\in\mathbb{N}}$ is an orthonormal basis of $\mathcal{H}$. The definition define a linear map $\mathrm{tr} : \mathcal{B}(\mathcal{H}) \to \mathbb{R} \cup \{+\infty\}$ and is well posed because does not depend on the chosen basis [RS$_1$, Sect.V.I].

Definition 3.4. *An operator $A \in \mathcal{B}(\mathcal{H})$ is called* **trace-class** *if and only if* $\mathrm{tr}\,|A| < \infty$. *We will denote the set of trace-class operator by $\mathcal{T}(\mathcal{H})$ (also denoted $\mathcal{T}_1$).*

The set $\mathcal{T}(\mathcal{H})$ is a subset of the set of compact operators $Com(\mathcal{H})$ and is a Banach space with the norm

$$\|A\|_1 = \mathrm{tr}\,|A|\,, \tag{3.8}$$

which satisfies the relation $\|A\| \le \|A\|_1$ [RS$_1$, Thm.VI.20]. We recall that a sequence $\{A_n\} \subset \mathcal{B}(\mathcal{H})$ is said to be *weakly convergent to* A if $\lim_{n\to\infty} \langle \phi \,,\, A_n\psi \rangle = \langle \phi \,,\, A\psi \rangle$ for all $\phi, \psi \in \mathcal{H}$ and will denote the weak limit $\mathrm{w.}\lim_{n\to\infty} A_n = A$. Similarly, we say that $\{A_n\} \subset \mathcal{B}(\mathcal{H})$ *converges ultraweakly* to A if $\lim_{n\to\infty} \mathrm{tr}(A_n\rho) = \mathrm{tr}(A\rho)$ for every $\rho \in \mathcal{T}(\mathcal{H})$. Ultraweak convergence implies weak convergence but on norm-bounded sequences they coincide. In particular they coincide if $A_n \to A \in \mathcal{B}(\mathcal{H})$.

As vector space, $\mathcal{T}(\mathcal{H})$ is stable under the composition with linear bounded operators and under the adjunction, *i.e.* if $A \in \mathcal{T}(\mathcal{H})$, $B \in \mathcal{B}(\mathcal{H})$ then AB, BA, $A^* \in \mathcal{T}(\mathcal{H})$, namely $\mathcal{T}(\mathcal{H})$ is a $*$-ideal of $\mathcal{B}(\mathcal{H})$. Moreover,

$$\|AB\|_1 \le \|A\|_1 \|B\|\,, \qquad \|BA\|_1 \le \|B\| \, \|A\|_1$$

This allows one to define for every $A \in \mathcal{T}(\mathcal{H})$ a map

$$\phi_A : B \mapsto \mathrm{tr}(AB), \tag{3.9}$$

which is a bounded linear functional on $\mathcal{B}(\mathcal{H})$. Or analogously, for every $B \in \mathcal{B}(\mathcal{H})$ the map

$$\varrho_B : A \mapsto \mathrm{tr}(AB) \tag{3.10}$$

is a bounded linear functional on $\mathcal{T}(\mathcal{H})$. These types of maps represent special classes of functionals as stated by the next theorem.

Theorem 3.5 ([RS$_1$] Thm.VIII.26). *The map ϕ is an isometric isomorphism of $\mathcal{T}(\mathcal{H})$ in $Com(\mathcal{H})^*$. The map ϱ is an isometric isomorphism of $\mathcal{B}(\mathcal{H})$ into $\mathcal{T}(\mathcal{H})^*$.*

It is also possible to define subspaces of $\mathcal{B}(\mathcal{H})$,$\mathcal{T}(\mathcal{H})$ and $Com(\mathcal{H})$ between which the above dualities still hold. We will denote $\mathcal{B}_s(\mathcal{H})$,$\mathcal{T}_s(\mathcal{H})$ and $Com_s(\mathcal{H})$ the set of linear bounded, trace-class and compact set of self-adjoint operators. It is still true that $\mathcal{T}_s(\mathcal{H}) = Com_s(\mathcal{H})^*$ and $\mathcal{B}_s(\mathcal{H}) = \mathcal{T}_s(\mathcal{H})^*$. We will denote $\mathcal{B}_s(\mathcal{H})^+$, $\mathcal{T}_s(\mathcal{H})^+$ the sets of self-adjoint non-negative linear and trace-class operators. Observe that

$$A \in \mathcal{T}_s(\mathcal{H})^+ \;\Leftrightarrow\; \mathrm{tr}(AB) \geq 0 \quad \forall B \in \mathcal{B}_s(\mathcal{H})^+,$$

and conversely

$$B \in \mathcal{B}_s(\mathcal{H})^+ \;\Leftrightarrow\; \mathrm{tr}(AB) \geq 0 \quad \forall A \in \mathcal{T}_s(\mathcal{H})^+. \tag{3.11}$$

Definition 3.6. *The* **state space** *of an Hilbert space $\mathcal{H}$ is defined as the Banach space $\mathcal{T}_s(\mathcal{H})$ with the norm $\|\cdot\|_1$. The* **states** *are defined as self-adjoint non-negative trace-class operators of trace one. The states are also called mixed states or density matrices.*

By the spectral theorem each state ρ admits a decomposition

$$\rho = \sum_{n\in\mathbb{N}} \lambda_n \left|\psi_n\right\rangle \left\langle\psi_n\right|^{1}, \qquad \lambda_n \geq 0 \text{ for all } n \in \mathbb{N}, \qquad \sum_{n\in\mathbb{N}} \lambda_n = 1. \tag{3.12}$$

where $\psi_n \in \mathcal{H}$ have norm one (it is always possible to find a decomposition in which $\{\psi_n\}_{n\in\mathbb{N}}$ is an orthonormal basis). A state is said to be *pure* if $\mathrm{tr}(\rho) = \mathrm{tr}(\rho^2)$, therefore if and only if $\rho = |\psi\rangle\langle\psi|$ for some $\psi \in \mathcal{H}$.

The definition of state generalizes the concept of wavefunction in the following sense. For each initial state $\psi_0 \in \mathcal{H}$ its evolution is given by the solution of the

[1] We make use hereafter of the standard Dirac notation for elements of an Hilbert space $\mathcal{H}$ endowed with an Hermitian product $S : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ [Co$_1$, Sect.II.B][Hall, Sect.3.12]. We denote an element $\psi \in \mathcal{H}$ with the symbol $|\psi\rangle$ (ket). We denote with the symbol $\langle\phi|$ (bra) the element of the dual space $\mathcal{H}^*$ defined by

$$\begin{array}{rccc} \langle\phi| : & \mathcal{H} & \longrightarrow & \mathbb{C} \\ & \psi & \mapsto & S(\phi,\psi) \end{array}$$

namely the dual element of $|\phi\rangle$ through the natural isomorphism between $\mathcal{H}$ and his dual space $\mathcal{H}^*$.

Therefore we choose to adopt the notation $\langle\cdot|\cdot\rangle$ for the Hermitian product. In this way given two elements $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ the complex number $S(\phi,\psi)$ is obtained by the evaluation of the functional $\langle\phi|$ on $|\psi\rangle$, *i.e.* $\langle\phi|\psi\rangle = S(\phi,\psi)$. Conversely, the "exterior product" $|\psi\rangle\langle\phi|$ denotes the linear operator

$$\begin{array}{rccc} |\psi\rangle\langle\phi| : & \mathcal{H} & \longrightarrow & \mathcal{H} \\ & |\xi\rangle & \mapsto & |\psi\rangle\langle\phi|\xi\rangle\,. \end{array}$$

Schrödinger equation, *i. e.* by the action of the one-parameter group $e^{itH/\hbar}$ on ψ_0. If we consider the pure state $\rho_0 = |\psi_0\rangle\langle\psi_0|$, it evolves accordingly to eq.(3.5)

$$\rho(t) = e^{iHt/\hbar}\rho_0 e^{-iHt/\hbar} = e^{iHt/\hbar}|\psi_0\rangle\langle\psi_0| e^{-iHt/\hbar} = |e^{-iHt/\hbar}\psi_0\rangle\langle e^{-iHt/\hbar}\psi_0| \quad (3.13)$$

which is exactly the pure state associated with $\psi(t) = e^{-iHt/\hbar}\psi_0$. Moreover, each expected value of an observable A can be computed by means of $\rho(t)$

$$\langle A\rangle_t = \langle\psi(t)\, , A\psi(t)\rangle = \mathrm{tr}(\rho(t)A). \quad (3.14)$$

Instead, if the system is prepared in a statistical mixture of states $\psi_k \in \mathcal{H}$, each one with probability $p_k \in [0,1]$ such that $\sum_k p_k = 1$, its initial state is described by

$$\rho_0 = \sum_k p_k |\psi_k\rangle\langle\psi_k|\, . \quad (3.15)$$

In fact the expected value of the observable $P_k := |\psi_k\rangle\langle\psi_k|$ on ρ_0 is

$$\langle P_k\rangle_0 = \mathrm{tr}(\rho_0 P_k) = p_k,$$

which means that the system has probability p_k of being in the state ψ_k. Even if this state is not pure its evolution is still given by eq. (3.6) and the expectation of observables by

$$\langle A\rangle_t = \mathrm{tr}(\rho(t)A) = \sum_k p_k\, \mathrm{tr}(P_k(t)A) = \sum_k p_k\, \mathrm{tr}(e^{iHt/\hbar}|\psi_k\rangle\langle\psi_k| e^{-iHt/\hbar}A). \quad (3.16)$$

Thus the expectation of an observable A on the state $\rho(t)$ is an average of the expectations of A on the wavefunctions $\psi_k(t)$, weighted as the initial mixture was.

3.4 Operations on state spaces

As pointed out in the previous section, the evolution of the state space of an Hilbert space $\mathcal{H}$ is sufficient to recover all the information about observable quantities, whatever the initial state of the system is. For this reason we are interested in studying general maps between state spaces, or elsewhere known as *operations.*

The map

$$\boldsymbol{T}_t : \rho \mapsto e^{-iHt/\hbar}\rho e^{iHt/\hbar}, \quad (3.17)$$

that we already encountered, is a linear bounded map on $\mathcal{T}_s(\mathcal{H})$ which is also trace preserving, *i. e.* $\mathrm{tr}(\boldsymbol{T}_t(\rho)) = \mathrm{tr}(\rho)$ (by the ciclicity of the trace), and positive according to the following definition.

Definition 3.7. *Let* $\boldsymbol{S} : \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_1)$ *be a linear map. We will say that* $\boldsymbol{S}$ *is* **positive** *if* $A \geq 0$ *implies* $\boldsymbol{S}(A) \geq 0$.

Moreover, a positive linear map is called **normal** *if for each sequence* $\{A_n\}_{n\in\mathbb{N}} \subset \mathcal{B}(\mathcal{H}_2)$ *such that* $\mathrm{w.}\lim_{n\to\infty} A_n = A \in \mathcal{B}(\mathcal{H}_2)$ *then* $\mathrm{w.}\lim_{n\to\infty} \boldsymbol{S}(A_n) = \boldsymbol{S}(A)$.

Moreover, a series of measurements on a quantum system with Hilbert space $\mathcal{H}$ can be seen as a positive linear bounded map $\boldsymbol{T}$ on $\mathcal{T}_s(\mathcal{H})$ (see [Da, Sect 2.2.1]) which generally satisfies

$$0 \leq \operatorname{tr}(\boldsymbol{T}(\rho)) \leq \operatorname{tr}(\rho), \qquad \forall \rho \in \mathcal{T}_s(\mathcal{H})^+. \tag{3.18}$$

For these reasons we are interested in classifying linear bounded maps on state spaces which satisfies also (3.18). The following results goes in that direction.

Lemma 3.8 ([Da, Lemma 2.2.2] **).** *If* $\boldsymbol{T} : \mathcal{T}_s(\mathcal{H}_1) \to \mathcal{T}_s(\mathcal{H}_2)$ *is a positive linear map then the adjoint* $\boldsymbol{T}^* : \mathcal{B}_s(\mathcal{H}_2) \to \mathcal{B}_s(\mathcal{H}_1)$ *is a positive linear normal map.*

Moreover,

$$0 \leq \boldsymbol{T}^*(\mathbb{1}) \leq \mathbb{1} \tag{3.19}$$

if and only if

$$0 \leq \operatorname{tr}(\boldsymbol{T}(\rho)) \leq \operatorname{tr}(\rho), \qquad \forall \rho \in \mathcal{T}_s(\mathcal{H}_1)^+.$$

Every normal positive linear map $\boldsymbol{S} : \mathcal{B}_s(\mathcal{H}_2) \to \mathcal{B}_s(\mathcal{H}_1)$ *is the adjoint of a unique positive linear map* $\boldsymbol{T} : \mathcal{T}_s(\mathcal{H}_1) \to \mathcal{T}_s(\mathcal{H}_2)$*.*

Proof. If $A \in \mathcal{B}_s(\mathcal{H}_2)$ and $\rho \in \mathcal{T}_s(\mathcal{H}_1)$, by Thm.3.5 $\boldsymbol{T}^*(A)$ is the unique element of $\mathcal{B}_s(\mathcal{H}_1)$ representing $\phi_A = \rho \mapsto \operatorname{tr}(A\boldsymbol{T}(\rho))$, *i. e.* such that

$$\operatorname{tr}(\boldsymbol{T}^*(A)\rho) = \operatorname{tr}(A\boldsymbol{T}(\rho)), \qquad \forall A \in \mathcal{B}_s(\mathcal{H}_2),\ \rho \in \mathcal{T}_s(\mathcal{H}_1).$$

Moreover, since

$$\operatorname{tr}(\boldsymbol{T}^*(A)\rho) = \operatorname{tr}(A\boldsymbol{T}(\rho)) \geq 0, \qquad \forall A \in \mathcal{B}_s(\mathcal{H}_2)^+,\ \rho \in \mathcal{T}_s(\mathcal{H}_1)^+,$$

then $\boldsymbol{T}^*(A) \geq 0$ by (3.11), so $\boldsymbol{T}^*$ is positive. Observe that

$$\operatorname{tr}(\rho) - \operatorname{tr}(\boldsymbol{T}(\rho)) = \operatorname{tr}((\mathbb{1} - \boldsymbol{T}^*(\mathbb{1}))\rho), \qquad \forall \rho \in \mathcal{T}_s(\mathcal{H}_1)^+$$

from which we have the equivalence between (3.18) and (3.19). If $\{A_n\}_{n\in\mathbb{N}} \subset \mathcal{B}(\mathcal{H})$ converge to $A \in \mathcal{B}(\mathcal{H})$ weakly, then A_n converge to A ultraweakly, so

$$\operatorname{tr}(\boldsymbol{T}^*(A_n)\rho) = \operatorname{tr}(A_n\boldsymbol{T}(\rho)) \to \operatorname{tr}(A\boldsymbol{T}(\rho)) = \operatorname{tr}(\boldsymbol{T}^*(A)\rho),$$

which means that $\boldsymbol{T}^*(A_n)$ converges to $\boldsymbol{T}^*(A)$ ultraweakly, then $\boldsymbol{T}^*(A_n) \to \boldsymbol{T}^*(A)$ weakly and $\boldsymbol{T}^*$ is normal.

This proves one implication of the one to one correspondence stated above. The converse descends again from Thm.3.5. □

Remark 3.9. The condition (3.19) must be understood in the following sense. The operation $\boldsymbol{T} : \mathcal{T}_s(\mathcal{H}_1) \to \mathcal{T}_s(\mathcal{H}_2)$ acts on density matrices ρ which represent ensembles according to (3.15). So $\boldsymbol{T}(\rho)$ contains information about the new distribution of the mixture as well as the form of the new state. In fact, from (3.15) we get

$$\boldsymbol{T}(\rho) = \sum_k p_k \boldsymbol{T}(|\psi_k\rangle\langle\psi_k|),$$

and normalizing each state of the new mixture

$$\boldsymbol{T}(\rho) = \sum_k p_k \operatorname{tr}(\boldsymbol{T}(|\psi_k\rangle\langle\psi_k|)) \frac{\boldsymbol{T}(|\psi_k\rangle\langle\psi_k|)}{\operatorname{tr}(\boldsymbol{T}(|\psi_k\rangle\langle\psi_k|))},$$

from which we see that

$$\operatorname{tr}(\boldsymbol{T}(\rho)) = \sum_k p_k \operatorname{tr}(\boldsymbol{T}(|\psi_k\rangle\langle\psi_k|)\mathbb{1}) = \sum_k p_k \operatorname{tr}(|\psi_k\rangle\langle\psi_k| \boldsymbol{T}^*(\mathbb{1})).$$

Thus the map $\boldsymbol{T}^*(\mathbb{1})$, commonly called *effect*, determines the probability of trasmission of a given state but not its form, given by $\boldsymbol{T}$. Since $0 \leq \boldsymbol{T}^*(\mathbb{1}) \leq 1$ then $0 \leq p_k \operatorname{tr}(\boldsymbol{T}(|\psi_k\rangle\langle\psi_k|)) \leq p_k \|\boldsymbol{T}^*(\mathbb{1})\| \leq p_k$. ⌟

An interesting case is when a linear positive map transforms pure states in pure states.

Definition 3.10. *Let $\boldsymbol{T} : \mathcal{T}_s(\mathcal{H}_1) \to \mathcal{T}_s(\mathcal{H}_2)$ be a positive linear map. We say that $\boldsymbol{T}$ is* **pure** *if $\boldsymbol{T}(\rho) \in \mathcal{T}_s(\mathcal{H}_2)^+$ is a pure element whenever $\rho \in \mathcal{T}_s(\mathcal{H}_1)^+$ is pure.*

Those type of maps admit a simple classification.

Theorem 3.11 ([Da, Thm 3.1] **).** *Every pure positive linear map $\boldsymbol{T} : \mathcal{T}_s(\mathcal{H}_1) \to \mathcal{T}_s(\mathcal{H}_2)$ is of one of the following form:*

(i)

$$\boldsymbol{T}(\rho) = B\rho B^* \tag{3.20}$$

where $B : \mathcal{H}_1 \to \mathcal{H}_2$ is bounded and linear;

(ii)

$$\boldsymbol{T}(\rho) = B\rho^* B^* \tag{3.21}$$

where $B : \mathcal{H}_1 \to \mathcal{H}_2$ is bounded and conjugate linear;

(iii)

$$\boldsymbol{T}(\rho) = \operatorname{tr}(\rho B)\,|\psi\rangle\langle\psi| \tag{3.22}$$

where $B \in \mathcal{B}(\mathcal{H}_1)^+$ and $\psi \in \mathcal{H}_2$.

In cases (i) and (ii) the operator B is uniquely determined up to a constant of modulus one.

This results gives a lot of information about invertible linear positive maps. In fact, if $\boldsymbol{T} : \mathcal{T}_s(\mathcal{H}_1) \to \mathcal{T}_s(\mathcal{H}_2)$ has a positive inverse $\boldsymbol{T}^{-1}$, then both $\boldsymbol{T}$,$\boldsymbol{T}^{-1}$ are pure. Moreover since $\boldsymbol{T}$ is pure $\boldsymbol{T}(\rho) = \boldsymbol{T}(\rho)^*$. Thus the following corollary is immediate.

Corollary 3.12. *Let $\boldsymbol{T} : \mathcal{T}_s(\mathcal{H}) \to \mathcal{T}_s(\mathcal{H})$ a positive linear map with positive inverse. Let also $\boldsymbol{T}$ be trace preserving. Then there exists a unitary or antiunitary map U on $\mathcal{H}$ such that*

$$\boldsymbol{T}(\rho) = U\rho U^*.$$

By duality a similar results holds for linear positive maps $\boldsymbol{S} : \mathcal{B}_s(\mathcal{H}) \to \mathcal{B}_s(\mathcal{H})$.

Corollary 3.13. *Let $\boldsymbol{S} : \mathcal{B}_s(\mathcal{H}) \to \mathcal{B}_s(\mathcal{H})$ a positive linear map with positive inverse. Let also $\boldsymbol{S}$ be unital, i. e. $\boldsymbol{S}(\mathbb{1}) = \mathbb{1}$. Then there exists a unitary or antiunitary map U on $\mathcal{H}$ such that*

$$\boldsymbol{S}(A) = UAU^*, \qquad A \in \mathcal{B}_s(\mathcal{H}).$$

There is a complex linear extension of S to $\mathcal{B}(\mathcal{H})$ which is either an algebra automorphism or an algebra antiautomorphism.

To conclude the section we recall that the map (3.17) happens to be a linear positive map with positive inverse, so $\{\boldsymbol{T}_t\}_{t\in\mathbb{R}}$ is a strongly continuous one-parameter group of those maps. The following theorem states that there are no other type of such groups.

Theorem 3.14. *Let $\boldsymbol{T}_t : \mathcal{T}_s(\mathcal{H}) \to \mathcal{T}_s(\mathcal{H})$ a strongly continuous one-parameter group of positive linear map such that*

$$\mathrm{tr}(\boldsymbol{T}_t(\rho)) = \mathrm{tr}(\rho), \qquad \forall \rho \in \mathcal{T}_s(\mathcal{H}).$$

Then there exists a self-adjoint operator H on $\mathcal{H}$ such that

$$\boldsymbol{T}_t(\rho) = e^{-iHt/\hbar}\rho e^{iHt/\hbar}, \qquad \forall t \in \mathbb{R}.$$

3.5 Dynamical semigroups

The assumption of having a closed system, namely an Hilbert space $\mathcal{H}$ with a state dynamics $\boldsymbol{T}_t : \mathcal{T}_s(\mathcal{H}) \to \mathcal{T}_s(\mathcal{H})$ that posses the group properties and moreover preserves probabilities, lead us to evolutions of Hamiltonian type (Thm 3.14). That means that the self-adjoint operator H on $\mathcal{H}$, which determines the state evoltution through (3.17), is completely determined by $\mathcal{H}$ and $\boldsymbol{T}_t$ and does not depend of any parameter or external factor.

For these reasons, one is induced to ask whether an evolution on the state space can in principle be related to an Hamiltonian on a larger Hilbert space. This Hilbert space should take into account all the part of the environment that affect the dynamics of the system, as an ideal quantization of the external world. We will call such a type of system an *open quantum system*.

Let $\mathcal{H}$ be the Hilbert space of the system, $\mathcal{H}_\varepsilon$ the Hilbert space of the environment and consider the tensor product $\mathcal{H} \otimes \mathcal{H}_\varepsilon$, the total space. Let H be a self-adjoint operator on $\mathcal{H}\otimes\mathcal{H}_\varepsilon$ and suppose that the initial state of the total system is factorized, namely $\rho \otimes \rho_\varepsilon \in \mathcal{T}(\mathcal{H}) \otimes \mathcal{T}(\mathcal{H}_\varepsilon)$. Therefore the evolution of the total system is

$$e^{-iHt/\hbar}(\rho \otimes \rho_\varepsilon)e^{iHt/\hbar},$$

and generally this is no more a factorized state (except in absence of interaction which is a trivial case). However, there exists a map on $\mathcal{T}(\mathcal{H} \otimes \mathcal{H}_\varepsilon)$ that act as a projection onto $\mathcal{T}(\mathcal{H})$, which means it gives a sort of *reduced state* in the following sense. Let us define a map $\mathrm{tr}_\varepsilon : \mathcal{T}(\mathcal{H}\otimes\mathcal{H}_\varepsilon) \to \mathcal{T}(\mathcal{H})$ such that on factorized states $\mathrm{tr}_\varepsilon(\rho\otimes\sigma) = \mathrm{tr}_{\mathcal{H}_\varepsilon}(\sigma)\rho$, then

$$\mathrm{tr}_{\mathcal{H}}(A\ \mathrm{tr}_\varepsilon(\rho\otimes\sigma)) = \mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}_\varepsilon}\left[(A\otimes\mathbb{1})(\rho\otimes\sigma)\right], \tag{3.23}$$

for each $A\in\mathcal{B}(\mathcal{H})$, where $\mathrm{tr}_{\mathcal{H}}$ is the trace on the Hilbert space $\mathcal{H}$. Observe that eq. (3.23) shows that tr_ε acts naturally on factorized states, reducing a state on $\mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}_\varepsilon}$ to a partial one which is compatible with the composition with $\mathrm{tr}_{\mathcal{H}}$. That map could be extended by duality. The application $A\mapsto A\otimes\mathbb{1}$ is a positive normal linear map from $\mathcal{B}(\mathcal{H})$ to $\mathcal{B}(\mathcal{H}\otimes\mathcal{H}_\varepsilon)$, then by Lemma 3.8

$$\mathrm{tr}_{\mathcal{H}}(A\ \mathrm{tr}_\varepsilon(\bar\rho)) = \mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}_\varepsilon}\left[(A\otimes\mathbb{1})\bar\rho\right]$$

defines a positive normal linear map for every $\bar\rho\in\mathcal{T}(\mathcal{H}\otimes\mathcal{H}_\varepsilon)$, which coincides with the one defined above for factorized states. We will call tr_ε *partial trace on* $\mathcal{H}_\varepsilon$. According to the argument above, we set

$$\mathbf{\Lambda}_t(\rho) := \mathrm{tr}_\varepsilon\left(e^{-iHt/\hbar}(\rho\otimes\rho_\varepsilon)e^{iHt/\hbar}\right) \tag{3.24}$$

which is a map on $\mathcal{T}(\mathcal{H})$ that describes the partial evolution of the subsystem $\mathcal{H}$ given an initial environment state ρ_ε.

The concept of partial trace can be translated into a similar one for observables. Given an environment state ρ_ε the map $\rho\mapsto\rho\otimes\rho_\varepsilon$ is positive linear from $\mathcal{T}(\mathcal{H})$ into $\mathcal{T}(\mathcal{H}\otimes\mathcal{H}_\varepsilon)$. Therefore by Lemma 3.8

$$\mathrm{tr}_{\mathcal{H}}(\mathbb{E}_{\rho_\varepsilon}(B)\rho) = \mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}_\varepsilon}\left[B(\rho\otimes\rho_\varepsilon)\right], \qquad \rho\in\mathcal{T}(\mathcal{H}) \tag{3.25}$$

defines a linear map $\mathbb{E}_{\rho_\varepsilon} : \mathcal{B}(\mathcal{H}\otimes\mathcal{H}_\varepsilon)\to\mathcal{B}(\mathcal{H})$ which is positive, normal and such that

$$\mathbb{E}_{\rho_\varepsilon}(A\otimes\mathbb{1}) = A\ \mathrm{tr}(\rho_\varepsilon).$$

We are now able to define the evolution of observables $X\in\mathcal{B}(\mathcal{H})$ given the initial environment state ρ_ε,

$$\mathbf{\Lambda}_t'(X) := \mathbb{E}_{\rho_\varepsilon}\left(e^{iHt/\hbar}(X\otimes\mathbb{1})e^{-iHt/\hbar}\right). \tag{3.26}$$

Remark 3.15. The map $\mathbf{\Lambda}_t : \mathcal{T}(\mathcal{H})\to\mathcal{T}(\mathcal{H})$ and $\mathbf{\Lambda}_t' : \mathcal{B}(\mathcal{H})\to\mathcal{B}(\mathcal{H})$ defined in (3.24) and (3.26) are dual. In fact

$$\begin{aligned}
\mathrm{tr}_{\mathcal{H}}\left(\mathbb{E}_{\rho_\varepsilon}\left(e^{iHt/\hbar}(X\otimes\mathbb{1})e^{-iHt/\hbar}\right)\rho\right) &= \mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}_\varepsilon}\left[e^{iHt/\hbar}(X\otimes\mathbb{1})e^{-iHt/\hbar}\rho\otimes\rho_\varepsilon\right]\\
&= \mathrm{tr}_{\mathcal{H}\otimes\mathcal{H}_\varepsilon}\left[(X\otimes\mathbb{1})e^{-iHt/\hbar}\rho\otimes\rho_\varepsilon e^{iHt/\hbar}\right]\\
&= \mathrm{tr}_{\mathcal{H}}\left(X\ \mathrm{tr}_\varepsilon\left(e^{-iHt/\hbar}\rho\otimes\rho_\varepsilon e^{iHt/\hbar}\right)\right)\\
&= \mathrm{tr}_{\mathcal{H}}(X\,\mathbf{\Lambda}_t(\rho)).
\end{aligned}$$

The map $\mathbf{\Lambda}_t$ is trace preserving if and only if $\mathrm{tr}\,\rho_\varepsilon = 1$. The map $\mathbf{\Lambda}_t'$ is unital if and only if $\mathrm{tr}\,\rho_\varepsilon = 1$, in fact $\mathbf{\Lambda}_t'(\mathbb{1}) = \mathbb{1}\ \mathrm{tr}\,\rho_\varepsilon$ (as Lemma 3.8 stated). ⌟

In conclusion, given an Hilbert space $\mathcal{H}\otimes\mathcal{H}_\varepsilon$ and a self-adjoint operator H acting on this space, there exists a way to define state's and observable's evolution of $\mathcal{H}$ coherently, which means by maps that: reduce the total dynamics on $\mathcal{T}(\mathcal{H}\otimes\mathcal{H}_\varepsilon)$ and $\mathcal{B}(\mathcal{H}\otimes\mathcal{H}_\varepsilon)$ to $\mathcal{T}(\mathcal{H})$ and $\mathcal{B}(\mathcal{H})$ preserving fundamental properties (positivity, normality, etc...); are compatible with the composition with (3.9),(3.10). This reduction maps suggest that the dynamics we defined cannot be reversible.

Those reasons lead us to the following

Definition 3.16. *Given an Hilbert space $\mathcal{H}$ we define a* **dynamical semigroup** *to be a one-parameter family of linear operators $\boldsymbol{T}_t : \mathcal{T}(\mathcal{H}) \to \mathcal{T}(\mathcal{H})$ for each $t \geq 0$, satisfying*

(i) *$\boldsymbol{T}_t$ positive for each $t \geq 0$;*

(ii) *$\boldsymbol{T}_t$ trace preserving for each $t \geq 0$;*

(iii) *$\boldsymbol{T}_0 = \mathbb{1}_{\mathcal{T}(\mathcal{H})}$, $\boldsymbol{T}_s\boldsymbol{T}_t\rho = \boldsymbol{T}_{t+s}\rho$ for all $s, t \geq 0$;*

(iv) *$\lim_{t\to 0} \|\boldsymbol{T}_t\rho - \rho\|_1 = 0$ for all $\rho \in \mathcal{T}(\mathcal{H})$.*

Remark 3.17. The Hamiltonian evolution law (3.17) is a dynamical semigroup. The one-parameter family $\boldsymbol{\Lambda}_t$ defined in (3.24) satisfies (i),(ii) and is continue but it is not generally a semigroup (see [Da, Sect. 10.4]). ⌟

It is useful to state an equivalent definition for the dual semigroup,

Definition 3.18 ([Li],[Pa, Sect. III.30] **).** *Given an Hilbert space $\mathcal{H}$ we will call* **dynamical semigroup** *(in the Heisenberg picture) a one-parameter family of linear operators $\boldsymbol{S}_t : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, $t \geq 0$ satisfying*

(a) *$\boldsymbol{S}_t(X) \geq 0$ for all $X \geq 0$ and $t \geq 0$;*

(b) *for all $t \geq 0$ $\boldsymbol{S}_t(\mathbb{1}) = \mathbb{1}$, $\|\boldsymbol{S}_t(X)\| \leq \|X\|$, $\boldsymbol{S}_t(X)^* = \boldsymbol{S}_t(X^*)$ and $\mathrm{w.}\lim_{n\to\infty} \boldsymbol{S}_t(X_n) = \boldsymbol{S}_t(X)$ whenever $\mathrm{w.}\lim_{n\to\infty} X_n = X$;*

(c) *$\boldsymbol{S}_0 = \mathbb{1}_{\mathcal{B}(\mathcal{H})}$, $\boldsymbol{S}_t\boldsymbol{S}_s = \boldsymbol{S}_{t+s}$ for all $t, s \geq 0$;*

(d) *$\lim_{t\to 0} \|\boldsymbol{S}_t(X) - X\|_1 = 0$ for all $X \in \mathcal{B}(\mathcal{H})$;*

We will call the dynamical semigroup **uniformly continuous** *if*

$$\lim_{t\to 0} \sup_{\|X\|\leq 1} \|\boldsymbol{S}_t(X) - X\| = 0$$

for all $X \in \mathcal{B}(\mathcal{H})$.

For a dynamical semigroup there exists a (generically unbounded) linear operator $L : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ defined on a ultraweakly dense domain $\mathcal{D}(L)$ such that

$$\lim_{t\to 0} \left\|L(X) - t^{-1}(\boldsymbol{S}_t(X) - X)\right\| = 0, \quad X \in \mathcal{D}(L).$$

L is called the *generator* of the semigroup. If the dynamical semigroup is uniformly continuous the generator L is a bounded linear operator on $\mathcal{H}$ and

$$\lim_{t\to 0} \left\| L - t^{-1}(\boldsymbol{S}_t - \mathbb{1}) \right\| = 0.$$

Remark 3.19. If $\boldsymbol{S}$ is identity preserving its dual semigroup $\boldsymbol{S}^*$ conserves probability *i.e.* $\mathrm{tr}(\boldsymbol{S}_t^*(\rho_0)) = \mathrm{tr}(\boldsymbol{S}_t^*(\rho_0)I) = \mathrm{tr}(\rho_0 \boldsymbol{S}_t(I)) = \mathrm{tr}(\rho_0) = 1$. The definition of normal map (b) is slightly different because we are considering maps on $\mathcal{B}(\mathcal{H})$ instead of $\mathcal{B}_s(\mathcal{H})$. ⌟

The map (3.24) satisfies (a),(b),(d) but is generally not a semigroup. For other examples we refer to [Pa, Ex. 30.1-5]. Nevertheless, one could try to understand under which conditions a dynamical semigroup $\boldsymbol{S}$ on $\mathcal{B}(\mathcal{H})$ admit a representation of type (3.26). It turns out that a condition stronger than the positivity is needed, as it will be discussed in the next Section.

3.6 Complete positivity

Consider a quantum system, whose pure states are described by $\mathcal{H}$, in a well defined region of space. Suppose that there exists a particle with n degrees of freedom localized very far away from the first system, such that they have no interaction with each other. The Hilbert space of the total system is $\mathcal{H} \otimes \mathbb{C}^n$ and if $\boldsymbol{S}$ is an operation on the system $\mathcal{H}$ that does not affect the distant particle, on factorized observables one has

$$\boldsymbol{S}^{(n)}(A \otimes B) = \boldsymbol{S}(A) \otimes B, \qquad A \in \mathcal{B}(\mathcal{H}),\ B \in \mathcal{B}(\mathbb{C}^n) \tag{3.27}$$

and $\boldsymbol{S}^{(n)}$ extends to a linear map on $\mathcal{B}(\mathcal{H} \otimes \mathbb{C}^n)$. The physical meaning of this map is clear, it is the trivial extension of an operation $\boldsymbol{S}$ on $\mathcal{H}$ to any larger system that includes $\mathcal{H}$, but in which it is still isolate. This inclusion must not change the physical meaning of our description, so $\boldsymbol{S}^{(n)}$ should be a positive linear map on $\mathcal{B}(\mathcal{H} \otimes \mathbb{C}^n)$ if $\boldsymbol{S}$ is positive linear on $\mathcal{B}(\mathcal{H})$. However, this is not true. If $\boldsymbol{S}$ is a positive linear map, $\boldsymbol{S}^{(n)}$ is not necessarily positive.

Example 3.20. Consider an Hamiltonian H_0 on $\mathcal{H}$, the one-parameter unitary group $e^{iH_0t/\hbar}$ and the dynamical semigroup $\boldsymbol{S}_t(A) = e^{iH_0t/\hbar}Ae^{-iH_0t/\hbar}$. Then, for every $n \in \mathbb{N}$ the map $\boldsymbol{S}_t^{(n)}$ on $\mathcal{B}(\mathcal{H} \otimes \mathbb{C}^n)$ defined on factorized states

$$\boldsymbol{S}_t^{(n)}(A \otimes B) = \boldsymbol{S}_t(A) \otimes B = e^{i(H_0 \otimes \mathbb{1})t/\hbar}(A \otimes B)e^{-i(H_0 \otimes \mathbb{1})t/\hbar},$$

extends to the map $\boldsymbol{S}_t^{(n)}(X) = e^{i(H_0 \otimes \mathbb{1})t/\hbar}Xe^{-i(H_0 \otimes \mathbb{1})t/\hbar}$. Therefore $\boldsymbol{S}_t^{(n)}$ is positive for all $n \in \mathbb{N}$.

To see that not every positive map is completely positive consider the transposition map $X \mapsto X^T$ acting on $\mathcal{B}(\mathbb{C}^n)$. ⌟

The above considerations should convince us that the positivity is not enough for an operation to have physical meaning.

Definition 3.21. *We will call a positive linear map* $\boldsymbol{S} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ **completely positive** *if for every* $n \in \mathbb{N}$ *the map* $\boldsymbol{S}^{(n)} : \mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathbb{C}^n) \to \mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathbb{C}^n)$ *defined by*

$$(X_{i,j})_{i,j=1}^n \mapsto (\boldsymbol{S}(X_{i,j}))_{i,j=1}^n , \qquad X_{i,j} \in \mathcal{B}(\mathcal{H}), \tag{3.28}$$

is positive.

Remark 3.22. The definition of $\boldsymbol{S}^{(n)}$ given in (3.27),(3.28) are equivalent given the isomorphism $\mathcal{B}(\mathcal{H} \otimes \mathbb{C}^n) \cong \mathcal{B}(\mathcal{H}) \otimes \mathcal{B}(\mathbb{C}^n)$. ⌟

Two fundamental results about completely positive maps are crucial to answer the question we asked at the end of previous section.

Theorem 3.23 (Stinespring, [Pa] Thm. III.29.6**).** *Let* $\mathcal{H}_1$, $\mathcal{H}_2$ *be Hilbert spaces and let* $\boldsymbol{S} : \mathcal{H}_2 \to \mathcal{H}_1$ *be a linear operator satisfying the following conditions:*

(a) $\boldsymbol{S}$ *is complete positive;*

(b) $\boldsymbol{S}(\mathbb{1}) = \mathbb{1}$, $\boldsymbol{S}(X)^* = \boldsymbol{S}(X^*)$, $\|\boldsymbol{S}(X)\| \leq \|X\|$ *and* $\mathrm{w.}\lim_{n\to\infty} \boldsymbol{S}(X_n) = \boldsymbol{S}(X)$ *whenever*
$\mathrm{w.}\lim_{n\to\infty} X_n = X$*;*

Then there exists a Hilbert space $\mathcal{K}$*, an isometry* $V : \mathcal{H}_1 \to \mathcal{H}_2 \otimes \mathcal{K}$ *such that:*

($\cdot$) $\boldsymbol{S}(X) = V^*(X \otimes \mathbb{1})V$ *for all* $X \in \mathcal{B}(\mathcal{H}_2)$*;*

($\cdot\cdot$) $\{(X \otimes \mathbb{1})V\psi \,|\, X \in \mathcal{B}(\mathcal{H}_2), \psi \in \mathcal{H}_1\}$ *is dense in* $\mathcal{H}_2 \otimes \mathcal{K}$*;*

Conversely, if $V : \mathcal{H}_1 \to \mathcal{H}_2 \otimes \mathcal{K}$ *is an isometry where* $\mathcal{K}$ *is any Hilbert space then the map* $\boldsymbol{S} : \mathcal{H}_2 \to \mathcal{H}_1$ *defined by* $\boldsymbol{S}(X) = V^*(X \otimes \mathbb{1})V$ *satisfies condition* (a),(b)*.*

Theorem 3.24 (Kraus, [Pa] Thm. III.29.6**).** *An operator* $\boldsymbol{S} : \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_1)$ *satisfies conditions* (a),(b) *of Thm* 3.23 *if and only if there exist operators* $L_j : \mathcal{H}_1 \to \mathcal{H}_2$*,* $j = 1, 2...$ *such that* $\sum_j L_j^* L_j = \mathbb{1}$ *is a strongly convergent sum and*

$$\boldsymbol{S}(X) = \sum_j L_j^* X L_j, \qquad \text{for all } X \in \mathcal{B}(\mathcal{H}_2). \tag{3.29}$$

If $dim\mathcal{H}_j = n_j < \infty$*,* $j = 1, 2$*, then the number of* $L_j's$ *can be restricted to be lesser or equal than* $n_1 n_2$*.*

Example 3.25. Consider the map $\boldsymbol{\Lambda}_t$ defined in (3.24) and let $\rho_\varepsilon = |\Omega\rangle\langle\Omega|$, $\Omega \in \mathcal{H}_\varepsilon$. Given $\{\phi_n\}_{n\in\mathbb{N}}$ basis of $\mathcal{H}_\varepsilon$ define the maps $E_n = \mathbb{1} \otimes |\Omega\rangle\langle\phi_n|$. Notice that

$$\sum_{n\in\mathbb{N}} E_n \bar{\rho} E_n^* = \mathrm{tr}_\varepsilon(\bar{\rho}) \otimes |\Omega\rangle\langle\Omega| \tag{3.30}$$

for each $\bar{\rho} = \rho \otimes \sigma \in \mathcal{T}(\mathcal{H}) \otimes \mathcal{T}(\mathcal{H}_\varepsilon)$, therefore it extends, by a density argument, to all $\mathcal{T}(\mathcal{H} \otimes \mathcal{H}_\varepsilon)$. Observe that the linear map $\pi : \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}_\varepsilon$, $\pi(\psi) = \psi \otimes \Omega$ has as dual map $\pi^* : \mathcal{H} \otimes \mathcal{H}_\varepsilon \to \mathcal{H}$, $\pi^*(\psi \otimes \phi) = \langle \Omega \,,\, \phi \rangle \, \psi$ and they are such that

$$\pi^*\pi = \mathbb{1}, \qquad \pi\rho\pi^* = \rho \otimes |\Omega\rangle\langle\Omega| \tag{3.31}$$

for each $\rho \in \mathcal{T}(\mathcal{H})$. From (3.30),(3.31) we obtain that

$$\sum_{n\in\mathbb{N}} E_n \bar{\rho} E_n^* = \operatorname{tr}_\varepsilon(\bar{\rho}) \otimes |\Omega\rangle\langle\Omega| = \pi \operatorname{tr}_\varepsilon(\bar{\rho})\pi^*$$

then

$$\operatorname{tr}_\varepsilon(\bar{\rho}) = \pi^* \sum_{n\in\mathbb{N}} E_n \bar{\rho} E_n^* \pi.$$

By the latter equality we can write

$$\begin{aligned}
\mathbf{\Lambda}_t(\rho) &= \operatorname{tr}_\varepsilon \left(e^{-iHt/\hbar}(\rho \otimes |\Omega\rangle\langle\Omega|) e^{iHt/\hbar} \right) \\
&= \pi^* \sum_{n\in\mathbb{N}} E_n e^{-iHt/\hbar}(\rho \otimes |\Omega\rangle\langle\Omega|) e^{iHt/\hbar} E_n^* \pi \\
&= \pi^* \sum_{n\in\mathbb{N}} E_n e^{-iHt/\hbar} \pi\rho\pi^* e^{iHt/\hbar} E_n^* \pi \\
&= \sum_{n\in\mathbb{N}} K_n \rho K_n^*
\end{aligned}$$

where $K_n = \pi^* E_n e^{-iHt/\hbar}\pi$. Its dual map $\mathbf{\Lambda}'_t$ is obtained by duality

$$\mathbf{\Lambda}'_t(X) = \sum_{n\in\mathbb{N}} K_n^* X K_n.$$

It is easy to verify that $\sum_{n\in\mathbb{N}} K_n^* K_n = \mathbb{1}$ strongly, so by the Kraus theorem $\mathbf{\Lambda}'_t$ is a completely positive map in case $\rho_\varepsilon = |\Omega\rangle\langle\Omega|$ is a pure state. ⌟

3.7 Quantum dynamical semigroups

In this section we conclude the discussion begun in Sect. 3.5 about open quantum systems. We will see that an observable evolution of type (3.26) is peculiar to a special group of dynamical semigroup.

Definition 3.26. *Given an Hilbert space $\mathcal{H}$ we will call* **quantum dynamical semigroup** *(in the Heisenberg picture) a one-parameter family of linear operators $\boldsymbol{S}_t : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, $t \geq 0$ satisfying* (b),(c),(d) *of Definition* 3.18 *and*

(a') *$\boldsymbol{S}_t$ is completely positive for all $t \geq 0$.*

As we noticed before, the uniform continuity of the semigroup implies the existence of the generator, which is a linear bounded operator on $\mathcal{B}(\mathcal{H})$. Then $\boldsymbol{S}_t(X) = e^{tL}(X)$ for all $t \geq 0$. Our first goal in this section is to find a general form for the generators of uniformly continuous quantum dynamical semigroups. Then we will see that each one of them is of the form (3.26).

Generators of uniformly continuous quantum dynamical semigroups were classified by Lindblad and Gorini, Kossakowski, Sudarshan in the 70'. Here we will state first a more general formulation of these results.

Theorem 3.27 ([Pa] Thm. III.30.12 **).** *An operator L on $\mathcal{B}(\mathcal{H})$ is the generator of a uniformly continuous quantum dynamical semigroup if and only if there exists: a Hilbert space $\mathcal{K}$, a bounded linear operator $V : \mathcal{H} \to \mathcal{H} \otimes \mathcal{K}$ and a bounded self-adjoint linear operator H on $\mathcal{H}$ satisfying*

(i) $L(X) = i[H, X] + \frac{1}{2}\{2V^*(X \otimes \mathbb{1})V - V^*VX - XV^*V\}$;

(ii) *the set* $\{(VX - (X \otimes \mathbb{1})V)\psi \mid X \in \mathcal{B}(\mathcal{H}),\ \psi \in \mathcal{H}\}$ *is dense in* $\mathcal{H} \otimes \mathcal{K}$.

From this statement one could recover the results of [Li] and [GKS] in their original (and often more useful) form.

Theorem 3.28 (Lindblad, [Li], [Pa] Thm. III.30.16 **).** *An operator L on $\mathcal{B}(\mathcal{H})$ is the generator of a uniformly continuous quantum dynamical semigroup if and only if there exists a sequence $\{L_j\}$ of bounded operators on $\mathcal{H}$ such that $\sum L_j^* L_j$ is strongly convergent and a bounded self-adjoint operator H on $\mathcal{H}$ satisfying*

$$L(X) = i[H, X] + \frac{1}{2}\sum_j \{2L_j^* X L_j - L_j^* L_j X - X L_j^* L_j\}. \tag{3.32}$$

Moreover the sequence $\{L_j\}$ could be chosen such that

(i) *The set* $\{\bigoplus_j [L_j, X]\psi \mid X \in \mathcal{B}(\mathcal{H}),\ \psi \in \mathcal{H}\}$ *is dense in* $\bigoplus_j \mathcal{H}$;

(ii) $\mathrm{tr}(\rho L_j) = 0$ *for each j, given a fixed state $\rho \in \mathcal{T}(\mathcal{H})$;*

(iii) *If* $\sum_j |c_j|^2 < \infty$ *and* $c_0 + \sum_j c_j L_j = 0$ *then* $c_j = 0$ *for each j.*

Theorem 3.29 (Gorini, Kossakoswki, Sudarshan [GKS]). *An operator L^* on $\mathcal{B}(\mathbb{C}^N)$ is the generator of a continuous quantum dynamical semigroup if and only if can be expressed in the following form*

$$L^*(\rho) = -i[H, \rho] + \frac{1}{2}\sum_{i,j=1}^{N^2-1} c_{ij}\{2L_i \rho L_j^* - L_j^* L_i \rho - \rho L_j^* L_i\} \tag{3.33}$$

where: $\{L_j\}$, $j = 1, ..., N^2 - 1$, is a sequence of bounded operator on $\mathcal{H}$ such that $\mathrm{tr}(L_j) = 0$, $\mathrm{tr}(L_i^* L_j) = \delta_{ij}$; H is a bounded self-adjoint operators on $\mathcal{H}$ such that $\mathrm{tr}(H) = 0$; $C = \{c_{ij}\}_{i,j=1}^{N^2-1}$ is a positive semidefinite complex matrix.

Remark 3.30. Here we stated the result for the dual generator. By duality one can recover the same form of the dual generator from equation (3.32) (observe that just one $*$ moved). In this statement the operators $\{L_j\}$ are required to form an orthonormal basis of the space of trace zero operators in $\mathcal{B}(\mathbb{C}^N)$. ⌟

Remark 3.31. The result of Gorini, Kossakowski and Sudarshan is the finite dimensional equivalent of Lindblad theorem. Given a unitary matrix $U = \{u_{ij}\}_{i,j=1}^{N^2-1}$ consider the base change

$$L'_j = (U\bar{L})_j = \sum_{k=1}^{N^2-1} u_{jk} L_k,$$

then

$$\begin{aligned}
-i[H,\rho] + \frac{1}{2}\sum_{i,j=1}^{N^2-1} c_{ij}\{2L_i\rho L_j^* - L_j^* L_i\rho - \rho L_j^* L_i\} = \\
&= -i[H,\rho] + \frac{1}{2}\sum_{i,j} c_{ij}\{2(\sum_k U_{ik}^* L'_k)\rho(\sum_h U_{jh}^* L'_h)^* \\
&\quad - (\sum_h \overline{u_{hj}} L'_h)^*(\sum_k \overline{u_{ki}} L'_k)\rho - \rho(\sum_h u_{hj} L'^*_h)(\sum_k \overline{u_{ki}} L'_k)\} \\
&= -i[H,\rho] + \frac{1}{2}\sum_{k,h}\Big(\sum_{i,j} \overline{u_{ki}} c_{ij} u_{hj}\Big)\{2L'_k\rho L'^*_h - L'^*_h L'_k\rho - \rho L'^*_h L'_k\} \\
&= -i[H,\rho] + \frac{1}{2}\sum_{k,h}\Big(\sum_{j} (\overline{U}C)_{kj} u_{hj}\Big)\{2L'_k\rho L'^*_h - L'^*_h L'_k\rho - \rho L'^*_h L'_k\} \\
&= -i[H,\rho] + \frac{1}{2}\sum_{k,h} (\overline{U}CU^T)_{kh}\{2L'_k\rho L'^*_h - L'^*_h L'_k\rho - \rho L'^*_h L'_k\} \\
&= -i[H,\rho] + \frac{1}{2}\sum_{k,h} \overline{(UCU^*)}_{kh}\{2L'_k\rho L'^*_h - L'^*_h L'_k\rho - \rho L'^*_h L'_k\}
\end{aligned}$$

By the positivity of the matrix C it is always possible to find a unitary matrix U such that UCU^* is a diagonal matrix $D = \{d_{ii}\}_{i=1}^{N^2-1}$ and every coefficient d_{ii} is non negative. Of course in this case $\sum(\sqrt{d_{jj}}L'_j)^*(\sqrt{d_{jj}}L'_j)$ is strongly convergent and one obtain the Lindblad form of the generator.

Conversely, Theorem (3.28) says that it is possible to choose the operators L_j with trace zero (choosing $\rho = I/N$ in (ii)). Condition (iii) guarantees that at most N^2-1 operators L_j are different from zero and that they are linearly independent *i.e.* $\mathrm{tr}(L_i^* L_j) = \delta_{ij}$. Then normalizing the L_j's, *i.e.* $L'_j = \mathrm{tr}(L_j^* L_j)^{-1/2} L_j$ we recall the GKS form of the generator with the diagonal matrix $\{\mathrm{tr}(L_j^* L_j)\}_{i=1}^{N^2-1}$(as usual, by adding a constant to H one could obtain a traceless and equivalent Hamiltonian). ⌟

The equation that generators of a quantum dynamical semigroups solve is called *Lindblad equation* and reads

$$\dot{X} = L(X) = i[H, X] + \frac{1}{2}\sum_j \{2L_j^* X L_j - L_j^* L_j X - X L_j^* L_j\} \tag{3.34}$$

for observables $X \in \mathcal{B}(\mathcal{H})$ and

$$\dot{\rho} = -i[H, X] + \frac{1}{2}\sum_j \{2L_j \rho L_j^* - L_j^* L_j \rho - \rho L_j^* L_j\} \tag{3.35}$$

for states $\rho \in \mathcal{T}(\mathcal{H})$.

We conclude with a theorem of Davies that classifies the form of finite dimensional uniformly continuous quantum dynamical semigroups.

Theorem 3.32 (Davies, [Da] Thm. 9.4.3 **).** *Let $\mathcal{H}$ be a finite-dimensional Hilbert space and $\boldsymbol{S}_t$ a uniformly continuous quantum dynamical semigroup on $\mathcal{B}(\mathcal{H})$. Then there exist an Hilbert space $\mathcal{K}$, a state $\rho = |\Omega\rangle\langle\Omega|$ on $\mathcal{K}$ and a strongly continuous one-parameter semigroup V_t of isometries on $\mathcal{H} \otimes \mathcal{K}$ such that*

$$\boldsymbol{S}_t(X) = \mathbb{E}_\rho\left(V_t^* X \otimes \mathbb{1} V_t\right)$$

for all $X \in \mathcal{B}(\mathcal{H})$ and all $t \geq 0$.

Example 3.33 (Damped harmonic oscillator)**.** As example of infinite dimensional quantum system we would illustrate the damped harmonic oscillator, namely a quantum harmonic oscillator coupled with an environment that stabilizes the average number of excitation of the system.

Consider the quantum harmonic oscillator $H = \hbar\omega(a^\dagger a + \frac{1}{2})$, where the *annihilator* a and the *creator* $a^\dagger$ are defined as

$$a^\dagger = \frac{1}{\sqrt{2}}(X - iP) \qquad a = \frac{1}{\sqrt{2}}(X + iP). \tag{3.36}$$

Consider the Lindblad operators

$$L_1 = \left(\frac{\gamma}{2}(\eta + 1)\right)^{\frac{1}{2}} a^\dagger \qquad L_2 = \left(\frac{\gamma}{2}\eta\right)^{\frac{1}{2}} a$$

where

$$\eta = \frac{1}{e^{\hbar\omega\beta} - 1}.$$

A general density operator for that system reads

$$\rho = \frac{1}{2}\sum_{n\leq m} c_{nm}|n\rangle\langle m| + c_{nm}^*|m\rangle\langle n| \qquad \sum_n c_{nn} = 1.$$

If ρ is a stationary state for the system it must satisfy $0 = \dot{\rho} = L(\rho)$ where L is given by (3.35). Notice that by going to the interaction picture, *i.e.* performing the coordinate change $e^{iHt/\hbar}$, we can consider $H = 0$. Then

$$
\begin{aligned}
0 = \; & \frac{\gamma}{2}(\eta+1)\left(2a\frac{1}{2}\sum_{n\le m}\Big[c_{nm}|n\rangle\langle m| + c^*_{nm}|m\rangle\langle n|\Big]a^\dagger - a^\dagger a\frac{1}{2}\sum_{n\le m}\Big[c_{nm}|n\rangle\langle m| + c^*_{nm}|m\rangle\langle n|\Big]\right. \\
& \qquad\qquad \left. -\frac{1}{2}\sum_{n\le m}\Big[c_{nm}|n\rangle\langle m| + c^*_{nm}|m\rangle\langle n|\Big]a^\dagger a\right) \\
& + \frac{\gamma}{2}\eta\left(2a^\dagger\frac{1}{2}\sum_{n\le m}\Big[c_{nm}|n\rangle\langle m| + c^*_{nm}|m\rangle\langle n|\Big]a - aa^\dagger\frac{1}{2}\sum_{n\le m}\Big[c_{nm}|n\rangle\langle m| + c^*_{nm}|m\rangle\langle n|\Big]\right. \\
& \qquad\qquad \left. -\frac{1}{2}\sum_{n\le m}\Big[c_{nm}|n\rangle\langle m| + c^*_{nm}|m\rangle\langle n|\Big]aa^\dagger\right) \\
= \; & \frac{\gamma}{4}(\eta+1)\left(2\sum_{n\le m}\Big[c_{nm}(a|n\rangle)(a|m\rangle)^* + c^*_{nm}\sqrt{m}\,|m-1\rangle\langle n-1|\sqrt{n}\Big]\right. \\
& \left. -\sum_{n\le m}\Big[c_{nm}n|n\rangle\langle m| + c^*_{nm}m|m\rangle\langle n|\Big] - \sum_{n\le m}\Big[c_{nm}|n\rangle\langle m|m + c^*_{nm}|m\rangle\langle n|n\Big]\right) \\
& + \frac{\gamma}{4}\eta\left(2\sum_{n\le m}\Big[c_{nm}\sqrt{n+1}\sqrt{m+1}\,|n+1\rangle\langle m+1| + c^*_{nm}\sqrt{n+1}\sqrt{m+1}\,|m+1\rangle\langle n+1|\Big]\right. \\
& \left. -\sum_{n\le m}\Big[c_{nm}(n+1)|n\rangle\langle m| + c^*_{nm}(m+1)|m\rangle\langle n|\Big] - \sum_{n\le m}\Big[c_{nm}(m+1)|n\rangle\langle m| + c^*_{nm}(n+1)|m\rangle\langle n|\Big]\right)
\end{aligned}
$$

$$
\begin{aligned}
= \; & \frac{\gamma}{2}(\eta+1)\sum_{n\le m}|n\rangle\langle m|\left(c_{n+1,m+1}\sqrt{(n+1)(m+1)} - \frac{n}{2}c_{n,m} - \frac{m}{2}c_{n,m}\right) \\
& \qquad\qquad |m\rangle\langle n|\left(c^*_{n+1,m+1}\sqrt{(n+1)(m+1)} - \frac{n}{2}c^*_{n,m} - \frac{m}{2}c^*_{n,m}\right) \\
& + \frac{\gamma}{2}\eta\sum_{n\le m, n\ge 1}|n\rangle\langle m|\left(c_{n-1,m-1}\sqrt{nm} - \frac{n+1}{2}c_{n,m} - \frac{m+1}{2}c_{n,m}\right) \\
& \qquad\qquad |m\rangle\langle n|\left(c^*_{n-1,m-1}\sqrt{nm} - \frac{n+1}{2}c^*_{n,m} - \frac{m+1}{2}c^*_{n,m}\right) \\
& + \frac{\gamma}{4}\eta\sum_{n=0,m\ge 0}c_{0,m}|0\rangle\langle m| + c^*_{0,m}|m\rangle\langle 0|(m+1) + c_{0,m}(m+1)|0\rangle\langle m| + c^*_{0,m}|m\rangle\langle 0|
\end{aligned}
$$

$$
\begin{aligned}
=&\frac{\gamma}{2}\sum_{1\le n\le m} |n\rangle\langle m| \Big[(\eta+1)\left(c_{n+1,m+1}\sqrt{(n+1)(m+1)}-\frac{n}{2}c_{n,m}-\frac{m}{2}c_{n,m}\right)\\
&\qquad+\eta\left(c_{n-1,m-1}\sqrt{nm}-\frac{n+1}{2}c_{n,m}-\frac{m+1}{2}c_{n,m}\right)\Big]\\
&+\frac{\gamma}{2}\sum_{1\le n\le m} |m\rangle\langle n| \Big[(\eta+1)\left(c^*_{n+1,m+1}\sqrt{(n+1)(m+1)}-\frac{n}{2}c^*_{n,m}-\frac{m}{2}c^*_{n,m}\right)\\
&\qquad+\eta\left(c^*_{n-1,m-1}\sqrt{nm}-\frac{n+1}{2}c^*_{n,m}-\frac{m+1}{2}c^*_{n,m}\right)\Big]\\
&+\frac{\gamma}{2}\sum_{0=n\le m} |0\rangle\langle m| \Big[(\eta+1)\left(c_{1,m+1}\sqrt{m+1}-\frac{m}{2}c_{0,m}\right)-\frac{1}{2}\eta\left(c_{0,m}\sqrt{nm}(m+1)c_{0,m}\right)\Big]\\
&+\frac{\gamma}{2}\sum_{0=n\le m} |m\rangle\langle 0| \Big[(\eta+1)\left(c^*_{1,m+1}\sqrt{m+1}+\frac{m}{2}c^*_{0,m}\right)-\frac{1}{2}\eta\left((m+1)c^*_{0,m-1}-\frac{n+1}{2}c^*_{n,m}+c^*_{0,m}\right)\Big]
\end{aligned}
$$

The solution of the previous equation could be found componentwise by induction on the indices m, n. More precisely, for each pair n, m we project the latter expression on the subspace $|n\rangle\langle m|$ and we impose that is null, *i. e.*

$$|n\rangle\langle n| L(\rho) |m\rangle\langle m| = 0$$

We begin by $n = m = 0$. The coefficient of the term $|0\rangle\langle 0|$ is zero if and only if

$$(\eta+1)(c_{1,1}\sqrt{1+0}-\frac{0}{2}c_{0,0})-\frac{\eta}{2}(c_{0,0}+c_{0,0})=0$$

which implies

$$c_{1,1}=\frac{\eta}{\eta+1}c_{0,0}.$$

For $n = 0, m \ge 1$ we obtain the condition

$$(\eta+1)c_{1,m+1}\sqrt{m+1}-\frac{m(\eta+1)}{2}c_{0,m}-\frac{(m+2)\eta}{2}c_{0,m}=0$$

that lead to the recursive relation

$$c_{1,m+1}=\frac{(\eta+\frac{1}{2})m+\eta}{\sqrt{m+1}}c_{0,m}.$$

For $n = m \ge 1$

$$(\eta+1)(c_{n+1,n+1}(n+1)-nc_{n,n})+\eta(c_{n-1,n-1}n-(n+1)c_{n,n})=0$$

which is

$$c_{n+1,n+1}=\frac{(2\eta+1)n+\eta}{(\eta+1)(n+1)}c_{n,n}-\frac{\eta n}{(\eta+1)(n+1)}c_{n-1,n-1}. \tag{3.37}$$

It can be easily shown by induction that the latter eq. is satisfied by

$$c_{n,n}=\left(\frac{\eta}{\eta+1}\right)^n c_{0,0}.$$

Then given that $\sum_n c_{n,n} = 1$, one obtains

$$c_{0,0} = \frac{1}{\eta + 1} = 1 - e^{-\hbar\omega\beta} \qquad c_{n,n} = e^{-\hbar\omega\beta n}(1 - e^{-\hbar\omega\beta}).$$

Thus, the population of each level, *i. e.* $c_{n,n} = Tr(\rho \, |n\rangle \, \langle n|)$, of a stationary state for the damped harmonic oscillator is given by the Boltzmann distribution.

The mean number of quanta in this state is the expectation of the number of particle $N = a^\dagger a$

$$\langle a^\dagger a \rangle = \sum n c_{n,n} = \eta,$$

which is the thermal average. If we define $N(t) := Tr(a^\dagger a \rho(t))$, *i. e.* the average number of quanta in the state ρ, then it satisfies the equation

$$\dot{N}(t) = Tr(a^\dagger a L(\rho(t)))$$

which reads

$$\dot{N}(t) = -\gamma N(t) + \gamma\eta.$$

The solution is

$$\begin{aligned} N(t) =& e^{-\gamma t} \left(N(0) + \int_0^t ds \; e^{\gamma s} \gamma\eta \right) \\ =& e^{-\gamma t} N(0) + \eta(1 - e^{-\gamma t}). \end{aligned}$$

Thus the average number of quanta of the system approaches, for $\gamma t \gg 1$ (which means on the scale of the inverse damping rate), the thermal average η. This happens for every initial data. ⌟

Chapter 4

Two-level closed and open quantum systems

In this chapter we will present our approach to the adiabatic controllability problem for an open quantum system. We will focus our attention to the case of a two-level system to illustrate the techniques used in our analysis. First we will introduce a set of coordinates for the state space of a finite dimensional quantum system. This allows to have a vectorial representation of the density matrix called vector of coherence. In these coordinates the Lindblad equation (an operator valued equation) translates into a set of ODEs that we can study as a classical dynamical system.

4.1 Vector of coherence

In this section we discuss the Bloch vector representation of density matrices for finite dimensional quantum systems. If $\mathcal{H} = \mathbb{C}^N$ it is always possible to choose a basis of $\mathcal{B}(\mathbb{C}^N)$, $\{F_i\}_{i=0}^{N^2-1}$ with $F_0 = \mathbb{1}$, $tr(F_j) = 0$ and $tr(F_i^* F_j) = N\delta_{ij}$ (the generalized Pauli basis). Then every state ρ on $\mathbb{C}^N$ admits the decomposition

$$\rho = \frac{tr(\rho\mathbb{1})}{tr(\mathbb{1})}\mathbb{1} + \sum_{j=1}^{N^2-1} \frac{tr(F_j^*\rho)}{tr(F_j^* F_j)} F_j = \frac{\mathbb{1}}{N} + \sum_{j=1}^{N^2-1} \frac{x_j}{N} F_j,$$

where

$$x_j := tr(F_j^*\rho), \quad j = 0, ..., N^2 - 1. \tag{4.1}$$

With respect to the previous decomposition we will call the coordinate vector $x = (x_0, ..., x_{N^2-1})$ the *vector of coherence of* ρ.

Then, by the spectral properties of density operators, namely $\sigma(\rho) \subset [0, 1]$

$$\frac{1}{N^2} tr(\mathbb{1}) + \sum_{j=1}^{N^2-1} \frac{|x_j|^2}{N^2} tr(F_j^* F_j) = tr(\rho^2) \leq 1 \quad \Rightarrow \quad \sum_{j=1}^{N^2-1} |x_j|^2 \leq N(1 - \frac{1}{N}) = N - 1.$$

The ball $B_N = \{x \in \mathbb{R}^N \mid \|x\|^2 \leq N-1\}$ is called in this context *Bloch ball.* We choose not to normalize the elements F_j's, but obviously by defining $F'_j = F_j/\sqrt{N}$ the relation $tr(F'^*_i F'_j) = \delta_{ij}$ holds, and

$$\rho = \frac{\mathbb{1}}{N} + \sum_{j=1}^{N^2-1} x'_j F'_j, \qquad x'_j = tr(F'^*_j \rho),\ j = 0, ..., N^2-1.$$

Then

$$\frac{1}{N^2} tr(\mathbb{1}) + \sum_{j=1}^{N^2-1} \left|x'_j\right|^2 = tr(\rho^2) \leq 1 \quad \Rightarrow \quad \sum_{j=1}^{N^2-1} \left|x'_j\right|^2 \leq (1 - \frac{1}{N}).$$

For simplicity of notation, in the following we will make use of the non normalized base. Notice that in the case $N = 2$, B_2 is the unit ball.

4.2 Two-level closed systems

In this section we briefly discuss the evolution of the density operator for a closed two-level quantum system in the Bloch representation. Let $\mathcal{H} = \mathbb{C}^2$ and $H \in \mathcal{B}(\mathbb{C}^2)$ be a self-adjoint operator, then H can be written

$$H = \begin{pmatrix} h_{00} & h_{01} \\ h_{10} & h_{11} \end{pmatrix}, \qquad \begin{cases} h_{00}, h_{11} \in \mathbb{R}, \\ h_{10} = \overline{h_{01}} \end{cases}$$

then it decomposes on the Pauli basis as

$$H = \frac{1}{2}\Big(\mathrm{tr}(H)\mathbb{1} + 2\,\mathrm{Re}(h_{01})\sigma_1 - 2\,\mathrm{Im}(h_{01})\sigma_2 + (h_{00} - h_{11})\sigma_3\Big). \tag{4.2}$$

Analogously, a density matrix ρ on $\mathbb{C}^2$, namely a self-adjoint positive matrix such that $tr(\rho) = 1$ and $\rho^2 < \rho$, *i. e.*

$$\rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}, \qquad \begin{cases} \rho_{00}, \rho_{11} \geq 0, \\ \rho_{10} = \overline{\rho_{01}}, \\ \rho_{00}\rho_{11} \geq |\rho_{01}|^2 \end{cases}$$

can be decomposed as

$$\rho = \frac{1}{2}\Big(\mathbb{1} + 2\,\mathrm{Re}(\rho_{01})\sigma_1 - 2\,\mathrm{Im}(\rho_{01})\sigma_2 + (\rho_{00} - \rho_{11})\sigma_3\Big),$$

therefore its vector of coherence $x = (x_0, x_1, x_2, x_3)$ is defined as in (4.1), *i. e.*

$$\begin{cases} x_0 = tr(\mathbb{1}\rho) = 1 \\ x_1 = tr(\sigma_1\rho) = \rho_{01} + \rho_{10} \\ x_2 = tr(\sigma_2\rho) = -i(\rho_{01} - \rho_{10}) \\ x_3 = tr(\sigma_3\rho) = \rho_{00} - \rho_{11} \end{cases} \tag{4.3}$$

We observe that

$$x_1^2 + x_2^2 + x_3^2 = 4\,\mathrm{Re}(\rho_{01})^2 + 4\,\mathrm{Im}(\rho_{01})^2 + (\rho_{00} - \rho_{11})^2 = 4\,|\rho_{01}|^2 + (\rho_{00} - \rho_{11})^2$$
$$\leq 4\rho_{00}\rho_{11} + (\rho_{00} - \rho_{11})^2 = (\rho_{00} + \rho_{11})^2 = 1,$$

and moreover

$$tr(\rho^2) = \frac{1}{2}(1 + x_1^2 + x_2^2 + x_3^2),$$

so $tr(\rho) = tr(\rho^2) = 1$ if and only if $x_1^2 + x_2^2 + x_3^2 = 1$, *i.e.* a state ρ is a pure state if and only if its vector of coherence is on the Bloch sphere of radius 1.

In Bloch coordinates the Heisenberg equation in Hartree units (so that in particular $\hbar = 1$ hereafter)

$$\dot{\rho} = -i[H, \rho] \tag{4.4}$$

translates into the following system of ODEs

$$\begin{cases} \dot{x}_1 = & -(h_{00} - h_{11})x_2 - 2\,\mathrm{Im}(h_{01})x_3 \\ \dot{x}_2 = & (h_{00} - h_{11})x_1 - 2\,\mathrm{Re}(h_{01})x_3 \\ \dot{x}_3 = & 2\,\mathrm{Im}(h_{01})x_1 + 2\,\mathrm{Re}(h_{01})x_2 \end{cases}, \tag{4.5}$$

which shortly reads

$$\dot{x} = A(h)x \qquad \text{where} \quad h = \Big(2\,\mathrm{Re}(h_{01}), -2\,\mathrm{Im}(h_{01}), h_{00} - h_{11}\Big) \tag{4.6}$$

is the vector of coordinates of $H - \mathrm{tr}(H)$ in the basis $\{\sigma_1, \sigma_2, \sigma_3\}$ (see (4.2)) and $A : \mathbb{R}^3 \to \mathcal{B}(\mathbb{R}^3)$ is defined

$$A(u) = \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix}. \tag{4.7}$$

Observe that $\dot{x} = A(h)x = h \wedge x$ and the matrix $A(h)$ is skew-symmetric *i.e.* $A(h)^T = -A(h)$, so the exponential matrix $e^{tA(h)}$ corresponds to a rotation around a fixed axis. Then the trajectory of a vector of coherence x in the Bloch ball is a circumference of fixed radius. Thus the *purity* of each state, namely $tr(\rho^2) = (1 + \|x\|^2)/2$, remains invariant during the dynamics. This is in agreement with equation (3.17).

When we consider a controlled system, we assume that the Hamiltonian $H = H(u)$ is affine with respect to the control variable $u \in \mathbb{R}^m$, $m \leq dim(\mathcal{H})$.

Assumption 4.1. *Assume that the Hamiltonian of a two-level system has the form*

$$H(u) = \frac{1}{2}\Big(E\sigma_3 + u_1\sigma_1 + u_2\sigma_2\Big), \qquad u = (u_1, u_2) \in \mathbb{R}^2 \tag{4.8}$$

where $E > 0$.

Remark 4.2. We choose to consider a system with a drift $H(0) = (E/2)\sigma_3$, because this uncontrolled Hamiltonian represents a standard two-level system with gap E between energy levels. The drift is chosen traceless, however this is not restrictive since two Hamiltonians which differ by $c\mathbb{1}$ generate the same state evolution, see eq.(3.17). We choose to have two control parameters to ensure that the system can be controlled by means of slowly varying controls. If fact, as seen in Example 2.31, one control is sufficient to achieve controllability, but in general this could have unbounded derivatives. ⌟

The Heisenberg equation in Bloch coordinates for this choice of H reads

$$\dot{x} = A(u_E)x \tag{4.9}$$

where

$$u_E = (u_1, u_2, E). \tag{4.10}$$

Equations (4.9) generates the rotation around the axis u_E, therefore the system has a set of equilibrium points, namely $\{cu_E \mid c \in \mathbb{R}\}$. Let us denote $\hat{u}_E = u_E / \|u_E\|$.

4.2.1 Slowly driven closed systems

The control law (4.8) allow to choose the rotation axis for the dynamics in Bloch coordinates. If we are able to change adiabatically the axis of rotation u_E, *i.e.* we can choose a control law such that $\|\dot{u}_E\| < \varepsilon \ll 1$, then we can ask if the equilibria of the system remain stable. More precisely, given a control function $u : [0,1] \to \mathbb{R}^2$ and an initial state x_0 such that

$$\|x_0 - \langle x_0 \,,\, \hat{u}_E(0)\rangle \,\hat{u}_E(0)\| < \delta,$$

we would prove that there exists ε small enough such that the solution $x(t)$ of

$$\dot{x} = A(u_E(\varepsilon t))x, \qquad t \in [0, 1/\varepsilon] \tag{4.11}$$

with initial condition $x(0) = x_0$ satisfies

$$\|x(t) - \langle x(t) \,,\, \hat{u}_E(\varepsilon t)\rangle \,\hat{u}_E(\varepsilon t)\| < \delta, \qquad \forall t \in [0, 1/\varepsilon].$$

Notice that with two controls u_E cannot span every unit vector $\hat{n} \in S^2_{\mathbb{R}}$. Assuming $(u_1, u_2) \in \mathbb{R}^2$, *i.e.* unbounded controls, $\hat{u}_E \in S^2_{\mathbb{R}} \cap \{x_3 > 0\}$. However we remark again that the we are interested in preserving the stability of equilibria.

To simplify the problem it is convenient to perform changes of coordinates on the system

$$i\dot{\psi} = H(u(t))\psi, \qquad \psi \in \mathbb{C}^2$$

where $H(u)$ has the form (4.8). Set

$$u_1(t) - iu_2(t) = v_1(t)e^{-2i\left(Et - \int_0^t v_3(\tau)d\tau\right)}, \qquad v_1(t), v_3(t) \in \mathbb{R} \tag{4.12}$$

and consider the time dependent transformation

$$V(t) = \begin{pmatrix} e^{2i\left(Et - \int_0^t v_3(\tau)d\tau\right)} & 0 \\ 0 & e^{-2i\left(Et - \int_0^t v_3(\tau)d\tau\right)} \end{pmatrix}. \tag{4.13}$$

Then $\phi = V(t)^{-1}\psi$ satisfies

$$i\dot{\phi} = \left[V^{-1}(t)H(u(t))V(t) - iV^{-1}(t)\frac{dV}{dt}(t)\right]\phi = H_{\rm rw}(v_1(t), 0, v_3(t))\phi$$

where the Hamiltonian $H_{\rm rw}$ is defined

$$H_{\rm rw}(v_1, v_2, v_3) = \frac{1}{2}\Big(v_1\sigma_1 + v_2\sigma_2 + v_3\sigma_3\Big). \tag{4.14}$$

In these new coordinates, the system become driftless. Notice that if $v_1(0) = 0$ the initial point of the control u is $u(0) = (0,0)$ or $u_E(0) = (0,0,E)$. When view in Bloch coordinates $H_{\rm rw}(v(t))$ corresponds to the generator $A(v(t))$ where $A(\cdot)$ was defined above.

Example 4.3. Now choose the particular control

$$v(t) = (v_1(t), 0, v_3(t)) = (2\sin\theta(t), 0, 2\cos\theta(t)), \qquad t \in [0,1] \tag{4.15}$$

which means that the time dependent Hamiltonian of the system is

$$H_{\rm rw}(v(t)) = \sin\theta(t)\sigma_1 + \cos\theta(t)\sigma_3. \tag{4.16}$$

If $\theta(t)$ is linear in time, the Schrödinger equation is integrable because there exists a time dependent change of coordinates $U(t) = \cos[\theta(t)/2]\sigma_3 + \sin[\theta(t)/2]\sigma_1$ such that in the new coordinates the dynamics is given by the Schrödinger equation of constant Hamiltonian

$$H'_{\rm rw} = \sigma_3 - \frac{\dot{\theta}}{2}\sigma_2.$$

Therefore the exponential of $H'_{\rm rw}$ is computed by the use of

$$e^{i(\gamma/2)[v_1\sigma_1 + v_2\sigma_2 + v_3\sigma_3]} = \cos(\gamma\left\|v\right\|/2)\mathbb{1} + i\frac{\sin(\gamma\left\|v\right\|/2)}{\left\|v\right\|}(v_1\sigma_1 + v_2\sigma_2 + v_3\sigma_3). \tag{4.17}$$

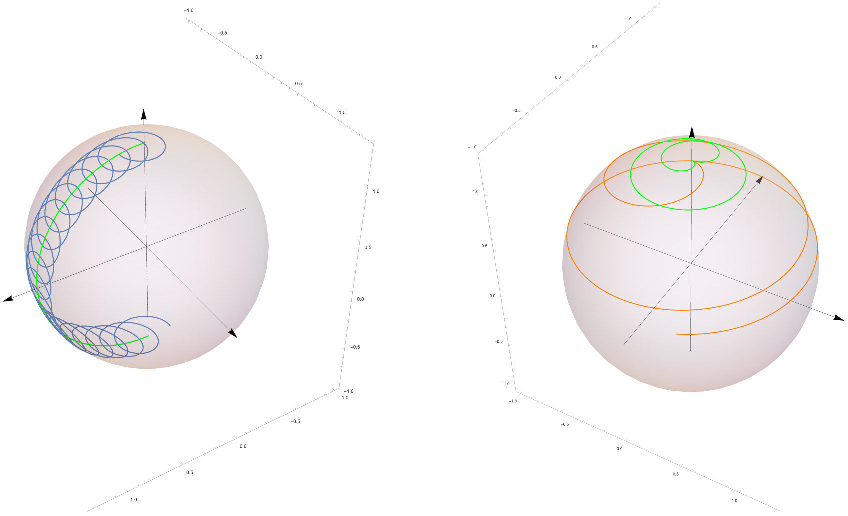
Choosing $\theta(t) = \varepsilon t$, the solution $\phi(t)$ to the slowly driven Schrödinger equation

$$i\dot{\phi} = H_{\rm rw}(v(\varepsilon t))\phi = [\sin(\varepsilon t)\sigma_1 + \cos(\varepsilon t)\sigma_3]\,\phi, \quad t \in [0, \vartheta/\varepsilon] \tag{4.18}$$

with initial datum $\phi(0) = \phi_0$ and $\vartheta \in (0, 2\pi]$ is

$$\phi(t) = U(t)e^{-iH'_{\rm rw}t}U(t)^{-1}\phi_0 = U(t)\left[\cos(\omega(\varepsilon)t)\mathbb{1} - i\frac{\sin(\omega(\varepsilon)t)}{\omega(\varepsilon)}\sigma_3 - i\frac{\varepsilon\sin(\omega(\varepsilon)t)}{2\omega(\varepsilon)}\sigma_2\right]\phi_0$$

Figure 4.1



(a) In blue a trajectory of system (4.16) with $\vartheta = \pi$, $\varepsilon = 0.01$. In green the vector $v/\|v\|$ where v is the control function (4.15). The trajectory remains stable around the slowly varying equilibrium point $v/\|v\|$.

(b) In green the vector $u_E/\|u_E\|$ where u_E is the control function (4.15) seen in the original coordinates. In orange the same control function multiplied by a constant factor of 20.

where $\omega(\varepsilon) = \sqrt{1+\varepsilon^2/4}$. Bloch coordinates $x(t) = (x_1(t), x_2(t), x_3(t))$ of $\rho(t) = |\phi(t)\rangle\langle\phi(t)|$ can now be computed by means of last equation and formula (3.13). Choosing as initial data $\rho_0 = \sigma_3$, *i.e.* $x(0) = (0,0,1)$, after some straightforward computation one obtains

$$
\begin{aligned}
x_1(t) &= -\frac{\varepsilon\omega}{2}\cos(\varepsilon t)\sin(2\omega t) + \left(\frac{1}{\omega^2} - \frac{\varepsilon^2}{8}\left(\omega^2 - \frac{1}{\omega^2}\right)\right)\sin(\varepsilon t) + \frac{\varepsilon^2}{8}\left(\omega^2 + \frac{1}{\omega^2}\right)\sin(\varepsilon t)\cos(2\omega t)\\
x_2(t) &= \varepsilon\sin(\omega t)^2\\
x_3(t) &= -\frac{\varepsilon\omega}{2}\sin(\varepsilon t)\sin(2\omega t) + \left(\frac{1}{\omega^2} - \frac{\varepsilon^2}{8}\left(\omega^2 - \frac{1}{\omega^2}\right)\right)\cos(\varepsilon t) + \frac{\varepsilon^2}{8}\left(\omega^2 + \frac{1}{\omega^2}\right)\cos(\varepsilon t)\cos(2\omega t)
\end{aligned}
$$

which is immediately recognized as $(v_1(\varepsilon t), 0, v_3(\varepsilon t)) + O(\varepsilon)$ (see Fig.4.1).

More generally if the initial state's coordinates are $x(0) = (x_1(0), x_2(0), x_3(0))$ with $\|x(0)\| = 1$ and $\|(0,0,1) - x(0)\| < \delta$ we can compute its evolution using the above argument. We arrive to

$$
\begin{aligned}
x_1(t) =& x_1(0)\left[-\frac{\varepsilon\omega}{2}\sin(\varepsilon t)\sin(2\omega t) - \left(\frac{1}{\omega^2} + \frac{\varepsilon^2}{8}\left(\omega^2 - \frac{1}{\omega^2}\right)\right)\cos(\varepsilon t)\cos(2\omega t) + \frac{\varepsilon^4}{32}\left(1 + \frac{1}{\omega^2}\right)\cos(\varepsilon t)\right]\\
&+ x_2(0)\left[\frac{1}{\omega}\cos(\varepsilon t)\sin(2\omega t) + \varepsilon\sin(\varepsilon t)\sin(\omega t)^2\right]\\
&+ x_3(0)\left[-\frac{\varepsilon\omega}{2}\cos(\varepsilon t)\sin(2\omega t) + \left(\frac{1}{\omega^2} - \frac{\varepsilon^2}{8}\left(\omega^2 - \frac{1}{\omega^2}\right)\right)\sin(\varepsilon t) + \frac{\varepsilon^2}{8}\left(\omega^2 + \frac{1}{\omega^2}\right)\sin(\varepsilon t)\cos(2\omega t)\right]
\end{aligned}
$$

$$x_2(t) = x_1(0)\frac{1}{\omega}\sin(2\omega t) + x_2(0)\frac{\varepsilon^2}{8}\left(\omega^2 - \frac{1}{\omega^2}\right) + x_2(0)\left(\frac{1}{\omega^2} - \frac{\varepsilon^4}{32}\left(1 + \frac{1}{\omega^2}\right)\right)\cos(2\omega t) + x_3(0)\varepsilon\sin(\omega t)^2$$

$$\begin{aligned} x_3(t) =& x_1(0)\left[-\frac{\varepsilon\omega}{2}\cos(\varepsilon t)\sin(2\omega t) + \left(\frac{1}{\omega^2} + \frac{\varepsilon^2}{8}\left(\omega^2 - \frac{1}{\omega^2}\right)\right)\sin(\varepsilon t)\cos(2\omega t) - \frac{\varepsilon^4}{32}\left(1 + \frac{1}{\omega^2}\right)\sin(\varepsilon t)\right] \\ &+ x_2(0)\left[-\frac{1}{\omega}\sin(\varepsilon t)\sin(2\omega t) + \varepsilon\cos(\varepsilon t)\sin(\omega t)^2\right] \\ &+ x_3(0)\left[-\frac{\varepsilon\omega}{2}\sin(\varepsilon t)\sin(2\omega t) + \left(\frac{1}{\omega^2} - \frac{\varepsilon^2}{8}\left(\omega^2 - \frac{1}{\omega^2}\right)\right)\cos(\varepsilon t) + \frac{\varepsilon^2}{8}\left(\omega^2 + \frac{1}{\omega^2}\right)\cos(\varepsilon t)\cos(2\omega t)\right] \end{aligned}$$

from which we can see that

$$\|(v_1(\varepsilon t), 0, v_3(\varepsilon t)) - x(t)\| \le \|(0,0,1) - x(0)\| + O(\varepsilon) < \delta, \qquad t \in [0, \vartheta/\varepsilon]$$

for $0 < \varepsilon$ small enough. ⌟

It is possible to generalize the result of the previous example to control functions $v : [0,1] \to \mathbb{R}^3 \setminus \{(0,0,0)\}$.

Theorem 4.4. *Let $v : [0,1] \to \mathbb{R}^3$, $v \in C^2([0,1])$ be a control function satisfying*

$$\min_{t\in[0,1]} \|v(t)\| > 0.$$

Let $x(0) \in \mathbb{R}^3 \setminus \{(0,0,0)\}$ be such that $\|x_0 - \langle x_0\,,\, \hat{v}(0)\rangle\,\hat{v}(0)\| < \delta$. There exist $\varepsilon > 0$ such that the solution $x(t)$ of the equation

$$\dot{x} = A(v(\varepsilon t))x, \qquad t \in [0, 1/\varepsilon]$$

satisfies

$$\|x(t) - \langle x(t)\,,\, \hat{v}(\varepsilon t)\rangle\,\hat{v}(\varepsilon t)\| < \delta, \qquad \forall t \in [0, 1/\varepsilon].$$

Remark 4.5 (Sketch of the proof of Thm.4.4)**.** The previous result follows from a generalization to evolutions on Banach spaces of standard quantum adiabatic results [AvFG]. In the hypothesis of the theorem 0 is eigenvalue of $A(v(t))$ for each t and is protected by a gap. Therefore, the projection P on the instantaneous eigenvector of eigenvalue 0 is well defined and $\ker A(v) \oplus \mathrm{Ran}\, A(v) = \mathbb{R}^3$. Notice that $P(t)x = \langle x\,,\, \hat{v}(t)\rangle\,\hat{v}(t)$. We define *propagator by parallel transport*[1] the collection of the maps $\{T(s,s')\}_{s,s'\in\mathbb{R}} \subset \mathrm{Aut}(\mathbb{R}^3)$, which are solution to the equation

$$\frac{\partial}{\partial s}T(s,s') = [\dot{P}(s), P(s)]T(s,s'), \qquad T(s',s') = \mathbb{1}. \tag{4.19}$$

[1]The definition above has a geometric counterpart in terms of an Ehresmann connection on the trivial vector bundle over $\mathbb{R}$ with fiber $\mathbb{R}^3$. The Ehresmann connection is a generalization of the Levi-Civita connection in Riemannian geometry, and defines parallel transport on general vector bundles [vWes, Part IV][Spi, Chap. 8].

In particular, they satisfy the *intertwining property* $P(s)T(s,s') = T(s,s')P(s')$. By [AvFG, Theorem 9]

$$\begin{aligned}\|(\mathbb{1}-P(t))x(t)\| &\leq \|(\mathbb{1}-P(t))(x(t)-T(t,0)x(0))\| + \|(\mathbb{1}-P(t))T(t,0)x(0)\| \\ &= \|(\mathbb{1}-P(t))x(t)-T(t,0)(\mathbb{1}-P(0))x(0)\| + \|T(t,0)(\mathbb{1}-P(0))x(0)\| \\ &\leq C\varepsilon\,\|x(0)\| + \|(\mathbb{1}-P(0))x(0)\|\end{aligned}$$

which is the claim of the theorem. ⌟

In the case of system (4.8) we can state a corollary of the previous theorem.

Corollary 4.6. *Let $u : [0,1] \to \mathbb{R}^2$, $u \in C^2([0,1])$ be a control function for the Hamiltonian (4.8). Let $x(0) \in \mathbb{R}^3 \backslash \{(0,0,0)\}$ be such that $\|x(0) - \langle x(0)\,,\, \hat{u}_E(0)\rangle\, \hat{u}_E(0)\| < \delta$. There exist $\varepsilon > 0$ such that the solution $x(t)$ of the equation*

$$\dot{x} = A(u_E(\varepsilon t))x, \qquad t \in [0, 1/\varepsilon]$$

satisfies

$$\|x(t) - \langle x(t)\,,\, \hat{u}_E(\varepsilon t)\rangle\, \hat{u}_E(\varepsilon t)\| < \delta, \qquad \forall t \in [0, 1/\varepsilon].$$

4.3 Two-level open systems

We will now obtain the general form of the equation $\dot{\rho} = L^*(\rho)$ in the Bloch coordinates where L^* is the generator in the form (3.33).

Given a generic matrix $C = \{c_{ij}\}$ which is assumed positive semidefinite (then Hermitian), and the standard Pauli basis $\{I, \sigma_1, \sigma_2, \sigma_3\}$, (3.33) reads

$$\begin{aligned}L^*(\rho) =& -i[H,\rho] + \frac{1}{2}\sum_{i,j=1}^{3} c_{ij}[2\sigma_i\rho\sigma_j^* - \rho\sigma_j^*\sigma_i - \sigma_j^*\sigma_i\rho] \\ =& -i[H,\rho] + \frac{1}{2}\sum_{j=1}^{3} c_{jj}[2\sigma_j\rho\sigma_j - \rho\sigma_j\sigma_j - (\mathbb{1})\rho] + \frac{1}{2}\sum_{i,j=1, i\neq j}^{3} c_{ij}[2\sigma_i\rho\sigma_j - \rho\sigma_j\sigma_i - \sigma_j\sigma_i\rho].\end{aligned}$$

From the elementary relation

$$\sigma_i\sigma_j = i\epsilon_{ijk}\sigma_k \tag{4.20}$$

where ϵ_{ijk} is the completely antisymmetric symbol[2], one obtains that if $k, h \in \{1,2,3\}$ and $k \neq h$ then $\sigma_k\sigma_h\sigma_k = -\sigma_h$. Thus, this implies

$$2\sigma_j\rho\sigma_j - 2\rho = -2\sum_i (1-\delta_{ji})x_i\sigma_i$$

[2] ϵ_{ijk} is 1 if (i,j,k) is an even permutation of $(1,2,3)$, -1 if it is an odd permutation, and 0 if any index is repeated.

and so

$$L^*(\rho) = -\,i[H,\rho] + \sum_{i,j=1}^{3} c_{jj}(\delta_{ji}-1)x_i\sigma_i + \frac{1}{2}\sum_{i,j=1,i\neq j}^{3} c_{ij}[2\sigma_i\rho\sigma_j - \rho(i\epsilon_{jik}\sigma_k) - (i\epsilon_{jik}\sigma_k)\rho].$$

Another elementary calculation based on (4.20) gives us $\sigma_i\rho + \rho\sigma_i = \sigma_i + x_i\mathbb{1}$, $i = 1, 2, 3$, from which

$$L^*(\rho) = -\,i[H,\rho] + \sum_{i,j=1}^{3} c_{jj}(\delta_{ji}-1)x_i\sigma_i + \frac{1}{2}\sum_{i,j=1,i\neq j}^{3} c_{ij}[2\sigma_i\rho\sigma_j + i\epsilon_{ijk}(\sigma_k + x_k\mathbb{1})].$$

Finally using

$$\sigma_i\rho\sigma_j = \frac{1}{2}(i\epsilon_{ijk}\sigma_k + x_i\sigma_j + x_j\sigma_i + ix_k\epsilon_{ikj}) = \frac{1}{2}i\epsilon_{ijk}(\sigma_k - x_k\mathbb{1}) + \frac{1}{2}(x_i\sigma_j + x_j\sigma_i),$$

we arrive at

$$\begin{aligned} L^*(\rho) = &-\,i[H,\rho] + \sum_{i,j=1}^{3} c_{jj}(\delta_{ji}-1)x_i\sigma_i + \frac{1}{2}\sum_{i,j=1,i\neq j}^{3} c_{ij}[(x_i\sigma_j + x_j\sigma_i) + i\epsilon_{ijk}(\sigma_k - x_k\mathbb{1}) \\ &+ i\epsilon_{ijk}(\sigma_k + x_k\mathbb{1})] \\ = &-\,i[H,\rho] + \sum_{i,j=1}^{3} c_{jj}(\delta_{ji}-1)x_i\sigma_i + \frac{1}{2}\sum_{i,j=1,i\neq j}^{3} c_{ij}[(x_i\sigma_j + x_j\sigma_i) + 2i\epsilon_{ijk}\sigma_k]. \end{aligned}$$

The latter equation in Bloch coordinates reads

$$\dot{x} = (A(h) + \Gamma)x + k \tag{4.21}$$

where $A(h)$ was obtained in (4.6) and

$$\Gamma = \begin{pmatrix} -2(c_{22}+c_{33}) & c_{12}+c_{21} & c_{13}+c_{31} \\ c_{12}+c_{21} & -2(c_{11}+c_{33}) & c_{32}+c_{23} \\ c_{13}+c_{31} & c_{32}+c_{23} & -2(c_{11}+c_{22}) \end{pmatrix}, \tag{4.22}$$

$$k = 2i(c_{23}-c_{32},\ c_{31}-c_{13},\ c_{12}-c_{21})^T = 4(-\operatorname{Im}(c_{23}),\ \operatorname{Im}(c_{13}),\ -\operatorname{Im}(c_{12}))^T. \tag{4.23}$$

Explicitly the equations are

$$\begin{cases} \dot{x_1} = & -2(c_{22}+c_{33})x_1 - (h_{00}-h_{11})x_2 + 2\operatorname{Re}(c_{12})x_2 - 2\operatorname{Im}(h_{01})x_3 + 2\operatorname{Re}(c_{13})x_3 - 4\operatorname{Im}(c_{23}) \\ \dot{x_2} = & (h_{00}-h_{11})x_1 + 2\operatorname{Re}(c_{12})x_1 - 2(c_{11}+c_{33})x_2 - 2\operatorname{Re}(h_{01})x_3 + 2\operatorname{Re}(c_{23})x_3 + 4\operatorname{Im}(c_{13}) \\ \dot{x_3} = & 2\operatorname{Im}(h_{01})x_1 + 2\operatorname{Re}(c_{13})x_1 + 2\operatorname{Re}(h_{01})x_2 + 2\operatorname{Re}(c_{23})x_2 - 2(c_{22}+c_{33})x_3 - 4\operatorname{Im}(c_{12}). \end{cases}$$

Observe that

$$\Gamma = (C + C^T) - 2tr(C)\mathbb{1} = 2\operatorname{Re}(C) - 2tr(C)\mathbb{1}.$$

Thus, the positivity of C translates to a compatibility condition between Γ and k. In fact, let us write C as

$$C = \mathrm{Re}(C) + i\,\mathrm{Im}(C),$$

then the condition $\langle z\,,\, Cz\rangle \geq 0$ reads

$$\langle z\,,\,(\mathrm{Re}(C) + i\,\mathrm{Im}(C))z\rangle = \langle z\,,\,\mathrm{Re}(C)z\rangle + \frac{i}{4}\,\langle z\,,\,k\wedge z\rangle \geq 0 \quad \forall\, z\in\mathbb{C}^3. \tag{4.24}$$

Given that

$$tr(\Gamma) = 2tr(C) - 2tr(C)tr(\mathbb{1}) = -4tr(C),$$

in terms of Γ and k, condition (4.24) reads

$$\langle z\,,\,\Gamma z\rangle - \frac{1}{2}tr(\Gamma)\,\|z\|^2 + \frac{i}{2}\,\langle z\,,\,k\wedge z\rangle \geq 0 \quad \forall\, z\in\mathbb{C}^3, \tag{4.25}$$

which we observe is invariant under rotations

$$\begin{aligned}\langle z\,,\,\Gamma z\rangle - \frac{1}{2}tr(\Gamma)\,\|z\|^2 + \frac{i}{2}\,\langle z\,,\,k\wedge z\rangle =& \\ = \left\langle Rz\,,\,R\Gamma(R^TR)z\right\rangle - \frac{1}{2}tr(R^TR\Gamma)\,\|Rz\|^2 + \frac{i}{2}\,\langle Rz\,,\,R(k\wedge z)\rangle& \\ = \left\langle Rz\,,\,(R\Gamma R^T)Rz\right\rangle - \frac{1}{2}tr(R\Gamma R^T)\,\|Rz\|^2 + \frac{i}{2}\,\langle Rz\,,\,Rk\wedge Rz\rangle\,.&\end{aligned}$$

Remark 4.7. The map

$$C = \mathrm{Re}(C) + i\,\mathrm{Im}(C) \mapsto (\Gamma, k)$$

is invertible from the subset of positive semidefinite matrices into the subset of elements $(\Gamma, k) \in M_{3\times 3}(\mathbb{R}) \times \mathbb{R}^3$ that satisfy (4.25) and such that $\Gamma \leq 0$.
In fact $C \geq 0$ implies that $\mathrm{Re}(C)$ is real symmetric and $\mathrm{Im}(C)$ is real antisymmetric as one can see from

$$\mathrm{Re}(C) = \frac{1}{2}(C + \overline{C}) = \frac{1}{2}(C + C^T), \qquad \mathrm{Im}(C) = \frac{1}{2i}(C - \overline{C}) = \frac{1}{2i}(C - C^T).$$

So first one notice from (4.23) that the map $\mathrm{Im}(C) \mapsto k$ is one to one. Then observe that $\Gamma_{ij} = 2\,\mathrm{Re}(c_{ij})$ for $i < j$ and $\Gamma_{ii} = -2\sum_{j\neq i} c_{jj}$, so

$$2c_{ii} = 2tr(C) + \Gamma_{ii} = -\frac{1}{2}tr(\Gamma) + \Gamma_{ii}.$$

⌟

From the discussion above we conclude that $\mathrm{Re}(C)$ is a symmetric non-negative matrix, hence it diagonalizes (the fact that Γ is symmetric for each C is true only in dimension 2, in general Γ has a mixed symmetry [AL, Sect. 2.4]). Moreover, it diagonalizes simultaneously with Γ. Performing the change of coordinates $y = Rx$ that diagonalize Γ, equation (4.21) become

$$\dot{y} = R(A(h) + \Gamma)R^T y + Rk$$

where $A(h)' = RA(h)R^T$ is skew-symmetric $\Gamma' = R\Gamma R^T$ is diagonal and the pair (Γ', Rk) satisfies (4.25). So, without loss of generality we can always assume $\mathrm{Re}(C)$ diagonal .

In conclusion, the evolution of a generic two-level open system is completely determined by a positive matrix C that we can assume in the form

$$C = \begin{pmatrix} c_{11} & -i\frac{k_3}{4} & i\frac{k_2}{4} \\ i\frac{k_3}{4} & c_{22} & -i\frac{k_1}{4} \\ -i\frac{k_2}{4} & i\frac{k_1}{4} & c_{33} \end{pmatrix} \tag{4.26}$$

and a skew-symmetric matrix $A(u)$

$$A(u) = \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix} \tag{4.27}$$

which corresponds to the generic (traceless) Hamiltonian $H(u) = (1/2)(u_1\sigma_1 + u_2\sigma_2 + u_3\sigma_3)$. Given this choice the Lindblad equation in Bloch coordinates reads

$$\dot{x} = (A(u) + \Gamma)x + k \tag{4.28}$$

where $k = (k_1, k_2, k_3)$ and Γ is the diagonal matrix

$$\begin{pmatrix} -\gamma_1 & 0 & 0 \\ 0 & -\gamma_2 & 0 \\ 0 & 0 & -\gamma_3 \end{pmatrix}, \qquad \text{whose elements are} \qquad \begin{cases} \gamma_1 := 2(c_{22} + c_{33}) \\ \gamma_2 := 2(c_{11} + c_{33}) \\ \gamma_3 := 2(c_{11} + c_{22}). \end{cases} \tag{4.29}$$

It is important to notice that, with these choices, equation (4.25) translates into the following set of inequalities (see [AL, Sect. 2.3.1])

$$\begin{aligned} \gamma_1 + \gamma_2 &\geq \gamma_3 \\ \gamma_2 + \gamma_3 &\geq \gamma_1 \\ \gamma_3 + \gamma_1 &\geq \gamma_2 \\ \gamma_i &\geq |k_i| \qquad i = 1, 2, 3 \\ \gamma_1^2 - (\gamma_2 - \gamma_3)^2 &\geq 4k_3^2 \\ \gamma_2^2 - (\gamma_1 - \gamma_3)^2 &\geq 4k_2^2 \\ \gamma_3^2 - (\gamma_1 - \gamma_2)^2 &\geq 4k_1^2. \end{aligned}$$

In particular these inequalities imply that if $\gamma_1\gamma_2\gamma_3 = 0$ then $k = 0$. This gives us a classification of open systems in two types. We will characterize each subcase in the following sections.

Remark 4.8 (Equilibrium points of the control system). We consider the system (4.28) where u is treated as control parameter. Let $\mathbb{E}$ be the set of points x such that $0 = \langle x\,,\,\dot{x}\rangle$, *i. e.*

$$\mathbb{E} := \{x \mid \langle x\,,\,\Gamma x + k\rangle = 0\} \tag{4.30}$$

Case 1 : $\gamma_1\gamma_2\gamma_3 \neq 0$

The set $\mathbb{E}$ is an ellipsoid. In fact

$$0 = \langle x\,,\,\Gamma x + k\rangle = \left\langle x\,,\,-\Gamma(x + \Gamma^{-1}k)\right\rangle,$$

which can be written as

$$\left\|\sqrt{-\Gamma}x + \frac{1}{2}(-\Gamma)^{-\frac{1}{2}}k\right\|^2 = \left\|\frac{1}{2}(-\Gamma)^{-\frac{1}{2}}k\right\|^2 \tag{4.31}$$

where $\sqrt{-\Gamma} = diag(\sqrt{\gamma_1}, \sqrt{\gamma_2}, \sqrt{\gamma_3})$. The origin always belong to $\mathbb{E}$. Moreover, if $x \in \mathbb{E} \setminus \{0\}$ then there exists $u_x \in \mathbb{R}^3$ such that $(A(u_x) + \Gamma)x + k = 0$. Last equation is in fact equivalent to

$$\langle y\,,\,(A(u_x) + \Gamma)\,x\rangle = \langle y\,,\,-k\rangle \qquad \forall y \in \mathbb{R}^3, \tag{4.32}$$

but it is enough to satisfy (4.32) for $y = e_i$, $i = 1,2,3$, where $\{e_1, e_2, e_3\}$ is an orthonormal basis. If we choose $e_3 = \Gamma x / \|\Gamma x\|$ and e_1, e_2 such that $e_1 \wedge e_2 = e_3$ we obtain the following equations for u_x

$$\begin{aligned}
\left\langle \frac{\Gamma x}{\|\Gamma x\|}\,,\,A(u_x)x\right\rangle &= \left\langle \frac{\Gamma x}{\|\Gamma x\|}\,,\,-k\right\rangle - \|\Gamma x\| \\
\langle e_1\,,\,A(u_x)x\rangle &= \langle e_1\,,\,-k\rangle \\
\langle e_2\,,\,A(u_x)x\rangle &= \langle e_2\,,\,-k\rangle
\end{aligned}$$

which admit always at least one solution.

Case 2 : $\gamma_1\gamma_2\gamma_3 = 0$

The set $\mathbb{E}$ is a line. Assume without loss of generality that $\gamma_3 = 0$ and $\gamma := \gamma_1 = \gamma_2$ (if $\gamma_i = \gamma_j = 0$ then $\gamma_k = 0$ for every triple of different indexes i, j, k).

$$0 = \langle x\,,\,\Gamma x\rangle = -\gamma x_1^2 - \gamma x_2^2 \quad \Leftrightarrow \quad x = (0, 0, x_3).$$

┘

Remark 4.9 (Invariance of the Bloch ball). If $\gamma_1\gamma_2\gamma_3 = 0$ then

$$\langle x\,,\,\dot{x}\rangle = \langle x\,,\,(A(u) + \Gamma)x + k\rangle = \langle x\,,\,\Gamma x\rangle \leq 0.$$

On the other hand, if $\gamma_1\gamma_2\gamma_3 \neq 0$ from the previous Remark we can see that $0 \leq \langle x\,,\,\dot{x}\rangle = \langle x\,,\,\Gamma x + k\rangle$ if and only if

$$\left\|\sqrt{-\Gamma}x + \frac{1}{2}(-\Gamma)^{-\frac{1}{2}}k\right\|^2 \leq \left\|\frac{1}{2}(-\Gamma)^{-\frac{1}{2}}k\right\|^2,$$

which means for x inside the ellipsoid $\mathbb{E}$. Therefore we will show that if x is such that $\langle x\,,\,\dot{x}\rangle = 0$ then $\|x\| \leq 1$, this implies $\mathbb{E} \subset B_1(0)$ and that the ball is invariant. Observe that from the inequality (4.25), choosing $z = e_1(x) + ie_2(x)$ where $e_1(x), e_2(x) \in \mathbb{R}^3$ are orthonormal vectors such that $x/\|x\| = e_1(x) \wedge e_2(x)$, we get

$$\left\langle e_1(x)\,,\,\left(\Gamma - \frac{1}{2}tr\Gamma\right)e_1(x)\right\rangle + \left\langle e_2(x)\,,\,\left(\Gamma - \frac{1}{2}tr\Gamma\right)e_2(x)\right\rangle + \langle e_1(x)\wedge e_2(x)\,,\,k\rangle \geq 0$$

$$-tr\Gamma + \left\langle \frac{x}{\|x\|}\,,\,k\right\rangle \geq \langle e_1(x)\,,\,-\Gamma e_1(x)\rangle + \langle e_2(x)\,,\,-\Gamma e_2(x)\rangle\,.$$

Similarly we could choose $z' = e_2(x) + ie_1(x)$ and this leads to

$$-tr\Gamma - \left\langle \frac{x}{\|x\|}\,,\,k\right\rangle \geq \langle e_1(x)\,,\,-\Gamma e_1(x)\rangle + \langle e_2(x)\,,\,-\Gamma e_2(x)\rangle\,.$$

Since $\langle x\,,\,\Gamma x + k\rangle = 0$

$$-tr\Gamma - \frac{1}{\|x\|}\langle x\,,\,-\Gamma x\rangle \geq \langle e_1(x)\,,\,-\Gamma e_1(x)\rangle + \langle e_2(x)\,,\,-\Gamma e_2(x)\rangle$$

$$-tr\Gamma \geq \langle e_1(x)\,,\,-\Gamma e_1(x)\rangle + \langle e_2(x)\,,\,-\Gamma e_2(x)\rangle + \frac{1}{\|x\|}\langle x\,,\,-\Gamma x\rangle$$

$$-tr\Gamma \geq -tr\Gamma - \left\langle \frac{x}{\|x\|}\,,\,-\Gamma\frac{x}{\|x\|}\right\rangle + \frac{1}{\|x\|}\langle x\,,\,-\Gamma x\rangle$$

therefore

$$\left\langle \frac{x}{\|x\|}\,,\,-\Gamma\frac{x}{\|x\|}\right\rangle \geq \left\langle \frac{x}{\|x\|}\,,\,-\Gamma\frac{x}{\|x\|}\right\rangle\|x\| \qquad \Leftrightarrow \qquad 1 \geq \|x\|\,.$$

⌟

Remark 4.10 (Bloch equations)**.** Following [GKS], we want to show that there exists an abstract characterization of the vectors k compatible with each matrix Γ in the form (4.29).

Let $k = -(A(u) + \Gamma)k_0$ where $k_0 \in \mathcal{K}_\Gamma$, a subset of $\mathbb{R}^3$ defined as follows

$$\mathcal{K}_\Gamma = \left\{ y \in \mathbb{R}^3 \mid \inf_{\|x\|=1}\langle x\,,\,-\Gamma(x-y) + y\wedge u\rangle \geq 0\right\},$$

Then equation (4.28) writes

$$\dot{x} = (A(u)+\Gamma)x + k = (A(u)+\Gamma)(x-k_0) = u\wedge(x-k_0) + \Gamma(x-k_0),$$

which is commonly known as *Bloch equation.* One observes immediately that if $k_0 \in \mathcal{K}_\Gamma$ then the unit ball is invariant under the dynamics, in fact

$$0 \leq \inf_{\|x\|=1}\langle x\,,\,-\Gamma(x-k_0) + k_0\wedge u\rangle = \inf_{\|x\|=1} -\langle x\,,\,(A(u)+\Gamma)(x-k_0)\rangle = \inf_{\|x\|=1} -\langle x\,,\,\dot{x}\rangle\,.$$

Moreover, if $k \in \mathcal{K}_\Gamma$ then $(\Gamma,\ k)$ satisfy the inequality (4.25). ⌟

To conclude this section we illustrate some examples of open systems which are physically interesting.

Example 4.11 (Lindblad eq. rotationally symmetric around the axis of the magnetic field)**.** Let us consider the equation (3.35) with

$$H(0) = \frac{1}{2}E\sigma_3, \quad L_1 = \sqrt{b_+}\sigma_+, \quad L_2 = \sqrt{b_-}\sigma_-, \quad L_3 = \sqrt{a}\sigma_3, \qquad a, b_+, b_- \geq 0$$

where $\sigma_\pm = 1/2(\sigma_1 \pm i\sigma_2)$, then

$$\dot{\rho} = \frac{1}{2}E(-y\sigma_1+x\sigma_2)+a(-x\sigma_1-y\sigma_2)+b_+(\sigma_3-\frac{1}{2}x\sigma_1-\frac{1}{2}y\sigma_2-z\sigma_3)+b_-(-\sigma_3-\frac{1}{2}y\sigma_1-\frac{1}{2}y\sigma_2-z\sigma_3)$$

that in Bloch coordinates reads

$$\begin{aligned}
\dot{x}_1 &= -(4a + b_+ + b_-)x_1 - Ex_2 \\
\dot{x}_2 &= Ex_1 - (4a + b_+ + b_-)x_2 \\
\dot{x}_3 &= -2(b_+ + b_-)x_3 + 2(b_+ - b_-)
\end{aligned} \tag{4.33}$$

which corresponds to

$$C = \begin{pmatrix} b_+ + b_- & -i\frac{b_+-b_-}{2} & 0 \\ i\frac{b_+-b_-}{2} & b_+ + b_- & 0 \\ 0 & 0 & 4a \end{pmatrix}.$$

Define

$$\Gamma = 4a + b_+ + b_- \qquad \gamma_+ = 2(b_+ + b_-) \qquad \gamma_- = 2(b_+ - b_-),$$

then

$$2\Gamma \geq \gamma_+ \geq |\gamma_-|\,.$$

Observe that if $\gamma_+ \neq 0$

$$\dot{x}_3 = -\gamma_+\left(x_3 - \frac{\gamma_-}{\gamma_+}\right),$$

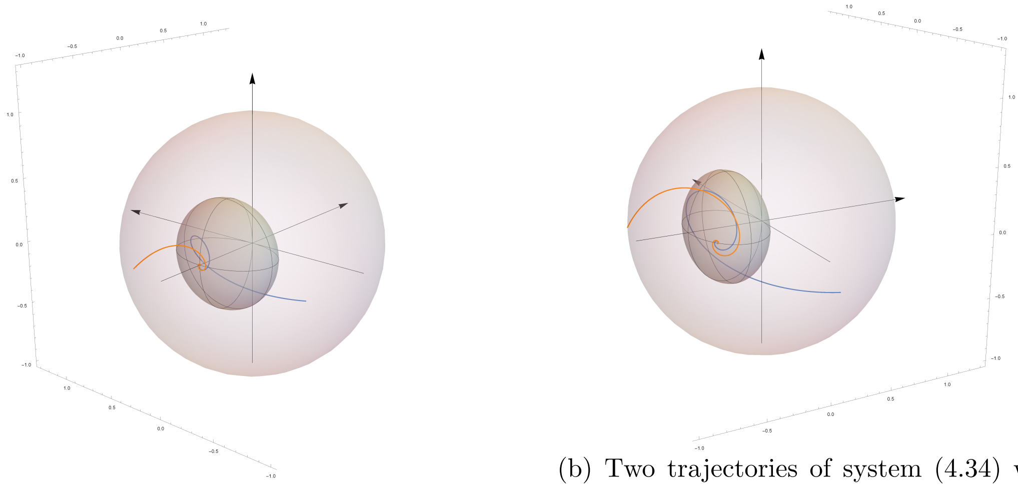
so the system has a unique fixed point $x_c = (0, 0, \frac{\gamma_-}{\gamma_+})$ with $\frac{\gamma_-}{\gamma_+} \in [-1, 1]$ (see Fig.4.2a). Otherwise, if $\gamma_+ = 0$ the entire x_3-axis consist of fixed points. The term L_3 causes a contraction on the x_1x_2-plane, the term L_1 induces a transition toward the point $(0, 0, 1)$ *i.e.* if $b_+ > 0$ and $b_- = 0$ then $\gamma_-/\gamma_+ = 1$. Conversely, L_2 induces a transition toward the point $(0, 0, -1)$. If we add to the Hamiltonian the control operators σ_1, σ_2

$$H(u_1, u_2) = \frac{1}{2}\Big(E\sigma_3 + u_1\sigma_1 + u_2\sigma_2\Big)$$

the equations becomes

$$\begin{aligned}
\dot{x}_1 &= -(4a + b_+ + b_-)x_1 - Ex_2 + u_2x_3 \\
\dot{x}_2 &= Ex_1 - (4a + b_+ + b_-)x_2 - u_1x_3 \\
\dot{x}_3 &= -u_2x_1 + u_1x_2 - 2(b_+ + b_-)x_3 + 2(b_+ - b_-).
\end{aligned} \tag{4.34}$$

Figure 4.2



(a) Two trajectories of system (4.33) with different initial points converging towards $(0, 0, \gamma_-/\gamma_+)$. Parameters are $a = 0, b_+ = 1, b_- = 4, E = 5$. In trasparency the ellipsoid (4.36).

(b) Two trajectories of system (4.34) with different initial points converging towards a point of the ellipsoid (4.36). The coordinates of the equilibrium point are given by (4.35) where parameters are $a = 0, b_+ = 1, b_- = 4, E = 5$ and $u_1 = 3, u_2 = 1.5$.

The coordinates of the fixed point are

$$\begin{aligned} x_1 =& \frac{\gamma_-}{\gamma_+ + \Gamma c_{E,\Gamma}(u_1^2 + u_2^2)} c_{E,\Gamma}(Eu_1 + \Gamma u_2) \\ x_2 =& \frac{\gamma_-}{\gamma_+ + \Gamma c_{E,\Gamma}(u_1^2 + u_2^2)} c_{E,\Gamma}(Eu_2 - \Gamma u_1) \\ x_3 =& \frac{\gamma_-}{\gamma_+ + \Gamma c_{E,\Gamma}(u_1^2 + u_2^2)} \qquad \text{where} \quad c_{E,\Gamma} = \frac{1}{E^2 + \Gamma^2}, \end{aligned} \tag{4.35}$$

which corresponds to a point of the surface

$$\Gamma(x_1^2 + x_2^2) + \gamma_+ \left(x_3 - \frac{\gamma_-}{2\gamma_+} \right)^2 = \frac{\gamma_-^2}{4\gamma_+}, \tag{4.36}$$

see Fig.4.2a,4.2b. Notice that the drift term does not affect the set of equilibrium point of the system.

With this notation of a two-level system spontaneously decaying from the excited state $|1\rangle$ to the ground state $|0\rangle$ while emitting a photon is given by

$$H(0) = \frac{1}{2} E\sigma_3, \qquad L_1 = \sqrt{b_-}\sigma_-.$$

In fact, the evolution of $|1\rangle\langle 1|$, which corresponds to $(0, 0, 1)$ in Bloch coordinates is $x_1(t) = x_2(t) = 0$, $x_3(t) = 2e^{-2b_-} - 1$. As noticed before every initial state converges toward $|0\rangle\langle 0|$ (see Fig.4.3). ⌟

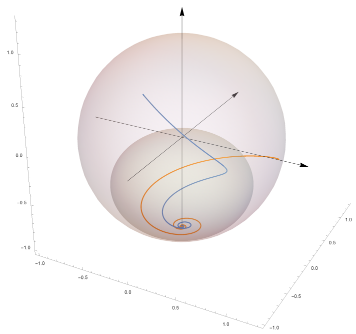


Figure 4.3: Decaying system. Two different trajectories of system (4.33) with $E = 1, a = 0, b_+ = 0, b_- = 1$. In transparency the ellipsoid (4.36).

4.3.1 Results of geometric control theory for open quantum systems

Geometric control tools for affine systems, presented in Section 2.1.4 were applied to finite dimensional open quantum system in the vector of coherence formulation. In particular in the work of Altafini [Alt], the case of two-level quantum system is considered in detail. We state here the main result of that paper.

Theorem 4.12 **(** [Alt, Thm. 5] **).** *Assume that the system*

$$i\frac{d}{dt}\psi = H(u)\psi = \left(H(0) + \sum_{k=1}^{m} u_k H_k\right)\psi, \qquad \psi \in \mathbb{C}^2$$

with $u \in U \subset \mathbb{R}^m$ *and* $-iH_k \in \mathfrak{su}(2)$ *is controllable. Then for a two-level system* (4.28) *we have:*

(a) *the system* (4.28) *is accessible in* $\overline{B_1(0)}$*,*

(b) *the system* (4.28) *is never small-time nor finite-time controllable in* $\overline{B_1(0)}$ *for* $\Gamma \neq 0$*.*

Under Assumption 4.8 the system

$$i\frac{d}{dt}\psi = H(u)\psi = \frac{1}{2}(E\sigma_3 + u_1\sigma_1 + u_2\sigma_2)\psi$$

is controllable by Theorem 2.24, so the previous results applies to our analysis. The result is partially negative, because controllability cannot be achieved on the whole Bloch ball. However, as in the case of closed system we want to see if adiabatic theory can be useful to produce robust controllability technique (on a smaller set).

4.4 Geometric Singular Perturbation

In this section we will recall briefly the main technique used in our analysis.

For closed systems the dynamics preserve the purity of the states, which also means that the equilibrium points of the system are stable but not asymptotically stable and every state follows a periodic orbit. In fact, by choosing a suitable control, one is able to modify these orbits in order to steer the system between states with equal purity. Similarly, for open systems, we saw in Remark 4.8 that exists a set of equilibrium points which depends on the Hamiltonian $H(u)$, and so on the control u. However, in contrast with the closed systems, we will show that every state converge towards the equilibrium set. Moreover, if we control the system adiabatically, once the state approaches the surface (4.30) it will follow the instantaneous critical point. We will show this by means of geometric singular perturbation techniques.

Consider the control equation

$$\dot{y} = g(y, u) \qquad y \in \mathbb{R}^n,\ u \in \mathbb{R}^m \tag{4.37}$$

and suppose that there exists a submanifold $\mathcal{E}$ of $\mathbb{R}^n$ such that

$$0 = g(y, u) \quad \forall y \in \mathcal{E}.$$

If $\operatorname{rank}(\frac{\partial g}{\partial y}) = n$ and $\operatorname{rank}(\frac{\partial g}{\partial u}) = k \leq m$ the manifold $\mathcal{E}$ admits a parametrization in terms of the control variable u given by the Implicit Function Theorem. We will denote this parametrization $h = h(u)$, so

$$0 = g(h(u), u) \quad \forall u \in \mathbb{R}^m.$$

Now choose a path in the control space $u_* : [0, 1] \to \mathbb{R}^m$ and consider the slowed system

$$y' = g(y, u_*(\varepsilon\tau)) \qquad \varepsilon \ll 1. \tag{4.38}$$

This time dependent problem could be seen as a multiscale system in which the time plays the role of the slow variable.

Introducing the variable $x := \varepsilon\tau$, we can rewrite (4.38)

$$\begin{cases} x' = \varepsilon & x(0) = 0 \\ y' = g(y, u_*(x)) & y(0) = y_0, \end{cases} \tag{4.39}$$

we should also consider the time scaling $t = \varepsilon\tau$ and the system

$$\begin{cases} \dot{x} = 1 & x(0) = 0 \\ \varepsilon\dot{y} = g(y, u_*(x)) & y(0) = y_0, \end{cases} \tag{4.40}$$

where we denoted with $\dot{}$ the derivative with respect to t and with $'$ the derivative with respect to τ.

In the following we will use the notation (4.39.ε_0),(4.40.ε_0) to denote (4.39),(4.40) for fixed $\varepsilon = \varepsilon_0$. We define also $y_c(x) := h(u_*(x))$ to not overweight the notation.

Remark 4.13. Observe that the manifold $\mathcal{E}' = \{(x, h(u_*(x))),\ x \in [0,1]\}$ consists entirely of critical points for the system (4.39.0), while (4.39.ε) has no critical point for $\varepsilon \neq 0$. This singularity in the nature of the dynamics of (4.39) is the characterizing feature of the singular perturbations problems. Instead, $\mathcal{E}'$ is the support of

$$(t, y_c(t)) = (t, h(u_*(t))) \quad t \in [0,1],$$

which is the unique solution of (4.40.0) with initial condition $y_0 = h(u_*(0)) = y_c(0)$. ⌟

We want to show that for ε sufficiently small and for $y_0 \in B_\rho(y_c(0))$, with ρ small enough, the solution $y(t,\varepsilon)$ of (4.40.ε) with initial condition y_0 is definitively near the solution $y_c(t)$, *i. e.*

$$y(t,\varepsilon) - y_c(t) = O(\varepsilon) \quad t \in [t_b, 1],$$

with $0 < t_b < 1$.

It is more convenient to study the system after the change of coordinates $\eta = y - h(u_*(x))$.

$$\begin{cases} x' = \varepsilon & x(0) = 0 \\ \eta' = g(\eta + h(u_*(x)), u_*(x)) - \varepsilon \frac{\partial h}{\partial u}(u_*(x)) u_*'(x) & \eta(0) = y_0 - h(u_*(0)) \end{cases} \tag{4.41}$$

$$\begin{cases} \dot{x} = 1 & x(0) = 0 \\ \varepsilon \dot{\eta} = g(\eta + h(u_*(x)), u_*(x)) - \varepsilon \frac{\partial h}{\partial u}(u_*(x)) \dot{u}_*(x) & \eta(0) = y_0 - h(u_*(0)) \end{cases} \tag{4.42}$$

where $\dot{u}_*, u_*'$ denote the same function which is the time derivative of u_*. The path of critical points is now $\{(x,0),\ x \in [0,1]\}$.

Theorem 4.14 (Tychonoff). *Consider the singular perturbation problem*

$$\dot{x} = f(t,x,y,\varepsilon), \qquad x(t_0) = \mu(\varepsilon) \tag{4.43}$$

$$\varepsilon \dot{y} = g(t,x,y,\varepsilon), \qquad y(t_0) = \nu(\varepsilon) \tag{4.44}$$

and let $y = h(t,x)$ be an isolated root of $0 = g(t,x,y,0)$. Assume that the following conditions are satisfied for all

$$(t, x, y - h(t,x), \varepsilon) \in [0, t_1] \times D_x \times D_y \times [0, \varepsilon_0]$$

for some domains $D_x \subset \mathbb{R}^q$ and $D_y \subset \mathbb{R}^n$, in which D_x is convex and contains the origin:

i) The functions f, g, $\partial f/\partial(x,y,\varepsilon)$, $\partial g/\partial(t,x,y,\varepsilon)$ are continuous; the functions $h(t,x)$ and $\partial g(t,x,y,0)/\partial y$ have continuous first partial derivatives with respect to their arguments; the initial data $\mu(\varepsilon)$ and $\nu(\varepsilon)$ are smooth functions of ε.

ii) The reduced problem

$$\dot{x} = f(t, x, h(t, x), 0), \qquad x(t_0) = \mu(0) \tag{4.45}$$

has a unique solution $\bar{x}(t) \in S$*, for* $t \in [t_0, t_1]$*, where* S *is a compact subset of* D_x*.*

iii) The origin is an exponentially stable equilibrium point of the boundary-layer model

$$\frac{\partial \eta}{\partial \tau} = g(\hat{t}, \hat{x}, \eta + h(\hat{t}, \hat{x}), 0), \qquad (\hat{t}, \hat{x}) \in [0, t_1] \times D_x \tag{4.46}$$

uniformly in $(\hat{t}, \hat{x})$*; let* $\mathcal{R}_y \subset D_y$ *be the region of attraction of*

$$\frac{\partial \eta}{\partial \tau} = g(t_0, \mu(0), \eta + h(t_0, \mu(0)), 0), \qquad \eta(0) = \nu(0) - h(t_0, \mu(0)) \tag{4.47}$$

and $\Omega_y \subset \mathcal{R}_y$ *a compact set.*

There exists a positive constant ε^* *such that for all* $\nu(0) - h(t_0, \mu(0)) \in \Omega_y$ *and* $0 < \varepsilon < \varepsilon^*$*, the singular perturbation problem* (4.43) *has a unique solution* $x(t, \varepsilon), y(t, \varepsilon)$ *on* $[t_0, t_1]$*, and*

$$x(t, \varepsilon) - \bar{x}(t) = O(\varepsilon)$$
$$y(t, \varepsilon) - h(t, \bar{x}(t)) - \hat{\eta}(t/\varepsilon) = O(\varepsilon)$$

hold uniformly for $t \in [t_0, t_1]$*, where* $\hat{\eta}$ *is the solution of the boundary-layer model* (4.46)*.*

Moreover, given any $t_b > t_0$*, there is* $\varepsilon^{**} \leq \varepsilon^*$ *such that*

$$y(t, \varepsilon) - h(t, \bar{x}(t)) = O(\varepsilon)$$

holds uniformly for $t \in [t_b, t_1]$ *whenever* $\varepsilon < \varepsilon^{**}$*.*

4.5 Slowly driven two-level open systems

In this Section we apply the geometric singular perturbation theory to the specific case of a two-level quantum open system, obtaining a result (Prop. 4.15) in the generic case $\gamma_1\gamma_2\gamma_3 \neq 0$. The idea is to obtain a result analogous to Theorem 4.4 or Corollary 4.6 for open systems.

Consider equation (4.28) where $u : [0, 1] \to \mathbb{R}^3$ is a fixed time dependent control function which varies slowly, *i. e.*

$$y' = (A(u(\varepsilon\tau)) + \Gamma)y + k, \qquad \tau \in [0, 1/\varepsilon], \quad \varepsilon \ll 1. \tag{4.48}$$

As we saw before in Section 4.3 this equation describes the dynamics of a two-level open quantum system which is slowly driven. Equivalently, we can consider the equation

$$\varepsilon\dot{y} = (A(u(t)) + \Gamma)y + k, \qquad t \in [0, 1], \quad \varepsilon \ll 1. \tag{4.49}$$

Case 1 : $\gamma_1\gamma_2\gamma_3 \neq 0$

Γ is negative definite and so is $A(u)+\Gamma$. In fact,

$$\langle y\,,\,(A(u)+\Gamma)y\rangle = \langle y\,,\,\Gamma y\rangle \leq 0,$$

then $0 \notin \sigma(A(u)+\Gamma)$. Therefore for each $u \in \mathbb{R}^3$ exists a unique fixed point of the dynamics which is $y_c(u) = -(A(u)+\Gamma)^{-1}k$. Linearizing around this point and performing the coordinates change $\eta = y - y_c(u)$ the system reads

$$\eta' = (A(u)+\Gamma)\eta - \varepsilon\frac{\partial y_c}{\partial u}(u(\varepsilon\tau))u'(\varepsilon\tau).$$

We observe that the origin is uniformly exponentially stable for

$$\eta' = (A(\hat{u})+\Gamma)\eta, \qquad \forall \hat{u} \in \{u(t) \mid t \in [0,1]\}$$

because, since $\hat{u}$ varies in a compact set

$$\sup_{\hat{u}} \sup_{\|y\|=1} \langle y\,,\,(A(\hat{u})+\Gamma)y\rangle = \max_{\|y\|=1} \langle y\,,\,\Gamma y\rangle < 0.$$

In conclusion Tychonoff theorem holds for this system (see Fig.4.4).

Proposition 4.15. *Consider the system* (4.49) *in the case* $\Gamma < 0$. *Let* $u : [0,1] \to \mathbb{R}^3$ *be a* $\mathcal{C}^1$ *control function and* $y_0 \in \overline{B_1(0)}$ *an arbitrarily initial data. For each* $t_b \in [0,1]$ *there exists* $\varepsilon^{**} > 0$ *such that for all* $\varepsilon < \varepsilon^{**}$ *the solution* $y_\varepsilon(t)$ *of equation* (4.49) *is such that*

$$\|y_\varepsilon(t) - y_c(u(t))\| = O(\varepsilon)$$

for all $t \in [t_b, 1]$, *where*

$$y_c(u) = -(A(u)+\Gamma)^{-1}k.$$

Case 2 : $\gamma_1\gamma_2\gamma_3 = 0$

Assume without loss of generality that $\gamma_3 = 0$ and $\gamma := \gamma_1 = \gamma_2$ (if $\gamma_i = \gamma_j = 0$ then $\gamma_k = 0$ for every triple of different indexes i,j,k). We observe that $(A(u)+\Gamma)y = 0$ has only the trivial solution iff

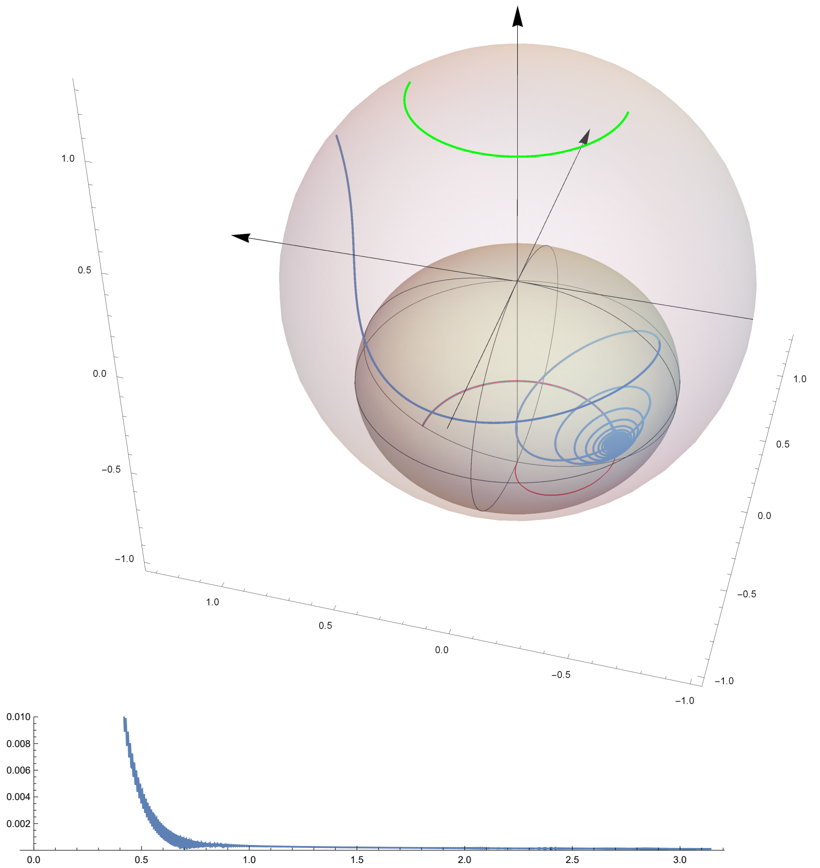
$$0 \notin \sigma(A(u)+\Gamma) \quad \Leftrightarrow \quad det(A(u)+\Gamma) \neq 0 \quad \Leftrightarrow \quad 4\gamma(u_1^2+u_2^2) \neq 0,$$

moreover

$$det(A(u)+\Gamma-\lambda\mathbb{1}) \geq 4\gamma(u_1^2+u_2^2) \qquad \text{if } \lambda \geq 0.$$

Therefore if $u_1^2+u_2^2 \neq 0$ the system has 0 as unique fixed point and $\sigma(A(u)+\Gamma) \subset \{z \mid \mathrm{Re}(z) < 0\}$, then it converges toward the origin. If $u_1 = u_2 = 0$ the entire y_3-axis consists of fixed points and the equation for y_3 decouples, so the system converges toward the point $(0,0,y_3(0))$.

Figure 4.4: Trajectory of system (4.34) (blue line) with control $u_1(t) = -t\sin(t)/\vartheta$, $u_2(t) = -t\sin(t)/\vartheta$. Parameters are $a = 0, b_+ = 0, b_- = 0.01, E = 2, \vartheta = \pi$ and $\varepsilon = 0.001$. In green the trace of $u_E/\|u_E\|$. In red the instantaneous equilibrium $y_c(u_E(t))$ given by (4.35). Below the plot of the distance between the blue and red trajectories.



In this case we can prove that the set of reachable points for $t \to \infty$ coincides with a compact subinterval of the segment $\{(0, 0, s) \mid s \in [0, 1]\}$. Indeed, assume (without lost of generality) that the initial state of the system lies in the plane $\{y = 0\}$, namely $y_0 = (y_1(0), 0, y_3(0))$, than we choose to apply a control of the form $u = (0, u_2, 0)$. Therefore the system reduces to

$$\begin{aligned}\dot{y}_1 &= -\gamma y_1 + 2u_2 y_3\\ \dot{y}_2 &= 0\\ \dot{y}_3 &= -2u_2 y_1.\end{aligned}$$

Solving the equations for y_1, y_3 under the constraint $4|u_2| > \gamma$, we obtain

$$\begin{pmatrix} y_1(t) \\ y_3(t) \end{pmatrix} = e^{-\gamma t/2} \begin{pmatrix} \cos(\omega t) + \frac{\gamma}{2\omega}\sin(\omega t) & -\frac{2u_2}{\omega}\sin(\omega t) \\ \frac{2u_2}{\omega}\sin(\omega t) & \cos(\omega t) - \frac{\gamma}{2\omega}\sin(\omega t) \end{pmatrix} \begin{pmatrix} y_1(0) \\ y_3(0) \end{pmatrix} \tag{4.50}$$

where the angular velocity $\omega := \sqrt{4u_2^2 - \gamma^2/4}$. So, one can see that

$$z_+ := \sup_{t\geq 0} y_3(t) = \sup_{t\geq 0} e^{-\gamma t/2}\left(\frac{2u_2}{\omega}\sin(\omega t) y_1(0) + \cos(\omega t) y_3(0) - \frac{\gamma}{2\omega}\sin(\omega t) y_3(0)\right) \tag{4.51}$$

and

$$z_- := \max_{t\geq 0} y_3(t) = \max_{t\geq 0} e^{-\gamma t/2}\left(\frac{2u_2}{\omega}\sin(\omega t) y_1(0) + \cos(\omega t) y_3(0) - \frac{\gamma}{2\omega}\sin(\omega t) y_3(0)\right) \tag{4.52}$$

are assumed for some finite value of t, namely t_+ and t_- (the function in the above parenthesis is periodic, so $y_3(t)$ assume is max and min value in $[0, 2\pi/\omega]$). Observe that for $\gamma = 0$ one has $\|y_0\| = \sup_{t\geq 0} y_3(t) = -\inf_{t\geq 0} y_3(t)$. Thus for every value $y_3^f \in [z_-, z_+]$ exists a time $t_f \in [0, \max\{t_-, t_+\}]$ such that $y_3(t_f) = y_3^f$ if $u(t) = (0, u_2, 0)$ for $t \in [0, t_f]$. Now defining $u(t) = (0, 0, E)$ for $t > t_f$ the systems converges exponentially fast to $(0, 0, y_3^f)$.

The result we obtained is partially satisfying. However, it could be a first step to study more general models of open quantum system. In particular, the main issue of our approach is the effectiveness of the Lindblad equation in the description of adiabatic open quantum systems. As we have seen in our analysis, the dynamics described by (4.28) is almost always a motion that converges exponentially fast to a unique equilibrium. In this framework the adiabatic theory cannot be effective because the convergence rate is accelerated when the time is slowed.

In literature, between the approaches to adiabatic open quantum systems, we are interested in the works of Lidar et al. [Lid$_1$],[Lid$_2$].In those papers the authors develop a physical model where to any variation of the Hamiltonian it corresponds a variation of the Lindblad operators. This is due to the fact that the dissipation/decoherence of the system occurs in the instantaneous energy eigenbasis.

Chapter 5

Controllability of spin-boson models

5.1 Introduction

In quantum mechanics one names spin-boson model an Hamiltonian that describe the interaction of a finite dimensional system, usually called spin, with one bosonic mode of a field. These type of models, arise in many different physical contexts, such as cavity QED, quantum optics and magnetic resonance. Two important spin boson models are the Rabi model and the Jaynes-Cummings model, which are also some of firsts ever introduced [Ra_1][Ra_2][JaCu].

In the field of quantum control the study of these models has recently begun. Their interest lies in the fact that are some of the simplest infinite dimensional systems. More precisely, their simplicity could be seen at the level of symmetries. In general, symmetries are an obstacle to controllability, because they imply the existence of invariant subspaces for the system dynamics. Therefore, the external control must necessarily break all the symmetries of the unperturbed system in order to achieve controllability. There are highly symmetric systems that cannot be controlled, *e.g.* the harmonic oscillator, which was proved to be uncontrollable by Mirrahimi and Rouchon [MiRo]. On the other hand, controllability was proved for the trapped ion model [EbLa][ErPu] and more recently for the Rabi Hamiltonian [BMPS]. So, one may wonder whether more symmetric models are controllable. The Jaynes-Cummings model in particular, has an additional conserved quantity than the Rabi model, namely the total number of excitations, and his controllability is an interesting matter. The question was posed by Rouchon [Ro] some years ago.

In this chapter we provide an answer to this question. In Theorem 5.1 we prove that the Jaynes-Cummings model is controllable for almost every value of the interaction parameter, *i.e.* up to a set S of measure zero. Then, in Theorem 5.2 we characterize the points of S as solutions to explicit equations. Our technique exploits three ingredients: the integrability of the model [JaCu]; a study of the resonances of the spectrum which allows to invoke the controllability criterion 2.40 presented in Sect. 2.2.3; a detailed analysis of the resonance condition.

As for the future perspective, an interesting task would be provide a constructive control method for the Jaynes-Cummings model. In this chapter, we make an explicit contruction of a non-resonant chain of connectedness (see Def.2.39). However, as far as we know, this fact implies the approximate controllability of the system only via a theorem [BCCS] whose proof is not constructive. As for a related problem, is known that the Jaynes-Cummings Hamiltonian (JCH) could be seen as an approximation of the Rabi Hamiltonian in an appropriate regime, as discussed by [Ro]. A rigorous mathematical proof of the latter claim could provide a deeper understanding of these two models.

5.2 The Jaynes-Cummings model

5.2.1 Definition of the model

In the Hilbert space $\mathcal{H} = L^2(\mathbb{R}) \otimes \mathbb{C}^2$ we consider the Schrödinger equation

$$i\hbar\,\partial_t \psi = H_{\mathrm{JC}}\psi$$

with Hamiltonian operator (JC Hamiltonian)

$$H_{\mathrm{JC}} \equiv H_{\mathrm{JC}}(g) = \frac{\hbar\omega}{2}(X^2 + P^2) \otimes \mathbb{1} + \frac{\hbar\Omega}{2}\mathbb{1} \otimes \sigma_z + \frac{\hbar g}{\sqrt{2}}(X \otimes \sigma_x - P \otimes \sigma_y) \tag{5.1}$$

where $\omega, \Omega \in \mathbb{R}_+$ and $g \in \mathbb{R}$ are constants, X is the position operator, *i. e.* $X\psi(x) = x\psi(x)$, and $P = -i\partial_x$. The operators $\sigma_x, \sigma_y, \sigma_z$ acting on $\mathbb{C}^2$ are given by the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The quantity $\Delta := \Omega - \omega$ is called *detuning* and measures the difference between the energy quanta of the two subsystems corresponding to the factorization of the Hilbert space.

By introducing the *creation* and *annihilation* operators for the harmonic oscillator, defined as usual by

$$a^\dagger = \frac{1}{\sqrt{2}}(X - iP) \qquad a = \frac{1}{\sqrt{2}}(X + iP), \tag{5.2}$$

and the *lowering* and *raising* operators

$$\sigma = \frac{1}{2}(\sigma_x - i\sigma_y) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \sigma^\dagger = \frac{1}{2}(\sigma_x + i\sigma_y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \tag{5.3}$$

the JC Hamiltonian (omitting tensors) reads

$$H_{\mathrm{JC}} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) + \frac{\hbar\Omega}{2}\sigma_z + \frac{\hbar g}{2}\left(a\sigma^\dagger + a^\dagger\sigma\right).$$

The popularity of this model relies on the fact that it is presumably the simplest model describing a two-level system interacting with a distinguished mode of a quantized bosonic field (the harmonic oscillator). It was introduced by Jaynes and Cummings in 1963 as an approximation to the Rabi Hamitonian

$$H_{\mathrm{R}} = H_{\mathrm{R}}(g) = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) + \frac{\hbar\Omega}{2}\sigma_z + \frac{\hbar g}{2}(a + a^\dagger)(\sigma + \sigma^\dagger). \tag{5.4}$$

The latter traces back to the early works of Rabi on spin-boson interactions [Ra_1, Ra_2], while in [JaCu] Jaynes and Cummings derived both (5.1) and (5.4) from a more fundamental model of non-relativistic Quantum Electro Dynamics (QED).

Nowadays, both Hamiltonians (5.1) and (5.4) are widely used in several fields of physics. Among them, one of the most interesting is cavity QED. In typical cavity QED experiments, atoms move across a cavity that stores a mode of a quantized electromagnetic field. During their passage in the cavity the atoms interact with the field: the Hamiltonians (5.1) and (5.4) aim to describe the interaction between the atom and the cavity, in different regimes [BRH, HaRa]. More precisely, (5.1) and (5.4) can be heuristically derived from a mathematical model of non-relativistic QED, the Pauli-Fierz model [Sp]; we refer to [Co_1] and the more recent [BMPS] for a discussion of this derivation.

The approximation consisting in replacing (5.4) with (5.1) is commonly known as the *rotating wave approximation* (or *secular approximation*), and is valid under the assumptions [Ro]

$$|\Delta| \ll \omega, \Omega \qquad g \ll \omega, \Omega \tag{5.5}$$

which mean that the harmonic oscillator and the two-level system are almost in resonance and the coupling strength is small compared to the typical energy scale. Heuristically, in this regime the probability of creating or destroying two excitations is negligible, thus one can remove the so-called *counter-rotating* terms $a^\dagger\sigma^\dagger$ and $a\sigma$ in (5.4) to obtain (5.1). More precisely, the justification of this approximation relies on separation of time scales, a well-know phenomenon in several areas of physics [PST_1, PST_2, PSpT]. Indeed, by rewriting the dynamics generated by (5.4) in the interaction picture with respect to

$$H_0 := H_{\mathrm{JC}}(0) = H_{\mathrm{R}}(0) = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) + \frac{\hbar\Omega}{2}\sigma_z, \tag{5.6}$$

one gets

$$\begin{aligned} e^{iH_0 t/\hbar}(H_{\mathrm{R}} - H_0)e^{-iH_0 t/\hbar} = & \frac{g}{2} \left(e^{-i(\Omega-\omega)t} a^\dagger \sigma + e^{i(\Omega-\omega)t} a \sigma^\dagger \right) \\ & + \frac{g}{2} \left(e^{-i(\Omega+\omega)t} a \sigma + e^{i(\Omega+\omega)t} a^\dagger \sigma^\dagger \right). \end{aligned} \tag{5.7}$$

One notices that the terms $a^\dagger\sigma$, $a\sigma^\dagger$ oscillate with frequency $|\omega - \Omega|$, while $a^\dagger\sigma^\dagger$, $a\sigma$ oscillate on the faster scale $\omega + \Omega$, so that the latter average to zero on the long time scale $|\omega - \Omega|^{-1}$. While the physical principles leading from (5.4) to (5.1) are clear, as we mentioned in the Introduction a rigorous mathematical justification for this approximation seems absent from the literature, as recently remarked in [Ro].

We use hereafter Hartree units, so that in particular $\hbar = 1$.

5.2.2 Spectrum of the JC Hamiltonian

While apparently similar, the JC Hamiltonian (5.1) and the Rabi Hamiltonian (5.4) are considerably different from the viewpoint of symmetries.

As operators, they are both infinitesimally small perturbation, in the sense of Kato [Ka], of the free Hamiltonian H_0 (defined in (5.6)), which has compact resolvent. Eigenvalues and eigenvectors of H_0 are easily obtained by tensorization, starting from the eigenvectors $\{e_1, e_{-1}\}$ of σ_z and the standard basis of $L^2(\mathbb{R})$ given by real eigenfunctions of $a^\dagger a$, namely the Hermite functions

$$|n\rangle = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} h_n(x)\, e^{-\frac{x^2}{2}}, \qquad n \in \mathbb{N}, \tag{5.8}$$

where h_n is the n-th Hermite polynomial. As well known, they satisfy

$$a^\dagger a\,|n\rangle = n\,|n\rangle\,, \qquad a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,, \qquad a\,|n\rangle = \sqrt{n}\,|n-1\rangle\,. \tag{5.9}$$

Then

$$H_0\,|n\rangle \otimes e_1 = E^0_{(n,1)}\,|n\rangle \otimes e_1, \quad H_0\,|n\rangle \otimes e_{-1} = E^0_{(n,-1)}\,|n\rangle \otimes e_{-1}$$

with

$$E^0_{(n,s)} = \omega(n + \frac{1}{2}) + s\frac{\Omega}{2}, \qquad n \in \mathbb{N},\ s \in \{-1, 1\}.$$

Since $(a + a^\dagger)\sigma_x$ and $(a\sigma^\dagger + a^\dagger\sigma)$ are infinitesimally H_0-bounded, by standard perturbation theory $\{H_{\mathrm{JC}}(g)\}_{g\in\mathbb{C}}$ and $\{H_{\mathrm{R}}(g)\}_{g\in\mathbb{C}}$ are analytic families (of type A) of operators with compact resolvent [Ka, Section VII.2]. Therefore, by Kato-Rellich theorem, the eingenvalues and eigenvectors of $H_{\mathrm{JC}}(g)$ and $H_{\mathrm{R}}(g)$ are analytic functions of the parameter g. Coefficients of the series expansion of eingenvalues and eigenvectors can be explicitly computed [RS$_4$].

From the viewpoint of symmetries, it is crucial to notice that, as compared to the Rabi Hamiltonian, the JC Hamiltonian has an additional conserved quantity, namely the total number of excitations, represented by the operator $C = a^\dagger a + \sigma^\dagger \sigma$. As a consequence, the JC Hamiltonian reduces to the invariant subspaces

$$\mathcal{H}_n = \mathrm{Span}\{|n\rangle \otimes e_1, |n+1\rangle \otimes e_{-1}\} \quad n \geq 0, \qquad \mathcal{H}_{-1} = \mathrm{Span}\{|0\rangle \otimes e_{-1}\}, \tag{5.10}$$

which are the subspaces corresponding to a fixed number of total excitations, *i.e.* $C \restriction_{\mathcal{H}_n} = n + 1$. Indeed, H_{JC} restricted to these subspaces reads

$$\begin{aligned} H_n(g) := H_{\mathrm{JC}}(g) \restriction_{\mathcal{H}_n} &= \begin{pmatrix} E^0_{(n,1)} & g\sqrt{n+1} \\ g\sqrt{n+1} & E^0_{(n+1,-1)} \end{pmatrix} \\ &= \omega(n+1)\mathbb{1} + \begin{pmatrix} \Delta/2 & g\sqrt{n+1} \\ g\sqrt{n+1} & -\Delta/2 \end{pmatrix}. \end{aligned} \tag{5.11}$$

Eigenvalues and eigenvectors of H_n are easily computed to be

$$H_{\mathrm{JC}}(g)\,|n,\nu\rangle = E_{(n,\nu)}\,|n,\nu\rangle\,, \qquad n\in\mathbb{N},\ \nu\in\{-,+\} \tag{5.12}$$

where

$$E_{(n,\nu)}(g) = \omega(n+1) + \nu\frac{1}{2}\sqrt{\Delta^2+4g^2(n+1)} \tag{5.13}$$
$$|n,+\rangle\,(g) = \cos(\theta_n/2)\,|n\rangle\otimes e_1 + \sin(\theta_n/2)\,|n+1\rangle\otimes e_{-1} \tag{5.14}$$
$$|n,-\rangle\,(g) = -\sin(\theta_n/2)\,|n\rangle\otimes e_1 + \cos(\theta_n/2)\,|n+1\rangle\otimes e_{-1} \tag{5.15}$$

and the *mixing angle* $\theta_n(g)\in[-\pi/2,\pi/2]$ is defined through the relation

$$\tan\theta_n := \frac{2g\sqrt{n+1}}{\omega-\Omega}. \tag{5.16}$$

Hereafter, we will omit the g-dependence of the eigenvectors $|n,\nu\rangle$ for the sake of a lighter notation. Observe that in the resonant case, *i.e.* $\Delta=0$, equation (5.16) implies $|\theta_n|=\pi/2$ for every $n\in\mathbb{N}$, hence the eigenvectors $|n,\nu\rangle$ are independent from g, while the eigenvalues still depend on it.

Moreover, depending on the sign of Δ, one has

$$\begin{array}{lll} E_{(n,+)}(0) = E^0_{(n,1)} & E_{(n,-)}(0) = E^0_{(n+1,-1)}, & \text{for } \Delta>0 \\ E_{(n,+)}(0) = E^0_{(n+1,-1)} & E_{(n,-)}(0) = E^0_{(n,1)}, & \text{for } \Delta<0 \\ E_{(n,\nu)}(0) = E^0_{(n+1,-1)} = E^0_{(n,1)}, & & \text{for } \Delta=0 \end{array}.$$

As we mentioned before, in view of Kato-Rellich theorem, the eigenvalues of $H_{\mathrm{JC}}(g)$ are analytic in g if a convenient labeling is chosen. The table above shows which function, among $g\mapsto E_{(n,+)}(g)$ and $g\mapsto E_{(n,-)}(g)$, provides the analytic continuations of the spectrum at the points $E^0_{(n,1)}$ or $E^0_{(n+1,-1)}$. When $\Delta=0$, in order to have analytic eigenvalues and eigenfunctions we must choose $E_{(n,\nu)}=\omega(n+1)+\nu\sqrt{n+1}g$.

The spurious eigenvector $|0\rangle\otimes e_{-1}$ with eigenvalue $E^0_{(0,-1)}=\Delta/2$ completes the spectrum of the JCH. Let us define

$$\delta \equiv \delta(\Delta) := \begin{cases} + & \text{if } \Delta\geq 0 \\ - & \text{if } \Delta<0 \end{cases}.$$

Throughout the paper we will use the notation $|-1,\delta\rangle := |0\rangle\otimes e_{-1}$ and $E_{(-1,\delta)} := E^0_{(0,-1)}$. We will denote a pair (n,ν) with a bold letter $\boldsymbol{n}$, meaning that the first component of $\boldsymbol{n}$ is the same not-bold letter while the second component is the corresponding Greek letter, namely

$$\boldsymbol{n}=(n,\nu),\quad \boldsymbol{n}(1)=n,\quad \boldsymbol{n}(2)=\nu.$$

Let also us define

$$f_n(g) := \frac{1}{2}\sqrt{\Delta^2+4g^2(n+1)}. \tag{5.17}$$

With this notation, we can write the spectrum of the JC Hamiltonian in a synthetic way as

$$\sigma\Big(H_{\rm JC}(g)\Big) = \{E_{\boldsymbol{n}}\}_{\boldsymbol{n}\in\mathcal{N}}, \qquad E_{\boldsymbol{n}}(g) = \omega(n+1) + \nu f_n(g) \tag{5.18}$$

where

$$\mathcal{N} := (\mathbb{N}\times\{-,+\}) \cup \{(-1,\delta(\Delta))\}. \tag{5.19}$$

Notice that the notation is coherent since

$$E_{(-1,\delta)} = \delta(\Delta) f_{-1}(g) = \delta(\Delta)\frac{|\Delta|}{2} = \frac{\Delta}{2} = E^0_{(0,-1)},$$

in agreement with the definition above. It will be also useful introduce the following sets

$$\mathfrak{N}_\pm := \mathbb{N} \cup \{\mp\delta(\Delta)1\} \tag{5.20}$$

which are copies of the natural numbers with $\{\,-1\,\}$ added to the set with the index $\delta(\Delta)$.

5.3 General setting and main result

In most of the physically relevant applications, the external control does not act on the spin part [BMPS, Sp]. Hence, we consider the JC dynamics with two different control terms acting only on the bosonic part, namely

$$H_1 = X \otimes \mathbb{1} \qquad H_2 = P \otimes \mathbb{1}. \tag{5.21}$$

To motivate our choice, we notice that – for example – in the cavity QED context the experimenters can only act on the electromagnetic field stored in the cavity. In this context the control terms H_1, H_2 correspond, respectively, to an external electric field and a magnetic field in the dipole approximation, see [BMPS, Section I.A], and the control functions $u_1(t), u_2(t)$ model the amplitudes of this external fields.

With the previous choice, the complete controlled Schrödinger dynamics reads

$$\begin{cases} i\partial_t\psi = \Big(H_{\rm JC}(g) + u_1(t)H_1 + u_2(t)H_2\Big)\psi \\ \psi(0) = \Psi_{\rm in} \in \mathcal{H}, \quad \Psi_{\rm fin} \in \mathcal{H} \quad \text{s.t. } \|\Psi_{\rm in}\| = \|\Psi_{\rm fin}\| \\ u_1, u_2 \in [0,c] \\ \omega, \Omega > 0 \\ |\Delta| \ll \omega, \Omega \end{cases} \tag{5.22}$$

Notice that the control functions u_1, u_2 are independent from each other so, as subcases, one can consider the system in which just one control is active. Obviously, controllability of the system in one of these two subcases implies controllability in the general case. This is exactly what we are going to prove. We consider the system

(5.22) in the subcases $u_1 \equiv 0$ or $u_2 \equiv 0$ and we prove that in each subcase the system is approximately controllable.

The following theorems are the main results of the paper.

Theorem 5.1 (Approximate controllability of JC dynamics). *The system* (5.22) *with* $u_1 \equiv 0$ *or* $u_2 \equiv 0$ *is approximately controllable for every* $g \in \mathbb{R} \setminus S_*$ *where* S_* *is a countable set.*

Theorem 5.2 (Characterization of the singular set). *The set* S_**, mentioned in Theorem 5.1, consists of the value* $g = 0$ *and those* $g \in \mathbb{R}$ *that satisfy one of the following equations:*

$$E_{(n+1,-)}(g) = E_{(n,\nu)}(g), \qquad (n,\nu) \in \mathcal{N} \tag{5.23}$$

$$2\omega = f_{m+1}(g) + f_m(g) - f_{n+1}(g) + f_n(g), \qquad n, m \in \mathfrak{N}_+ \tag{5.24}$$

$$2\omega = f_{m+1}(g) - f_m(g) - f_{n+1}(g) + f_n(g), \quad n, m \in \mathfrak{N}_-,\ m < n \tag{5.25}$$

$$2\omega = f_{m+1}(g) + f_m(g) - f_{n+1}(g) - f_n(g), \quad n, m \in \mathfrak{N}_-,\ m > n \tag{5.26}$$

where $\mathcal{N}$, $\mathfrak{N}_\pm$ *and* f_n *are defined in* (5.19),(5.20) *and* (5.17)*, respectively.*

The proof of Theorem 5.1 follows two main steps: we introduce a Hilbert basis of eigenvectors of H_{JC}, namely $\{|\boldsymbol{n}\rangle\}_{\boldsymbol{n}\in\mathcal{N}}$, and analyze the action of the control operators on it in order to show that all levels are coupled for every value of the parameter g except a countable set (see Section 5.4.1). We then construct a subset $\mathcal{C}_0$ of $\mathcal{N}^2$ and prove that it is a non-resonant chain of connectedness (see Section 5.4.2). The claim then follows from the application of the general result by Boscain et al., namely Theorem 2.40.

To prove Theorem 5.2 we carefully analyze the resonances of the system, which are solution to the forthcoming equation (5.33). By proving that the latter has a countable number of solutions, we conclude that relevant pairs of energies are not resonant for every $g \in \mathbb{R}$ except the values in a countable set which will be characterized in the proof.

5.4 Proof of Theorem 5.1

5.4.0 Preliminaries

Preliminarily, we have to show that Assumption 2.32 is satisfied by

$$(iH_{\mathrm{JC}}(g),\ iH_j,\ \mathbb{R},\ \{|\boldsymbol{n}\rangle\}_{\boldsymbol{n}\in\mathcal{N}}), \quad \text{for } g \in \mathbb{R} \setminus S_0,\ j \in \{1,2\},$$

where S_0 is a countable set. Notice that the index set $\mathcal{N}$ plays the role of the countable set $\mathcal{I}$ in Definition 2.39.

We have already shown that $\{|\boldsymbol{n}\rangle\}_{\boldsymbol{n}\in\mathcal{N}}$ is a Hilbert basis of eigenfunctions for $H_{\mathrm{JC}}(g)$. Since H_j is infinitesimally H_0-bounded ($H_j \ll H_0$ for short) for $j \in \{1,2\}$, then $H_j \ll H_{\mathrm{JC}}(g)$ for $j \in \{1,2\}$ (see [RS$_4$, Exercise XII.11]). Hence (A$_2$) holds.

Moreover, this implies that $H_{\mathrm{JC}}(g) + wH_j$ is self-adjoint on $\mathcal{D}(H_{\mathrm{JC}}) = \mathcal{D}(H_0)$ for every $w \in \mathbb{R}$ (see [RS$_2$, Theorem X.12]) and so (A$_3$) is satisfied.

As for assumption (A$_4$), we observe that in view of the analyticity of the eigenvalues, there are just countable many values of g which correspond to eigenvalue intersections. With the only exception of these values, the eigenvalues are simple, so (A$_4$) and Assumption 2.32 hold automatically for every $g \in \mathbb{R} \setminus S_0$, where S_0 is the countable set corresponding to the eigenvalue intersections.

On the other hand, we can further restrict the set of singular points from S_0 to $S_1 \subset S_0$. Indeed, if two eigenvalues intersect in a point g_*, say $E_{\boldsymbol{n}}(g_*) = E_{\boldsymbol{m}}(g_*)$, property (A$_4$) is still satisfied (by the same orthonormal system) provided that $\langle \boldsymbol{m} | H_j | \boldsymbol{n} \rangle (g_*) = 0,\ j \in \{1, 2\}$.

Observe that, given $n \in \mathbb{N}$,

$$|m - n| > 2 \quad \Rightarrow \quad \langle \boldsymbol{m} | H_j | \boldsymbol{n} \rangle (g) = 0 \quad \forall g \in \mathbb{R},\ j \in \{1, 2\}. \tag{5.27}$$

Hence, *a priori* the only possibly problematic points are solutions to the following equations

$$E_{\boldsymbol{m}}(g) = E_{\boldsymbol{n}}(g) \qquad \boldsymbol{m}, \boldsymbol{n} \in \mathcal{N}, \quad \boldsymbol{m} \neq \boldsymbol{n}, \quad |m - n| \leq 2. \tag{5.28}$$

By direct investigation, and using (5.18), one notices that there are solutions only in the following cases (for $\boldsymbol{n} = (n, \nu) \in \mathcal{N}$):

$$E_{\boldsymbol{n}}(g) = E_{(n+1,-)}(g) \quad \text{which is satisfied if and only if} \tag{5.29}$$
$$|g| = G^{(1)}_{\boldsymbol{n}} := \sqrt{\omega^2(2n+3) - \nu\sqrt{4\omega^4(n^2+3n+2) + \omega^2\Delta^2}};$$

$$E_{\boldsymbol{n}}(g) = E_{(n+2,-)}(g) \quad \text{which is satisfied if and only if} \tag{5.30}$$
$$|g| = G^{(2)}_{\boldsymbol{n}} := \sqrt{2\omega^2(n+2) - \nu\sqrt{4\omega^4(n^2+4n+3) + \omega^2\Delta^2}};$$

$$E_{(n,+)}(g) = E_{(n,-)}(g) \quad \text{which is satisfied if and only if} \tag{5.31}$$
$$g = 0 \quad \text{and} \quad \Delta = 0.$$

We will establish *a posteriori* whether we have indeed to exclude those points by the analysis in the next subsection, after looking at the action of the control operators.

5.4.1 Coupling of energy levels

To apply Theorem 2.40 to our case we need to build a non resonant chain of connectedness. As observed before in (5.27), the control operators do not couple most of the pairs.

The coupling between remaining pairs is easily checked by using (5.3), (5.9), (5.14), and (5.15). For the sake of a shorter notation, we set $c_n := \cos(\theta_n/2)$ and

$s_n := \sin(\theta_n/2)$. Some straightforward calculations for H_1 yield the following result:

$$\begin{aligned}
\langle n,-|\, H_1\, |n,+\rangle &= 0\\
\langle n+1,+|\, H_1\, |n,+\rangle &= \frac{1}{\sqrt{2}}(\sqrt{n+1}c_nc_{n+1}+\sqrt{n+2}s_ns_{n+1}) \neq 0\\
\langle n+2,+|\, H_1\, |n,+\rangle &= 0\\
\langle n+1,-|\, H_1\, |n,-\rangle &= \frac{1}{\sqrt{2}}(\sqrt{n+1}c_nc_{n+1}+\sqrt{n+2}s_ns_{n+1}) \neq 0\\
\langle n+2,-|\, H_1\, |n,-\rangle &= 0\\
\langle n+1,-|\, H_1\, |n,+\rangle &= \frac{1}{\sqrt{2}}(\sqrt{n+2}s_nc_{n+1}-\sqrt{n+1}c_ns_{n+1}) \neq 0 \qquad \Leftrightarrow g\neq 0
\end{aligned}$$

$$\begin{aligned}
\langle n+2,-|\, H_1\, |n,+\rangle &= 0\\
\langle n+1,+|\, H_1\, |n,-\rangle &= \frac{1}{\sqrt{2}}(\sqrt{n+2}c_ns_{n+1}-\sqrt{n+1}s_nc_{n+1}) \neq 0 \qquad \Leftrightarrow g\neq 0\\
\langle n+2,+|\, H_1\, |n,-\rangle &= 0\\
\langle 0,-|\, H_1\, |{-1},\delta\rangle &= \frac{c_0}{\sqrt{2}} \geq \frac{1}{2}\\
\langle 0,+|\, H_1\, |{-1},\delta\rangle &= \frac{s_0}{\sqrt{2}} \neq 0 \Leftrightarrow g\neq 0.
\end{aligned}$$

From these computations we see that (compare with (5.29),(5.30)) in the points $\{G^{(2)}_{\boldsymbol{n}}\}_{\boldsymbol{n}\in\mathcal{N}}$ the system still satisfies Assumption 2.32, while in the points $\{G^{(1)}_{\boldsymbol{n}}\}_{\boldsymbol{n}\in\mathcal{N}}$ does not. The point $g=0$ is never solution to (5.29) or (5.30) in view of the assumption $|\Delta| \ll \omega$. Moreover, since $\langle n,-|\, H_1\, |n,+\rangle = 0$ for every $g\in\mathbb{R}$, the system still satisfies Assumption 2.32 for $g=0$, notwithstanding (5.31).

The same results hold for H_2. Moreover, in each of the previous cases one has

$$\langle \boldsymbol{m}|\, H_2\, |\boldsymbol{n}\rangle = i\,\langle \boldsymbol{m}|\, H_1\, |\boldsymbol{n}\rangle\,.$$

We conclude that Assumption (A_4) is satisfied for every $g\in\mathbb{R}\setminus S_1$, where $S_1 := \{G^{(1)}_{\boldsymbol{n}}\}_{\boldsymbol{n}\in\mathcal{N}}$.

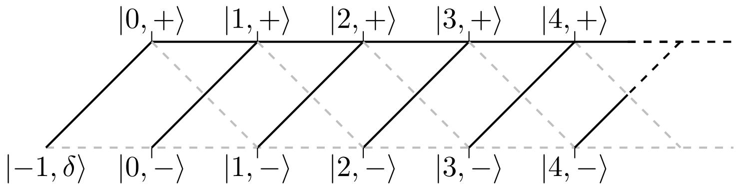
5.4.2 Non-resonances of relevant pairs

Knowing exactly the pairs of levels coupled by the control terms, we claim that the set (illustrated in Figure 1)

$$\mathcal{C}_0 = \big\{\big[(n+1,+),(n,+)\big],\ \big[(n+1,+),(n,-)\big] \mid n\in\mathbb{N}\big\} \cup \big\{\big[(0,+),(-1,\delta)\big]\big\} \quad (5.32)$$

is a non-resonant chain of connectedness for every $g\in\mathbb{R}\setminus S_2$, where $S_2\subset\mathbb{R}$ is a countable set.

Figure 5.1: Schematic representation of the eigenstates of the JC Hamiltonian and the chain of connectedness $\mathcal{C}_0$, in the case $\delta(\Delta) = -$. Thick black lines correspond to pairs of eigenstates in the chain $\mathcal{C}_0$. Gray dashed lines correspond instead to pairs of eigenstates coupled by the control which are not in $\mathcal{C}_0$.



To prove this claim, we have to show that for every $g \in \mathbb{R} \setminus S_2$ each pair of eigenstates in $\mathcal{C}_0$ has no resonances with every other pair coupled by the control term. In view of the computation above, there are just four types of pairs coupled, as illustrated in Figure 1 and 2. So, we define S_2 as the set of the solutions g to the following equations:

$$|E_{\boldsymbol{k}}(g) - E_{\boldsymbol{l}}(g)| = |E_{\boldsymbol{s}}(g) - E_{\boldsymbol{t}}(g)| \tag{5.33}$$

where $[\boldsymbol{k}, \boldsymbol{l}] \in \mathcal{C}_0$ and

$$\begin{aligned}[\boldsymbol{s}, \boldsymbol{t}] \in \mathcal{C}_0 \cup \big\{ \big[(n+1, -), (n, -)\big],\ \big[(n+1, -), (n, +)\big] \mid n \in \mathbb{N} \big\} \\ \cup \big\{ \big[(0, -), (-1, \delta)\big] \big\} .\end{aligned} \tag{5.34}$$

It is enough to prove that the set of solutions to the latter equations is countable. Observe that, by the analyticity of the functions $g \mapsto E_{\boldsymbol{k}}(g) - E_{\boldsymbol{l}}(g)$, equation (5.33) may have at most countable many solutions unless is identically satisfied. Thus, we need to show that

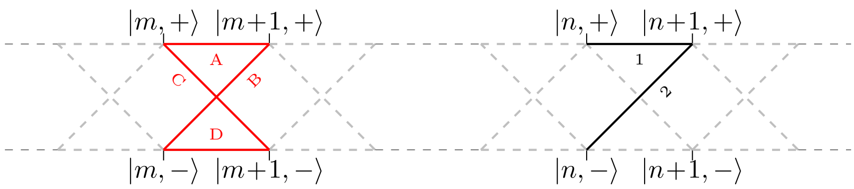
$$E_{\boldsymbol{k}}(g) - E_{\boldsymbol{l}}(g) = \pm (E_{\boldsymbol{s}}(g) - E_{\boldsymbol{t}}(g))$$

is not satisfied for some value g or, equivalently, that the Taylor expansions of r.h.s. and l.h.s. differ in at least a point. The same argument was used in [BMPS], where the authors computed the perturbative expansion of the eigenvalues of the Rabi Hamiltonian up to forth order in g. In our case, the model is exactly solvable,so that we can compute the series expansions in $g = 0$ directly from expression (5.13). An explicit computation yields the Taylor expansion:

$$\begin{aligned} &E_{\boldsymbol{n}} = \omega(n+1) + \nu \left(\tfrac{|\Omega - \omega|}{2} + \tfrac{n+1}{|\Omega - \omega|} g^2 - \tfrac{(n+1)^2}{|\Omega - \omega|^3} g^4 + o\left(g^4\right) \right) && \text{for } \Delta \neq 0 \\ &E_{\boldsymbol{n}} = \omega(n+1) + \nu \sqrt{n+1} g && \text{for } \Delta = 0. \end{aligned}$$

It is now easy to check, mimicking Step 2 in the proof of [BMPS], that for every choice of the indices in equation (5.33) the r.h.s. and l.h.s. have different series expansion at $g = 0$. We are not going to detail this calculation, since in the next Section we will analyze in full detail equations (5.33), in order to characterize the set S_2. By setting $S_* = S_1 \cup S_2$, the proof of Theorem 5.1 is concluded.

Figure 5.2: Classification of the arcs representing pairs of eigenstates coupled by the control operator. On the left-hand panel, red arcs and labels show the classification of generic arcs in four different types $\{A, B, C, D\}$. On the right-hand panel, black arcs of the set $\mathcal{C}_0$ are classified in two types $\{1, 2\}$. Labels correspond to the cases enumerated in the proof of Theorem 5.2.



5.5 Proof of Theorem 5.2

In this proof we will discuss the resonances of the pairs of eigenstates in the chain $\mathcal{C}_0$, defined in (5.32). Our aim is to provide conditions to determine whether, for a particular value of g, resonances are present or not. This requires a direct investigation of equation (5.33). Since these computations are rather long, we prefer to collect them in this section, not to obscure the simplicity of the proof of Theorem 5.1 with the details on the characterization of the set S_*.

Let us recall that the sets $\mathfrak{N}_\pm$ defined in (5.20) include both the natural numbers, and -1 is added to the one, among $\mathfrak{N}_+$ and $\mathfrak{N}_-$, whose label equals $\delta(\Delta)$.

In each of the following subcases the existence of solutions to equation (5.33) is discussed, for every choice of the indices compatible with the constraints (5.34). The mathematical arguments are based on elementary properties of functions $f_n(g) = \frac{1}{2}\sqrt{\Delta^2 + 4g^2(n+1)}$, which are summarized in Lemma 5.3 in the Appendix.

Case 1: Assume $[\boldsymbol{k}, \boldsymbol{l}] = [(n+1,+),(n,+)]$, $n \in \mathfrak{N}_+$. This assumption correspond to select the black arc labeled by 1 in the graph in Figure 5.2. We investigate the possible resonances between the selected arc and the other arcs, classified according to their qualitative type (see the labels in the left-hand panel of Figure 5.2). This analysis amounts to consider, with the help of Lemma 5.3 (properties (F.1)-(F.3)), the following subcases:

(1.A) $[\boldsymbol{s}, \boldsymbol{t}] = \big[(m+1,+),(m,+)\big]$, $m \in \mathfrak{N}_+$, $m \neq n$. Equation (5.33) reads

$$f_{n+1}(g) - f_n(g) = f_{m+1}(g) - f_m(g)$$

which is satisfied if and only if $g = 0$, because $f_{n+1}(g) - f_n(g)$ is strictly decreasing in n for $g \neq 0$ in view of (F.3).

(1.B) $[\boldsymbol{s}, \boldsymbol{t}] = \big[(m+1,+),(m,-)\big]$, $m \in \mathfrak{N}_-$. Equation (5.33) reads

$$f_{n+1}(g) - f_n(g) = f_{m+1}(g) + f_m(g)$$

which is satisfied if and only if $g = 0$ and $\Delta = 0$.
Indeed, by (F.2) one has

$$f_{n+1}(g) - f_n(g) \leq 2\,|g|\left(\sqrt{n+2} - \sqrt{n+1}\right) = \frac{2\,|g|}{\sqrt{n+2} + \sqrt{n+1}}.$$

For $\Delta < 0$, one has $n \in \mathfrak{N}_+ = \mathbb{N}$ and $m \in \mathfrak{N}_- = \mathbb{N} \cup \{-1\}$, as illustrated in Figure 1. Hence, for $g \neq 0$,

$$\begin{aligned} f_{n+1}(g) - f_n(g) \leq \frac{2\,|g|}{\sqrt{2}+1} < |g| &\leq |g|\,(\sqrt{m+2} + \sqrt{m+1}) \\ &\leq f_{m+1}(g) + f_m(g), \end{aligned}$$

and the last inequality is strict whenever $\Delta \neq 0$.
Analogously, for $\Delta > 0$ one has $n \in \mathfrak{N}_+ = \mathbb{N} \cup \{-1\}$ and $m \in \mathfrak{N}_- = \mathbb{N}$. Hence, for $g \neq 0$,

$$\begin{aligned} f_{n+1}(g) - f_n(g) \leq 2\,|g| < |g|\,(\sqrt{m+2} + \sqrt{m+1}) \\ \leq f_{m+1}(g) + f_m(g). \end{aligned}$$

As above, the last inequality is strict whenever $\Delta \neq 0$.

(1.C) $[\boldsymbol{s}, \boldsymbol{t}] = \big[(m+1, -), (m, +)\big]$, $m \in \mathfrak{N}_+$. Equation (5.33) reads

$$\omega + f_{n+1}(g) - f_n(g) = |\omega - f_{m+1}(g) - f_m(g)|\,.$$

If $|g| < G^{(1)}_{m,+}$ one has

$$f_{n+1}(g) - f_n(g) = -f_{m+1}(g) - f_m(g),$$

which implies $g = 0$ and $\Delta = 0$ because $-f_{m+1}(g) - f_m(g) \leq 0 \leq f_{n+1}(g) - f_n(g)$, and the first inequality is strict whenever $\Delta \neq 0$, while the second inequality is strict whenever $g \neq 0$.
On the other hand, if $|g| \geq G^{(1)}_{m,+}$ the equation above reads

$$2\omega = f_{m+1}(g) + f_m(g) - f_{n+1}(g) + f_n(g) \qquad (5.24)$$

which has two solutions because the r.h.s. is equal to $|\Delta|$ in zero (and $|\Delta| \ll \omega$ in view of (5.22)) and is strictly increasing in $|g|$. Indeed, one easily sees that

$$\begin{aligned} &\partial_g \left(f_{m+1}(g) + f_m(g) - f_{n+1}(g) + f_n(g)\right) = \\ &\qquad g\left(\frac{m+2}{f_{m+2}(g)} + \frac{m+1}{f_m(g)} - \frac{n+2}{f_{n+1}(g)} + \frac{n+1}{f_n(g)}\right) =: g C_{m,n}(g) \end{aligned}$$

where $C_{m,n}(g) > 0$ for every choice of indices $n, m \in \mathcal{N}_+$ and $\Delta \neq 0$. For $\Delta = 0$ the r.h.s. of (5.24) is $|g|\,(\sqrt{m+2} + \sqrt{m+1} - \sqrt{n+2} + \sqrt{n+1})$ which is clearly strictly increasing in $|g|$.

(1.D) $[\boldsymbol{s},\boldsymbol{t}] = \big[(m+1,-),(m,-)\big],\ m \in \mathfrak{N}_-$. Equation (5.33) reads

$$\omega + f_{n+1}(g) - f_n(g) = |\omega - f_{m+1}(g) + f_m(g)|$$

Then if $|g| < G^{(1)}_{m,-}$

$$f_{n+1}(g) - f_n(g) = -f_{m+1}(g) + f_m(g),$$

which is satisfied if and only if $g = 0$ because $f_{n+1}(g) - f_n(g) \geq 0 \geq -f_{m+1}(g) + f_m(g)$ and the inequalities are strict whenever $g \neq 0$. If instead $|g| \geq G^{(1)}_{m,-}$, the equation reads

$$2\omega = f_{m+1}(g) - f_m(g) - f_{n+1}(g) + f_n(g) \qquad (5.25)$$

which has two solutions if and only if $m < n$. Indeed, $f_{n+1}(g) - f_n(g)$ is decreasing in n in view of (F.3) and the derivative of the r.h.s. is

$$\partial_g \left(f_{m+1}(g) - f_m(g) - f_{n+1}(g) + f_n(g)\right) = \\ g\left(\frac{m+2}{f_{m+2}(g)} - \frac{m+1}{f_m(g)} - \frac{n+2}{f_{n+1}(g)} + \frac{n+1}{f_n(g)}\right) =: gD_{m,n}(g).$$

The function $D_{m,n}(g)$ is strictly positive for every $\Delta \neq 0$ and $m \in \mathcal{N}_-$, $n \in \mathcal{N}_+$ with $m < n$ because $\frac{n+2}{f_{n+1}(g)} - \frac{n+1}{f_n(g)}$ is strictly decreasing in n. For $\Delta = 0$ the r.h.s. of (5.25) is $|g|\left(\sqrt{m+2} - \sqrt{m+1} - \sqrt{n+2} + \sqrt{n+1}\right)$ which is positive if and only if $m < n$, and is clearly strictly increasing in $|g|$.

In view of the above analysis, there exist non trivial resonances (for $g \neq 0$) in cases (1.C), and (1.D) for $m < n$. In such circumstances, equations (5.24),(5.25) have two solutions each.As for the trivial value $g = 0$, the system exhibits multiple resonances, as noted in all previous cases. Hence, $g = 0$ has to be included in the set of resonant points.

Case 2: Assume $[\boldsymbol{k},\boldsymbol{l}] = [(n+1,+),(n,-)],\ n \in \mathfrak{N}_-$. This assumption corresponds to select the black arc labeled by 2 in the graph in Figure 5.2. As before, we proceed by considering the following sub-cases:

(2.A) By symmetry, this case reduces to the subcase (1.B). As already noticed, a solution exists if and only if $g = 0$ and $\Delta = 0$.

(2.B) $[\boldsymbol{s},\boldsymbol{t}] = \big[(m+1,+),(m,-)\big],\ m \in \mathfrak{N}_-,\ m \neq n$. The corresponding equation reads

$$f_{n+1}(g) + f_n(g) = f_{m+1}(g) + f_m(g)$$

which has only the trivial solution $g = 0$.

(2.C) $[\boldsymbol{s},\boldsymbol{t}] = \big[(m+1,-),(m,+)\big]$, $m \in \mathfrak{N}_+$. Equation (5.33) reads

$$\omega + f_{n+1}(g) + f_n(g) = |\omega - f_{m+1}(g) - f_m(g)| .$$

Then if $|g| < G^1_{m,+}$ the equation above become

$$f_{n+1}(g) + f_n(g) = -f_{m+1}(g) - f_m(g)$$

which clearly implies that $g = 0$ and $\Delta = 0$.
On the other hand, if $|g| \geq G^1_{m,+}$ the equation reads

$$2\omega = f_{m+1}(g) + f_m(g) - f_{n+1}(g) - f_n(g) \qquad (5.26)$$

which has non trivial solutions if and only if $m > n$ because f_n is increasing in n for $g \neq 0$. Since the r.h.s. is strictly increasing in $|g|$, as one can see using an argument similar to case (1.C), the latter equation has two solutions if $m > n$.

(2.D) $[\boldsymbol{s},\boldsymbol{t}] = \big[(m+1,-),(m,-)\big]$, $m \in \mathfrak{N}_-$. Equation (5.33) reads

$$\omega + f_{n+1}(g) + f_n(g) = |\omega - f_{m+1}(g) + f_m(g)| .$$

If $|g| < G^1_{m,-}$ the above equation reads

$$f_{n+1}(g) + f_n(g) = -f_{m+1}(g) + f_m(g)$$

which is satisfied if and only if $g = 0$ and $\Delta = 0$, since $-f_{m+1}(g) + f_m(g) \leq 0 \leq f_{n+1}(g) + f_n(g)$, and the first inequality is strict whenever $g \neq 0$, while the second inequality is strict whenever $\Delta \neq 0$. If, instead, $|g| \geq G^1_{m,-}$, the above equation becomes

$$2\omega = f_{m+1}(g) - f_m(g) - f_{n+1}(g) - f_n(g),$$

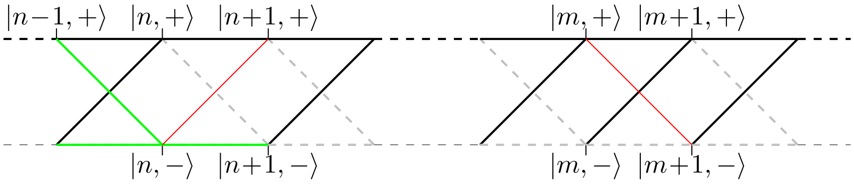
which has no solution since the r.h.s. is non-positive for every $g, \Delta \in \mathbb{R}$ and $n, m \in \mathcal{N}_-$.

In summary, as far as Case 2 is concerned, there exist non trivial resonances (for $g \neq 0$) only in the case (2.C) for $m > n$, and in such case equation (5.26) has exactly two solutions.

Recalling the definition of $\mathcal{C}_0$ (see (5.32)), one notices that every element of $\mathcal{C}_0$ is non-resonant with every other element of $\mathcal{C}_0$ except for the trivial value $g = 0$, in view of the analysis of the cases (1.A), (1.B), (2.A) and (2.B).

The proof above exhibits equations (5.24), (5.25) and (5.26) appearing in the statement of Theorem 5.2, as the equations which characterize the values of g in S_2, namely those values such that an arc in $\mathcal{C}_0$ is resonant with some arc (not in $\mathcal{C}_0$) non-trivially coupled by the interaction. As we said before, the value $g = 0$ is included in S_2.

Figure 5.3: Disconnection of the chain $\mathcal{C}_0$ for the value $g_{2.n}(m)$. In red resonant arcs. In green the possible choices to reconnect the node $|n,-\rangle$.



Finally, one has to include in S_* those values of g for which some eigenspace has dimension 2 and the corresponding eigenvectors are coupled. These values, defining the set S_1, have been already characterized by equation (5.23), whose solutions are exhibited in (5.29).

In view of Theorem 2.40, we conclude that the system is approximately controllable for every $g \in \mathbb{R} \setminus S_*$, where $S_* = S_1 \cup S_2$ is characterized by equations (5.23), (5.24), (5.25), and (5.26). This concludes the proof of Theorem 5.2.

5.6 Further improvements

We have seen that equations (5.24),(5.25),(5.26) specify points $g \in \mathbb{R}$ for which $\mathcal{C}_0$ fails to be a non-resonant chain of connectedness. However for each of such points, we can think of suitably modify $\mathcal{C}_0$ to replace resonant arcs and preserve the connectedness of the chain. Notice that $\mathcal{C}_0$ is composed by arcs of type A and B, thus to replace one of them in case of resonances we must use arcs of type C,D (see Fig.5.2). Therefore it is necessary to check resonances between arcs of type C,D.

Let us illustrate the problem with an example. Denote with $g_{2.n}(m) \in \mathbb{R}$ the positive solution of equation (5.26), *i. e.* $g \geq 0$ such that

$$2\omega = f_{m+1}(g) + f_m(g) - f_{n+1}(g) - f_n(g), \qquad n, m \in \mathfrak{N}_-,\ m > n$$

is satisfied. Recall that $g_{2.n}(m)$ is a resonant point between the arcs $\big[(n,-),(n+1,+)\big]$ and $\big[(m,+),(m+1,-)\big]$ (in red in Fig.5.3). In this point we have to remove the arc $\big[(n,-),(n+1,+)\big]$ from $\mathcal{C}_0$ because is resonant, thus the node $|n,-\rangle$ disconnects. We have three possible choices to restore the connectedness: add one arc between $\big[(n-1,-),(n,-)\big],\big[(n,-),(n+1,-)\big],\big[(n-1,+),(n,-)\big]$ to the chain (in green in Fig.5.3). One choice seems more natural, since by eq.(5.26) $\big[(n-1,+),(n,-)\big]$ is never resonant with $\big[(n,-),(n+1,+)\big]$ we can consider

$$\mathcal{C}_{2.n}(m) = \mathcal{C}_0 \cup \{\big[(n-1,+),(n,-)\big]\} \setminus \{\big[(n,-),(n+1,+)\big]\}.$$

Remain to verify that $\mathcal{C}_{2.n}(m)$ is non-resonant for $g = g_{2.n}(m)$. This means to check that every arc of $\mathcal{C}_{2.n}(m)$ has no resonances at the value $g_{2.n}(m)$. Therefore to ensure that no arc of type A has resonances in $g_{2.n}(m)$ it must not be solution of the following equations

$$\begin{aligned} 2\omega &= f_{t+1}(g) + f_t(g) - f_{s+1}(g) + f_s(g), \qquad \forall s,t \in \mathfrak{N}_+ \\ 2\omega &= f_{t+1}(g) - f_t(g) - f_{s+1}(g) + f_s(g), \qquad \forall s,t \in \mathfrak{N}_-,\ t < s \end{aligned}$$

(these are equations (5.24),(5.25) for each possible choice of the indexes). Moreover we have to check resonances of $\big[(n-1,+),(n,-)\big]$ which is an arc of type C.

At the moment, we don't have a general method to solve systems of equations of type (5.24),(5.25) or (5.26), and to affirm that they have not a common solution. Notice that the analysis is complicated by the fact that we have general parameters ω, Ω under the unique assumption (5.5).

The results of this Chapter are collected in [PP].

Appendix 5.A

The following Lemma contains a list of useful elementary properties of the functions $\{f_n\}_{n\in\mathbb{N}}$, which have been used in the proof of Theorem 5.2 (Section 5.5).

Lemma 5.3. *Let f_n, $n \in \mathbb{N}$, be defined as in* (5.17). *Then*

(F.1) $f_m(g) - f_n(g) \geq 0$ *if and only if* $m \geq n$*;*

(F.2) $f_{n+1}(g) - f_n(g) \leq 2\,|g|\,(\sqrt{n+2} - \sqrt{n+1})$*;*

(F.3) $f_{n+1}(g) - f_n(g)$ *is strictly increasing w.r.to* $|g|$*, and strictly decreasing in* n*;*

Proof. Property (F.1) follows from the monotonicity of the square root. As for (F.2), one notices that

$$f_{n+1}(g) - f_n(g) \leq \frac{2g^2}{\sqrt{\Delta^2 + 4g^2(n+2)}}$$

which is equivalent to

$$(\Delta^2 + 4g^2(n+2)) - \sqrt{\Delta^2 + 4g^2(n+2)}\sqrt{\Delta^2 + 4g^2(n+1)} \leq 4g^2$$

which follows from the fact that

$$(\Delta^2 + 4g^2(n+1)) \leq \sqrt{\Delta^2 + 4g^2(n+2)}\sqrt{\Delta^2 + 4g^2(n+1)}.$$

Then,

$$\begin{aligned} f_{n+1}(g) - f_n(g) &\leq \frac{2g^2}{\sqrt{\Delta^2 + 4g^2(n+2)}} \leq \frac{2g^2}{2\,|g|\,\sqrt{n+2}} \\ &\leq 2\,|g|\,(\sqrt{n+2} - \sqrt{n+1}). \end{aligned}$$

Notice that the last inequality is strict whenever $g \neq 0$.

As for (F.3), one sets

$$F(x,y) := \frac{1}{2}\sqrt{\Delta^2 + 4x^2 y} \quad \text{and} \quad G(x,y) := y/\sqrt{\Delta^2 + 4x^2 y},$$

so that $f_n(g) = F(g, n+1)$ and $\partial_g f_n(g) = 2g\, G(g, n+1)$. Observe that for $y \geq 0$ one has

$$\frac{\partial G}{\partial y} = \frac{1}{\sqrt{\Delta^2 + 4x^2 y}} \left(1 - \frac{2x^2 y}{\Delta^2 + 4x^2 y}\right) > 0$$

and also

$$\frac{\partial^2 G}{\partial y^2} = \frac{4x^2}{(\Delta^2 + 4x^2 y)^{3/2}} \left(-1 + \frac{3y}{4} \frac{4x^2}{\Delta^2 + 4x^2 y}\right) \leq 0,$$

and the latter is equal to 0 if and only if $x = 0$. Then, one has (with an innocent abuse of notation concerning $\partial_n f_n(g)$)

$$\begin{aligned} \partial_g (f_{n+1} - f_n)(g) =& 2g(G(g, n+2) - G(g, n+1)) \quad \begin{cases} > 0 & \text{for } g > 0 \\ < 0 & \text{for } g < 0 \end{cases} ; \\ \partial_n (f_{n+1} - f_n)(g) =& \frac{\partial F}{\partial y}(g, n+2) - \frac{\partial F}{\partial y}(g, n+1) \\ =& g^2 \left(\frac{1}{\sqrt{\Delta^2 + 4g^2(n+2)}} - \frac{1}{\sqrt{\Delta^2 + 4g^2(n+1)}} \right) < 0. \end{aligned}$$

The monotonicity properties claimed in the statement follow immediately.

□

Chapter 6

Towards an adiabatic derivation of the Jaynes-Cummings model

In this Chapter we present some preliminary results concerning the derivation of the Jaynes-Cummings Hamiltonian as an approximation of the Rabi Hamiltionian in a suitable regime. The limit that we investigate is the so called *rotating wave approximation* which we will see as an adiabatic limit. The precise meaning of the approximation is the usual in quantum mechanics: closeness of the evolution operators in the norm of $\mathcal{B}(\mathcal{H})$.

6.1 Time scales identification

In the physics literature, as we briefly mentioned in Sect.5.2, one finds applications of the Rabi and Jaynes-Cummings models in different fields. What is usually stated is that those Hamiltonians exhibits different behaviours depending on the range of the fundamental parameters ω, Ω, g. We are interested in the so called *weak-coupling limit*, in which the assumptions are

$$|\Delta| \ll \omega, \Omega \qquad g \ll \omega, \Omega \tag{6.1}$$

and the *rotating wave approximation* (RWA) is supposed to hold [Ro],[AGJ]. The heuristic explanation we gave in Sect.5.2 is a way to introduce a time dependence in the Rabi Hamiltonian and identify the different time scales. Indeed, performing the time-dependent change of coordinates $\psi' = e^{iH_0 t}\psi$, the function ψ' satisfies the Schrödinger equation $i\partial_t \psi' = H'_{\mathrm{R}}(t)\psi'$[1] where H'_{R} was obtained in (5.7) and is

$$H'_{\mathrm{R}}(t) = e^{iH_0 t}(H_{\mathrm{R}} - H_0)e^{-iH_0 t} = \frac{g}{2}(e^{-i(\Omega-\omega)t}a^\dagger\sigma + e^{i(\Omega-\omega)t}a\sigma^\dagger) + \frac{g}{2}(e^{-i(\Omega+\omega)t}a\sigma + e^{i(\Omega+\omega)t}a^\dagger\sigma^\dagger). \tag{6.2}$$

[1]Throughout the chapter we will make use of Hartree units, so that in particular $\hbar = 1$

From the previous Hamiltonian (H_{R} in the interaction frame) ones notices two different frequencies, namely $|\omega - \Omega|$ and $\omega + \Omega$, which are of different order given (6.1). To have a dimensionless parameter we choose

$$\varepsilon := \frac{|\omega - \Omega|}{\omega + \Omega} \tag{6.3}$$

instead of $|\Delta|$ as small parameter. Therefore, terms $a^\dagger \sigma, a\sigma^\dagger$ oscillate with frequency of $O(1)$ as $\varepsilon \to 0$[2] on the time-scale $\tau = \varepsilon t$, while $a^\dagger \sigma^\dagger, a\sigma$ oscillate with frequency $O(\varepsilon^{-1})$ as $\varepsilon \to 0$[3] on the time-scale τ, so they average to zero on time intervals of $O(1)$ as $\varepsilon \to 0$.

Notice that apparently no relations are assumed between ε and g. In principle this should mean that the limits $\varepsilon \to 0$ and $g \to 0$ could be performed in any order and the approximation will hold. Moreover, from equation (6.2) we observe that the order of oscillations does not depend from g, which seems an argument in favour of the independence of the two limits. However, observing that

$$H_{\mathrm{R}} = (\omega - \Omega + \Omega)(a^\dagger a + \frac{1}{2}) + \frac{\Omega}{2}\sigma_3 + g(a + a^\dagger)(\sigma + \sigma^\dagger)$$

we can choose to apply the transformation $\phi = e^{i\Omega t(a^\dagger a + 1/2)} e^{i(\Omega t/2)\sigma_3} \psi$ (assume $\omega > \Omega$), to obtain another interaction frame

$$\begin{aligned} H''_{\mathrm{R}}(t) &= (\omega - \Omega)(a^\dagger a + \frac{1}{2}) + g(e^{-2i\Omega t} a + e^{2i\Omega t} a^\dagger)(e^{-2i\Omega t}\sigma + e^{2i\Omega t}\sigma^\dagger) \\ &= \varepsilon(\omega + \Omega)(a^\dagger a + \frac{1}{2}) + g(a^\dagger \sigma + a\sigma^\dagger) + g(e^{2i\Omega t} a^\dagger \sigma^\dagger + e^{-2i\Omega t} a\sigma) \\ &= H''_{\mathrm{JC}} + g(e^{2i\Omega t} a^\dagger \sigma^\dagger + e^{-2i\Omega t} a\sigma), \end{aligned} \tag{6.4}$$

where the time dependence is all contained in the term $e^{2i\Omega t} a^\dagger \sigma^\dagger + e^{-2i\Omega t} a\sigma$. In our hypothesis the latter time-dependent term average to zero on every scale $\tau = \phi(\varepsilon, g)t$ where $\lim_{(\varepsilon,g)\to(0,0)} \phi(\varepsilon, g) = 0$ (so ε or g are possible choices) but the order of the limits seems important. More precisely, spectral properties of $H''_{\mathrm{R}}(t)$ strongly depend on the relation between ε and g. For each $\varepsilon > 0$ the operator $H''_{\mathrm{R}}(t)$ has pure point spectrum, while for $\varepsilon = 0$ it doesn't.

To state a rigorous result we must take into account this problem.

[2]Here and thereafter we make use of the Landau symbols of which we briefly recall the definition. Let f, ϕ be two functions: we say that $f(x) = o(\phi(x))$ as $x \to x_0$ if $\lim_{x\to x_0} f(x)/\phi(x) = 0$; we say that $f(x) = O(\phi(x))$ as $x \to x_0$ if there exist constants $M, \delta > 0$ such that $|f(x)| \leq M\,|\phi(x)|$ for each x s.t. $0 < |x - x_0| < \delta$.

[3]In the following we will omit the expression "as $x \to x_0$" after $o(\phi(x))$ or $O(\phi(x))$ when is clear which kind of limit we are considering. In particular, since we consider only limits of variables that go to zero, $o(x^\alpha)$ and $O(x^\alpha)$ with $\alpha \in \mathbb{R}$ will denote respectively "$o(x^\alpha)$ as $x \to 0$" and "$O(x^\alpha)$ as $x \to 0$".

6.1.1 Statement of the result

We recall that H_{JC} leaves invariant the subspaces $\mathcal{H}_n$ defined in (5.10). Thus a general invariant subspaces for H_{JC} reads

$$\bigoplus_{n\in\mathbb{N}} \mathcal{H}_{i_n}$$

where $\{i_n\}_{n\in\mathbb{N}} \subset \mathbb{N}$. Denote with P_j the projection operator on $\mathcal{H}_j$, $j \in \mathbb{N}$. Then for each $E \in \mathbb{N}$ we define Π_E as the sum

$$\Pi_E = \sum_{j=-1}^{E} P_j. \tag{6.5}$$

The result we claim is standard in the context of Adiabatic theories (see [Teu]), in which one consider the difference between the evolution operators generated by the two Hamiltonian in question (in our case $e^{-iH_{\mathrm{R}}\frac{t}{\varepsilon}}$ and $e^{-iH_{\mathrm{JC}}\frac{t}{\varepsilon}}$), and looks for an estimate in terms of the small parameter ε. The bounding term must vanish in the limit $\varepsilon \to 0$ to affirm that the two dynamics exhibit the same behaviour in the adiabatic limit. In many cases this type of bound can be achieved only on a subspace of the state space (see for example the Born-Oppenheimer approximation [Teu, Sect.1.2]), therefore it is necessary to evaluate the difference of the two evolutions when projected on that subspace. This subspace is usually identified starting from physical consideration (for example, in the Born-Oppenheimer case, the kinetic energy of the nuclei must be bounded to have a uniform estimate). In our setting the subspace on which evaluate the difference is $\oplus_{n=-1}^{E}\mathcal{H}_n$, so that the corresponding projector is Π_E. In conclusion, the estimate that we want to prove is

$$\left\| \left(e^{-iH_{\mathrm{R}}\frac{t}{\varepsilon}} - e^{-iH_{\mathrm{JC}}\frac{t}{\varepsilon}} \right) \Pi_E \right\| \leq \sum_{j=1}^{M} C_j g^{\alpha_j} \varepsilon^{\beta_j} (1+t) \tag{6.6}$$

for all $t \geq 0$ and for some $\alpha_j, \beta_j \in \mathbb{R}$, $0 < C_j < \infty$, $j = 1, ..., M$.

However, to understand if such a bound is achievable one must ensure first that the subspace Π_E is approximately invariant for the total dynamics, which in our case is the Rabi dynamics. This estimate is preliminary to (6.6) and for this reason we prove in this Chapter the following

Theorem 6.1. *For each $E \in \mathbb{N}$ there exists a constant $C < \infty$ such that for all $t \geq 0$*

$$\left\| (\mathbb{1} - \Pi_E) e^{-iH_{\mathrm{R}}\frac{t}{\varepsilon}} \Pi_E \right\| \leq C \frac{g}{\varepsilon} t. \tag{6.7}$$

Remark 6.2. The previous estimate says that Π_E is an approximately invariant subspace for the Rabi dynamics when the ratio $g/\varepsilon \to 0$ as $(\varepsilon, g) \to (0,0)$, *i. e.* when $g = o(\varepsilon)$. We want to understand if is possible to improve the estimate (6.7) to have a weaker relation between ε and g. ⌟

6.2 Proof of Theorem 6.1

6.2.1 Preliminary estimates

With the notation of Chapter 5 (5.6) we write the Hamiltonians (5.4),(5.1) as

$$H_{\mathrm{R}}(g) = H_0 + \sqrt{2}gX \otimes \sigma_1 \tag{6.8}$$

$$H_{\mathrm{JC}}(g) = H_0 + \frac{g}{\sqrt{2}}(X \otimes \sigma_1 - P \otimes \sigma_2). \tag{6.9}$$

We recall that

$$X \otimes \sigma_1, P \otimes \sigma_2 << H_0,$$

so that $H_{\mathrm{JC}}, H_{\mathrm{R}}$ are self-adjoint operators on $\mathcal{D}(H_0)$ and essentially self-adjoint on each core of H_0 (see Sect.5.4.0). More precisely for every $\alpha > 0$ and $\psi \in \mathcal{D}(H_0)$

$$\|X \otimes \sigma_1 \psi\| \leq \alpha^{\frac{1}{2}} \|H_0 \psi\| + \left(2\alpha + \frac{2}{\alpha}\right)^{\frac{1}{2}} \|\psi\|$$

$$\|P \otimes \sigma_2 \psi\| \leq \alpha^{\frac{1}{2}} \|H_0 \psi\| + \left(2\alpha + \frac{2}{\alpha}\right)^{\frac{1}{2}} \|\psi\|,$$

from which the following estimates descend

$$\|H_{\mathrm{R}}\psi\| \leq (1 + \sqrt{2\alpha}g) \|H_0\psi\| + 2g \left(\alpha + \frac{1}{\alpha}\right)^{\frac{1}{2}} \|\psi\| \tag{6.10}$$

$$\|H_{\mathrm{JC}}\psi\| \leq (1 + \sqrt{2\alpha}g) \|H_0\psi\| + 2g \left(\alpha + \frac{1}{\alpha}\right)^{\frac{1}{2}} \|\psi\| \tag{6.11}$$

$$\|H_{\mathrm{R}}\psi\| \leq \left(1 + \frac{\sqrt{2\alpha}g}{1 - \sqrt{2\alpha}g}\right) \|H_{\mathrm{JC}}\psi\| + \frac{2g}{1 - \sqrt{2\alpha}g} \left(\alpha + \frac{1}{\alpha}\right)^{\frac{1}{2}} \|\psi\| \tag{6.12}$$

$$\|H_{\mathrm{JC}}\psi\| \leq \left(1 + \frac{\sqrt{2\alpha}g}{1 - \sqrt{2\alpha}g}\right) \|H_{\mathrm{R}}\psi\| + \frac{2g}{1 - \sqrt{2\alpha}g} \left(\alpha + \frac{1}{\alpha}\right)^{\frac{1}{2}} \|\psi\|, \tag{6.13}$$

($\alpha > 0$ small enough) *i.e.* H_{JC} and H_{R} are bounded with respect to each other with relative bound 1. Moreover, notice that since $\mathcal{D}(H_{\mathrm{R}}) = \mathcal{D}(H_{\mathrm{JC}}) = \mathcal{D}(H_0)$ it is obvious that each eigenvector of H_{JC} is in the domain of H_{R}. In addition, as one can see from (5.8), $|n, \nu\rangle$ belongs to the Schwartz space $\mathcal{S}(\mathbb{R})$, namely the set of rapidly decreasing functions on $\mathbb{R}$ (see [RS$_1$, Sect.V.3]). The Schwartz space $\mathcal{S}(\mathbb{R})$ is a core of H_{R} and is invariant in the sense that $H_{\mathrm{R}}^m |n, \nu\rangle \in \mathcal{S}(\mathbb{R})$ for every $m \in \mathbb{N}$, thus $|n, \nu\rangle \in \mathcal{D}(H_R^m)$ for every $m, n \in \mathbb{N}$, $\nu = \pm$.

6.2.2 Step 1

We start the proof with a standard argument. Since Π_E is invariant for H_{JC}, *i. e.* $\Pi_E H_{\mathrm{JC}} = H_{\mathrm{JC}}\Pi_E$, it commutes with $e^{-iH_{\mathrm{JC}}\frac{t}{\varepsilon}}$. Then

$$\begin{aligned}\left\|(\mathbb{1}-\Pi_E)e^{-iH_{\mathrm{R}}\frac{t}{\varepsilon}}\Pi_E\right\| &= \left\|(\mathbb{1}-\Pi_E)(e^{-iH_{\mathrm{R}}\frac{t}{\varepsilon}} - e^{-iH_{\mathrm{JC}}\frac{t}{\varepsilon}})\Pi_E\right\| \\ &= \left\|(\mathbb{1}-\Pi_E)e^{-iH_{\mathrm{JC}}\frac{t}{\varepsilon}}\frac{-i}{\varepsilon}\int_0^t d\tau\,\left[e^{iH_{\mathrm{JC}}\frac{\tau}{\varepsilon}}(H_{\mathrm{R}}-H_{\mathrm{JC}})\right]e^{-iH_{\mathrm{R}}\frac{\tau}{\varepsilon}}\Pi_E\right\| \\ &= \left\|e^{-iH_{\mathrm{JC}}\frac{t}{\varepsilon}}\frac{-ig}{\varepsilon}\int_0^t d\tau\,(\mathbb{1}-\Pi_E)\left[e^{iH_{\mathrm{JC}}\frac{\tau}{\varepsilon}}\left(a^\dagger\sigma^\dagger + a\sigma\right)\right]e^{-iH_{\mathrm{R}}\frac{\tau}{\varepsilon}}\Pi_E\right\|.\end{aligned} \tag{6.14}$$

We want to exploit the oscillating terms that are contained in last integral. More precisely, the operator $e^{iH_{\mathrm{JC}}\frac{\tau}{\varepsilon}}$ in the basis of the eigenvectors of H_{JC} is a multiplication by an oscillating phase $e^{iE_{\boldsymbol{n}}\frac{\tau}{\varepsilon}}$, $\boldsymbol{n} \in \mathcal{N}$. Therefore our next task will be to rewrite $e^{iH_{\mathrm{JC}}\frac{\tau}{\varepsilon}}\left(a^\dagger\sigma^\dagger + a\sigma\right)$ on this basis.

Remark 6.3 (Riemann-Lebesgue lemma)**.** The usual method to estimate an integral that contains an oscillating term is through the Riemann-Lebesgue lemma. Consider the integral

$$\begin{aligned}\int_0^t d\tau\, e^{i(c+o(\varepsilon))\frac{\tau}{\varepsilon}} f(\tau) &= \int_0^t d\tau\,\frac{d}{d\tau}\left(-i\frac{\varepsilon}{c+o(\varepsilon)}e^{i(c+o(\varepsilon))\frac{\tau}{\varepsilon}}\right)f(\tau) \\ &= \left[-i\frac{\varepsilon}{c+o(\varepsilon)}e^{i(c+o(\varepsilon))\frac{\tau}{\varepsilon}}f(\tau)\right]_0^t + i\frac{\varepsilon}{c+o(\varepsilon)}\int_0^t d\tau\, e^{i(c+o(\varepsilon))\frac{\tau}{\varepsilon}}f'(\tau).\end{aligned}$$

If f is sufficiently regular and has compact support in $(0,t)$ we get the estimate

$$\left|\int_0^t d\tau\, e^{i(c+o(\varepsilon))\frac{\tau}{\varepsilon}} f(\tau)\right| \le \frac{\varepsilon}{|c+o(\varepsilon)|}\left\|f'\right\|_{L^1}.$$

Moreover, if f has n derivatives we can iterate the trick to get

$$\left|\int_0^t d\tau\, e^{i(c+o(\varepsilon))\frac{\tau}{\varepsilon}} f(\tau)\right| \le \frac{\varepsilon^n}{|c+o(\varepsilon)|^n}\left\|f^{(n)}\right\|_{L^1}.$$

⌟

For the sake of a lighter notation we denote

$$\underline{\theta}_n := \frac{\theta_n}{2} \tag{6.15}$$

here and thereafter. We compute $a^\dagger\sigma^\dagger + a\sigma$ on the basis of eigenvectors of H_{JC}, namely $\{|\boldsymbol{n}\rangle\}_{\in\mathcal{N}}$ (see (5.8)),

$$\begin{aligned}(a^\dagger\sigma^\dagger + a\sigma)\,|n,+\rangle = & \quad \sqrt{n}\cos\frac{\theta_n}{2}\,|n-1\rangle\otimes e_{-1} + \sqrt{n+2}\sin\frac{\theta_n}{2}\,|n\rangle\otimes e_1 \\ = & \quad \sqrt{n}\cos\underline{\theta}_n\Big(\sin\underline{\theta}_{n-2}\,|n-2,+\rangle + \cos\underline{\theta}_{n-2}\,|n-2,-\rangle\Big) \\ & +\sqrt{n+2}\sin\underline{\theta}_n\Big(\cos\underline{\theta}_{n+2}\,|n+2,+\rangle - \sin\underline{\theta}_{n+2}\,|n+2,-\rangle\Big)\end{aligned}$$

$$\begin{aligned}(a^\dagger\sigma^\dagger + a\sigma)\,|n,-\rangle = & \quad -\sqrt{n}\sin\underline{\theta}_n\,|n-1\rangle\otimes e_{-1} + \sqrt{n+2}\cos\underline{\theta}_n\,|n+2\rangle\otimes e_1 \\ = & \quad -\sqrt{n}\sin\underline{\theta}_n\Big(\sin\underline{\theta}_{n-2}\,|n-2,+\rangle + \cos\underline{\theta}_{n-2}\,|n-2,-\rangle\Big) \\ & +\sqrt{n+2}\cos\underline{\theta}_n\Big(\cos\underline{\theta}_{n+2}\,|n+2,+\rangle - \sin\underline{\theta}_{n+2}\,|n+2,-\rangle\Big).\end{aligned}$$

Notice that $a^\dagger\sigma^\dagger$, $a\sigma$ act as raising and lowering operators (sometimes called *ladder operators*) on the subspaces $\mathcal{H}_n$

$$\mathrm{Ran}\left(a^\dagger\sigma^\dagger\restriction_{\mathcal{H}_n}\right)\subset\mathcal{H}_{n+2},\qquad \mathrm{Ran}\left(a\sigma\restriction_{\mathcal{H}_n}\right)\subset\mathcal{H}_{n-2}, \tag{6.16}$$

thus we denote

$$A_n^+ := a^\dagger\sigma^\dagger\restriction_{\mathcal{H}_n} = a^\dagger\sigma^\dagger P_n,\qquad A_n^- := a\sigma\restriction_{\mathcal{H}_n} = a\sigma P_n. \tag{6.17}$$

Then the coefficient matrix of $a^\dagger\sigma^\dagger + a\sigma$ in the basis $\{|\boldsymbol{n}\rangle\}_{\in\mathcal{N}}$ appears as

$$\begin{pmatrix} 0 & 0 & A_1^- & & & & & & & \\ 0 & 0 & 0 & A_2^- & \ddots & & & & & \\ A_{-1}^+ & 0 & 0 & 0 & \ddots & & & & & \\ & A_0^+ & 0 & 0 & \ddots & & & & & \\ & & A_1^+ & \ddots & \ddots & & & & & \\ & & & \ddots & \ddots & A_{n-1}^- & & & & \\ & & & & \ddots & 0 & 0 & A_n^- & & \\ & & & & \ddots & 0 & 0 & 0 & A_{n+1}^- \\ & & & & & A_{n-2}^+ & 0 & 0 & 0 \\ & & & & & & A_{n-1}^+ & 0 & 0 \\ & & & & & & & A_n^+ & \end{pmatrix} \tag{6.18}$$

where $A_n^\pm : \mathcal{H}_n \to \mathcal{H}_{n\pm2}$ acts as

$$A_n^+ = \sqrt{n+2}\begin{pmatrix} \sin\underline{\theta}_n\cos\underline{\theta}_{n+2} & \cos\underline{\theta}_n\cos\underline{\theta}_{n+2} \\ -\sin\underline{\theta}_n\sin\underline{\theta}_{n+2} & -\cos\underline{\theta}_n\sin\underline{\theta}_{n+2}\end{pmatrix} \tag{6.19}$$

$$A_n^- = \sqrt{n}\begin{pmatrix} \sin\underline{\theta}_{n-2}\cos\underline{\theta}_n & -\sin\underline{\theta}_{n-2}\sin\underline{\theta}_n \\ \cos\underline{\theta}_{n-2}\cos\underline{\theta}_n & -\cos\underline{\theta}_{n-2}\sin\underline{\theta}_n\end{pmatrix}. \tag{6.20}$$

when seen as linear maps from $\mathbb{C}^2$ with basis $\{|n,+\rangle, |n,-\rangle\}$ onto $\mathbb{C}^2$ with basis $\{|n\pm 2,+\rangle, |n\pm 2,-\rangle\}$. Observe that $(A^-_{n+2})^\dagger = A^+_n$.

The evolutor $e^{iH_{\mathrm{JC}}\frac{t}{\varepsilon}}$ assumes in this basis the block form

$$\begin{pmatrix} e^{i\frac{-\varepsilon(\Omega+\omega)}{2}\frac{\tau}{\varepsilon}} & & & \\ & e^{iH_0\frac{\tau}{\varepsilon}} & & \\ & & e^{iH_1\frac{\tau}{\varepsilon}} & \\ & & & \ddots \end{pmatrix}$$

therefore

$$e^{iH_{\mathrm{JC}}\frac{t}{\varepsilon}}(a^\dagger\sigma^\dagger + a\sigma) = \tag{6.21}$$

$$\begin{pmatrix}
0 & 0 & \Gamma_1^- & & & & & & \\
0 & 0 & 0 & \Gamma_2^- & & & & & \\
\Gamma_{-1}^+ & 0 & 0 & 0 & \ddots & & & & \\
 & \Gamma_0^+ & 0 & 0 & \ddots & \ddots & & & \\
 & & \Gamma_1^+ & \ddots & \ddots & \ddots & \Gamma_{n-1}^- & & \\
 & & & \ddots & \ddots & 0 & 0 & \Gamma_n^- & \\
 & & & & \ddots & 0 & 0 & 0 & \Gamma_{n+1}^- \\
 & & & & & \Gamma_{n-2}^+ & 0 & 0 & 0 \\
 & & & & & & \Gamma_{n-1}^+ & 0 & 0 \\
 & & & & & & & \Gamma_n^+ &
\end{pmatrix}$$

where

$$\Gamma_n^+ = e^{iH_{n+2}\frac{\tau}{\varepsilon}}A_n^+ = \sqrt{n+2}\begin{pmatrix} e^{iE_{(n+2,+)}\frac{\tau}{\varepsilon}}\sin\underline{\theta}_n\cos\underline{\theta}_{n+2} & e^{iE_{(n+2,+)}\frac{\tau}{\varepsilon}}\cos\underline{\theta}_n\cos\underline{\theta}_{n+2} \\ -e^{iE_{n+2,-}\frac{\tau}{\varepsilon}}\sin\underline{\theta}_n\sin\underline{\theta}_{n+2} & -e^{iE_{n+2,-}\frac{\tau}{\varepsilon}}\cos\underline{\theta}_n\sin\underline{\theta}_{n+2} \end{pmatrix} \tag{6.22}$$

$$\Gamma_n^- = e^{iH_{n-2}\frac{\tau}{\varepsilon}}A_n^- = \sqrt{n}\begin{pmatrix} e^{iE_{(n-2,+)}\frac{\tau}{\varepsilon}}\cos\underline{\theta}_n\sin\underline{\theta}_{n-2} & -e^{iE_{(n-2,+)}\frac{\tau}{\varepsilon}}\sin\underline{\theta}_n\sin\underline{\theta}_{n-2} \\ e^{iE_{(n-2,-)}\frac{\tau}{\varepsilon}}\cos\underline{\theta}_n\cos\underline{\theta}_{n-2} & -e^{iE_{(n-2,-)}\frac{\tau}{\varepsilon}}\sin\underline{\theta}_n\cos\underline{\theta}_{n-2} \end{pmatrix}. \tag{6.23}$$

By means of $\Gamma_n^\pm$, the integrand of (6.14) reads

$$\begin{aligned}
(\mathbb{1}-\Pi_E)\Big[e^{iH_{\mathrm{JC}}\frac{\tau}{\varepsilon}}\Big(a^\dagger\sigma^\dagger + a\sigma\Big)\Big]e^{-iH_{\mathrm{R}}\frac{\tau}{\varepsilon}}\Pi_E &= \\
&= (\mathbb{1}-\Pi_E)\left[\sum_{n\geq 1}(\Gamma_n^- + \Gamma_n^+)P_n + \Gamma_0^+P_0 + \Gamma_{-1}^+P_{-1}\right]e^{-iH_{\mathrm{R}}\frac{\tau}{\varepsilon}}\Pi_E \\
&= \left[\sum_{n>E+2}\Gamma_n^-P_n + \sum_{n>E-2}\Gamma_n^+P_n\right]e^{-iH_{\mathrm{R}}\frac{\tau}{\varepsilon}}\Pi_E
\end{aligned}$$

expanding $P_n = \sum_{\nu=\pm} |\boldsymbol{n}\rangle\langle\boldsymbol{n}| = \sum_{\nu=\pm} |n,\nu\rangle\langle n,\nu|$ the latter row is equal to

$$= \Bigg[\sum_{\substack{\boldsymbol{n}\in\mathcal{N} \\ n>E+2}} \Gamma_n^- |\boldsymbol{n}\rangle\langle\boldsymbol{n}| + \sum_{\substack{\boldsymbol{n}\in\mathcal{N} \\ n>E-2}} \Gamma_n^+ |\boldsymbol{n}\rangle\langle\boldsymbol{n}| \Bigg] e^{-iH_{\mathrm{R}}\frac{\tau}{\varepsilon}} \sum_{\substack{\boldsymbol{m}\in\mathcal{N} \\ m\leq E}} |\boldsymbol{m}\rangle\langle\boldsymbol{m}| \,.$$

We define

$$p_{\boldsymbol{n},\boldsymbol{m}}(\varepsilon, g, t) := \langle\boldsymbol{n}| e^{-iH_{\mathrm{R}}t} |\boldsymbol{m}\rangle \,, \tag{6.24}$$

and rewriting the latter row once again we arrive at

$$(\mathbb{1} - \Pi_E)\Big[e^{iH_{\mathrm{JC}}\frac{\tau}{\varepsilon}}\Big(a^\dagger\sigma^\dagger + a\sigma\Big)\Big]e^{-iH_{\mathrm{R}}\frac{\tau}{\varepsilon}}\Pi_E = \tag{6.25}$$

$$= \sum_{\substack{\boldsymbol{n}\in\mathcal{N} \\ n>E+2}} \sum_{\substack{\boldsymbol{m}\in\mathcal{N} \\ m\leq E}} p_{\boldsymbol{n},\boldsymbol{m}}(\varepsilon, g, \tau/\varepsilon)\Gamma_n^- |\boldsymbol{n}\rangle\langle\boldsymbol{m}| \tag{6.26}$$

$$+ \sum_{\substack{\boldsymbol{n}\in\mathcal{N} \\ n>E-2}} \sum_{\substack{\boldsymbol{m}\in\mathcal{N} \\ m\leq E}} p_{\boldsymbol{n},\boldsymbol{m}}(\varepsilon, g, \tau/\varepsilon)\Gamma_n^+ |\boldsymbol{n}\rangle\langle\boldsymbol{m}| \,. \tag{6.27}$$

In the following we will always omit the ε and g dependence of functions $p_{\boldsymbol{n},\boldsymbol{m}}$ for the sake of a lighter notation.

To summarize, to estimate (6.14) we decomposed the integrand on subspaces $\mathcal{H}_n$. Each subspace $\mathcal{H}_m$, $m \leq E$ evolves under the operator $\left(a^\dagger\sigma^\dagger + a\sigma\right) e^{-iH_{\mathrm{R}}\frac{\tau}{\varepsilon}}$ and gives a contribution on $\mathcal{H}_n$ which is

$$\sum_{\substack{\nu=\pm \\ n>E+2}} \sum_{\mu=\pm} p_{n,\nu,m,\mu}(\tau/\varepsilon)\Gamma_n^- |n,\nu\rangle\langle m,\mu| + \sum_{\substack{\nu=\pm \\ n>E-2}} \sum_{\mu=\pm} p_{n,\nu,m,\mu}(\tau/\varepsilon)\Gamma_n^+ |n,\nu\rangle\langle m,\mu| \,.$$

Each one of these eight terms is proportional to an oscillating phase produced by the action of $\Gamma_n^\pm$ on $|n,\nu\rangle$. Consider for example, $\nu = +$ in the previous expression, then

$$\begin{aligned} p_{n,+,m,\mu}(\tau/\varepsilon)\Gamma_n^- |n,+\rangle\langle m,\mu| &= \\ &= \sqrt{n}\, p_{n,+,m,\mu}(\tau/\varepsilon) e^{iE_{(n-2,+)}\frac{\tau}{\varepsilon}} \cos\underline{\theta}_n \sin\underline{\theta}_{n-2} |n-2,+\rangle\langle m,\mu| \,. \end{aligned} \tag{6.28}$$

In the latter term one recognizes: the oscillating phase; the coefficient p which is ε-dependent; the term $\cos\underline{\theta}_n \sin\underline{\theta}_{n-2}$ which depend on ε and g through $\underline{\theta}_n, \underline{\theta}_{n-2}$ but are bounded; the rank one operator $|n-2,+\rangle\langle m,\mu|$. Each other term of (6.26),(6.27) has the same structure. Therefore to bound (6.14) by means of the Riemann-Lebesgue lemma we need information about the regularity and the summability of coefficients $p_{\boldsymbol{n},\boldsymbol{m}}$.

6.2.3 Regularity of p coefficients

From conserved quantities and expectations of certain observables we can recover regularity and summability properties of coefficients $p_{\boldsymbol{n},\boldsymbol{m}}$.

(i) The dynamics is unitary. Observe that for each $\boldsymbol{m} \in \mathcal{N}$

$$e^{-iH_{\mathrm{R}}t} |\boldsymbol{m}\rangle = \sum_{\boldsymbol{n}\in\mathcal{N}} \langle \boldsymbol{n}| e^{-iH_{\mathrm{R}}t} |\boldsymbol{m}\rangle |\boldsymbol{n}\rangle ,$$

and being the vector on the left of norm one

$$1 = \sum_{\boldsymbol{n}\in\mathcal{N}} |p_{\boldsymbol{n},\boldsymbol{m}}(t)|^2 , \tag{6.29}$$

then $|p_{\boldsymbol{n},\boldsymbol{m}}(t)| \leq 1$, *i. e.* $p_{\boldsymbol{n},\boldsymbol{m}} \in L^\infty(\mathbb{R})$, and $p_{\boldsymbol{n},\boldsymbol{m}} \in l^2(\mathcal{N})$ uniformly in t.

(ii) The energy of the system is conserved, moreover H_{JC} is finite on the evolution of each initial state $|\boldsymbol{m}\rangle$, $\boldsymbol{m} \in \mathcal{N}$ because

$$\begin{aligned} \left|\langle \boldsymbol{m}| e^{iH_{\mathrm{R}}t} H_{\mathrm{JC}} e^{-iH_{\mathrm{R}}t} |\boldsymbol{m}\rangle\right| &\leq \left\|e^{-iH_{\mathrm{R}}t} |\boldsymbol{m}\rangle\right\| \left\|H_{\mathrm{JC}} e^{-iH_{\mathrm{R}}t} |\boldsymbol{m}\rangle\right\| \\ &\leq A \left\|H_{\mathrm{R}} e^{-iH_{\mathrm{R}}t} |\boldsymbol{m}\rangle\right\| + B \left\|e^{-iH_{\mathrm{R}}t} |\boldsymbol{m}\rangle\right\| \\ &\leq A^2 \left\|H_{\mathrm{JC}} |\boldsymbol{m}\rangle\right\| + AB \left\||\boldsymbol{m}\rangle\right\| + B \\ &\leq A^2 E_{\boldsymbol{m}} + AB + B \\ &= (1 + O(g))E_{\boldsymbol{m}} + O(g) < \infty \end{aligned}$$

where A, B are the constants that appear in the estimates (6.12),(6.13),

$$A = \left(1 + \frac{\sqrt{2\alpha}g}{1 - \sqrt{2\alpha}g}\right), \qquad B = \frac{2g}{1 - \sqrt{2\alpha}g} \left(\alpha + \frac{1}{\alpha}\right)^{\frac{1}{2}} .$$

We compute the following expectation

$$\begin{aligned} \langle \boldsymbol{m}| e^{iH_{\mathrm{R}}t} H_{\mathrm{JC}} e^{-iH_{\mathrm{R}}t} |\boldsymbol{m}\rangle &= \sum_{\boldsymbol{n},\boldsymbol{n}'\in\mathcal{N}} \langle \boldsymbol{m}| e^{iH_{\mathrm{R}}t} |\boldsymbol{n}\rangle \langle \boldsymbol{n}| H_{\mathrm{JC}} |\boldsymbol{n}'\rangle \langle \boldsymbol{n}'| e^{-iH_{\mathrm{R}}t} |\boldsymbol{m}\rangle \\ &= \sum_{\boldsymbol{n},\boldsymbol{n}'\in\mathcal{N}} \overline{p}_{\boldsymbol{m},\boldsymbol{n}}(t) E_{\boldsymbol{n}} \delta_{\boldsymbol{n}=\boldsymbol{n}'} p_{\boldsymbol{n}',\boldsymbol{m}}(t) \\ &= \sum_{\boldsymbol{n}\in\mathcal{N}} E_{\boldsymbol{n}} |p_{\boldsymbol{n},\boldsymbol{m}}(t)|^2 \end{aligned}$$

thus by the previous estimate

$$\sum_{\boldsymbol{n}\in\mathcal{N}} E_{\boldsymbol{n}} |p_{\boldsymbol{n},\boldsymbol{m}}(t)|^2 \leq (1 + O(g))E_{\boldsymbol{m}} + O(g) < \infty \tag{6.30}$$

Observe that $E_{\boldsymbol{n}}$ is a function of g, but for every fixed values of $\hat{g}$ only a finite number of terms in the sum (6.30) are negative. In fact, recall that

$$E_{\boldsymbol{n}}(g) = \omega(n+1) + \nu\frac{1}{2}\sqrt{\Delta^2 + 4g^2(n+1)}, \tag{6.31}$$

then $E_{n,+} \geq \omega(n+1)$ and

$$E_{n,-}(g) = 0 \qquad \Leftrightarrow \qquad g = \sqrt{\omega^2(n+1) - \frac{\Delta^2}{4(n+1)}} \underset{n\to\infty}{\to} \infty. \tag{6.32}$$

Analogously, for the second power of H_{JC} holds

$$\begin{aligned}\sum_{\boldsymbol{n}\in\mathcal{N}} E_{\boldsymbol{n}}^2 \left|p_{\boldsymbol{n},\boldsymbol{m}}(t)\right|^2 &= \langle\boldsymbol{m}|\, e^{iH_{\mathrm{R}}t} H_{\mathrm{JC}}^2 e^{-iH_{\mathrm{R}}t} \,|\boldsymbol{m}\rangle \\ &\leq \left\| H_{\mathrm{JC}} e^{-iH_{\mathrm{R}}t}\,|\boldsymbol{m}\rangle\right\| \left\| H_{\mathrm{JC}} e^{-iH_{\mathrm{R}}t}\,|\boldsymbol{m}\rangle\right\| < \infty\end{aligned}$$

which means that $n\, p_{\boldsymbol{n},\boldsymbol{m}} \in l^2(\mathcal{N})$ uniformly in t because

$$\begin{aligned}2\omega(n+1) \geq& E_{n,+} \geq \omega(n+1) \\ \omega(n+1) \geq& E_{n,-} \geq \omega(n+1)[1 - O(\varepsilon) - O(g)]\end{aligned}$$

hold definitively in $n \in \mathbb{N}$ (see Appendix 6.A).

(iii) We compute the time derivative of $p_{\boldsymbol{n},\boldsymbol{m}}(t)$,

$$\frac{d\,p_{\boldsymbol{n},\boldsymbol{m}}}{dt}(t) = \langle\boldsymbol{n}|\,(-iH_{\mathrm{R}})e^{-iH_{\mathrm{R}}t}\,|\boldsymbol{m}\rangle\,,$$

thus

$$\begin{aligned}\sum_{\boldsymbol{n}\in\mathcal{N}} \left|\frac{d\,p_{\boldsymbol{n},\boldsymbol{m}}}{dt}(t)\right|^2 &= \sum_{\boldsymbol{n}\in\mathcal{N}} \left|\langle\boldsymbol{n}|\, H_{\mathrm{R}} e^{-iH_{\mathrm{R}}t}\,|\boldsymbol{m}\rangle\right|^2 \\ &= \mathrm{tr}\left(H_{\mathrm{R}} e^{-iH_{\mathrm{R}}t}\,|\boldsymbol{m}\rangle\langle\boldsymbol{m}|\, e^{iH_{\mathrm{R}}t} H_{\mathrm{R}}\right) \\ &= \mathrm{tr}\left(H_{\mathrm{R}}^2\,|\boldsymbol{m}\rangle\langle\boldsymbol{m}|\right) \\ &= \langle\boldsymbol{m}|\, H_{\mathrm{R}}^2\,|\boldsymbol{m}\rangle < \infty\end{aligned}$$

because of (6.12). So $\frac{d\,p_{\boldsymbol{n},\boldsymbol{m}}}{dt} \in L^\infty(\mathbb{R})$ and $e^{-iH_{\mathrm{R}}t}\,|\boldsymbol{m}\rangle \in L^2(\mathbb{R})$ for every t. Similarly

$$\frac{d^k\,p_{\boldsymbol{n},\boldsymbol{m}}}{dt^k}(t) = \langle\boldsymbol{n}|\,(-iH_{\mathrm{R}})^m e^{-iH_{\mathrm{R}}t}\,|\boldsymbol{m}\rangle\,,$$

and

$$\begin{aligned}\sum_{\boldsymbol{n}} \left|\frac{d^k\,p_{\boldsymbol{n},\boldsymbol{m}}}{dt^k}(t)\right|^2 &= \sum_{\boldsymbol{n}} \left|\langle\boldsymbol{n}|\, H_{\mathrm{R}}^k e^{-iH_{\mathrm{R}}t}\,|\boldsymbol{m}\rangle\right|^2 \\ &= Tr\left(H_{\mathrm{R}}^k e^{-iH_{\mathrm{R}}t}\,|\boldsymbol{m}\rangle\langle\boldsymbol{m}|\, e^{iH_{\mathrm{R}}t} H_{\mathrm{R}}^k\right) \\ &= \langle\boldsymbol{m}|\, H_{\mathrm{R}}^{2k}\,|\boldsymbol{m}\rangle\end{aligned}$$

which is bounded because $|\boldsymbol{m}\rangle \in \mathcal{D}(H_{\mathrm{R}}^k)$ for all $k \in \mathbb{N}$, as we noticed in Sect.6.2.1. For the second power, $k = 2$, we can explicitly compute

$$\begin{aligned}H_{\mathrm{R}}(H_{\mathrm{R}}\,|\boldsymbol{m}\rangle) =& H_{\mathrm{R}}\left(H_{\mathrm{JC}}\,|\boldsymbol{m}\rangle + g(a^\dagger\sigma^\dagger + a\sigma)\,|\boldsymbol{m}\rangle\right) \\ =& H_{\mathrm{R}}\left(E_{\boldsymbol{m}}\,|\boldsymbol{m}\rangle + gA_m^+\,|\boldsymbol{m}\rangle + gA_m^-\,|\boldsymbol{m}\rangle\right) \\ =& E_{\boldsymbol{m}}^2\,|\boldsymbol{m}\rangle + gH_{\mathrm{JC}}A_m^+\,|\boldsymbol{m}\rangle + gH_{\mathrm{JC}}A_m^-\,|\boldsymbol{m}\rangle + E_{\boldsymbol{m}}g(A_m^+ + A_m^-)\,|\boldsymbol{m}\rangle \\ &+ g^2(A_{m+2}^+ + A_{m+2}^-)A_m^+\,|\boldsymbol{m}\rangle + g^2(A_{m-2}^+ + A_{m-2}^-)A_m^-\,|\boldsymbol{m}\rangle\,.\end{aligned} \tag{6.33}$$

One recognize from the latter that

$$\begin{aligned}g^2A_{m-2}^-A_m^-\,|\boldsymbol{m}\rangle &\in \mathcal{H}_{m-4} \\ gH_{\mathrm{JC}}A_m^-\,|\boldsymbol{m}\rangle + gE_{\boldsymbol{m}}A_m^-\,|\boldsymbol{m}\rangle &\in \mathcal{H}_{m-2} \\ E_{\boldsymbol{m}}^2\,|\boldsymbol{m}\rangle + g^2A_{m+2}^-A_m^+\,|\boldsymbol{m}\rangle + g^2A_{m-2}^+A_m^-\,|\boldsymbol{m}\rangle &\in \mathcal{H}_m \\ gH_{\mathrm{JC}}A_m^+\,|\boldsymbol{m}\rangle + gE_{\boldsymbol{m}}A_m^+\,|\boldsymbol{m}\rangle &\in \mathcal{H}_{m+2} \\ g^2A_{m+2}^+A_m^+\,|\boldsymbol{m}\rangle &\in \mathcal{H}_{m+4}\end{aligned}$$

and being all operators in the previous expression bounded, is clear that $\langle\boldsymbol{m}|\,H_{\mathrm{R}}^4\,|\boldsymbol{m}\rangle < \infty$.

In summary, for the second derivative $k = 2$, holds $\frac{d^2\,p_{\boldsymbol{n},\boldsymbol{m}}}{dt^2}(t) \in L^\infty(\mathbb{R})$, $\frac{d^2\,p_{\boldsymbol{n},\boldsymbol{m}}}{dt^2}(t) \in l^2(\mathcal{N})$.

6.2.4 Step 2

Consider the summand

$$S_1 := \sum_{n>E+2}\sum_{\substack{\boldsymbol{m}\in\mathcal{N}\\ m\le E}} p_{n,+,\boldsymbol{m}}(\tau/\varepsilon)\Gamma_n^-\,|n,+\rangle\,\langle\boldsymbol{m}| \tag{6.34}$$

in equation (6.26). It has other three analogous terms that complete the integrand (6.25). We will estimate this sample term in details, since the others can be estimated in the same way.

Expanding (6.34) as in (6.28) and integrating as in (6.14) we get

$$\begin{aligned}
&\left\| e^{-iH_{\mathrm{JC}}\frac{t}{\varepsilon}} \frac{g}{2\varepsilon} \int_0^t d\tau \sum_{\substack{n>E+2\\ \boldsymbol{m}\in\mathcal{N}\\ m\leq E}} \sqrt{n} p_{n,+,\boldsymbol{m}}(\tau/\varepsilon) e^{iE_{(n-2,+)}\frac{\tau}{\varepsilon}} \cos\underline{\theta}_n \sin\underline{\theta}_{n-2} \left|n-2,+\right\rangle \left\langle \boldsymbol{m}\right| \right\| \\
&\leq \frac{g}{\varepsilon} \int_0^t d\tau \left\| \sum_{\substack{n>E+2\\ \boldsymbol{m}\in\mathcal{N}\\ m\leq E}} \sqrt{n} p_{n,+,\boldsymbol{m}}(\tau/\varepsilon) e^{iE_{(n-2,+)}\frac{\tau}{\varepsilon}} \cos\underline{\theta}_n \sin\underline{\theta}_{n-2} \left|n-2,+\right\rangle \left\langle \boldsymbol{m}\right| \right\| \\
&\leq \frac{g}{\varepsilon} \int_0^t d\tau \sum_{\substack{\boldsymbol{m}\in\mathcal{N}\\ m\leq E}} \left\| \sum_{n>E+2} \sqrt{n} p_{n,+,\boldsymbol{m}}(\tau/\varepsilon) e^{iE_{(n-2,+)}\frac{\tau}{\varepsilon}} \cos\underline{\theta}_n \sin\underline{\theta}_{n-2} \left|n-2,+\right\rangle \left\langle \boldsymbol{m}\right| \right\| \\
&\leq \frac{g}{\varepsilon} \int_0^t d\tau \sum_{\substack{\boldsymbol{m}\in\mathcal{N}\\ m\leq E}} \left\| \sum_{n>E+2} \sqrt{n} p_{n,+,\boldsymbol{m}}(\tau/\varepsilon) e^{iE_{(n-2,+)}\frac{\tau}{\varepsilon}} \cos\underline{\theta}_n \sin\underline{\theta}_{n-2} \left|n-2,+\right\rangle \right\| \left\| \left|\boldsymbol{m}\right\rangle \right\| \\
&\leq \frac{g}{\varepsilon} \int_0^t d\tau \sum_{\substack{\boldsymbol{m}\in\mathcal{N}\\ m\leq E}} \left(\sum_{n>E+2} n \left|p_{n,+,\boldsymbol{m}}(\tau/\varepsilon)\right|^2 \right)^{\frac{1}{2}}.
\end{aligned}$$

Since we proved that $\sum_{\boldsymbol{n}} n \left|p_{n,+,\boldsymbol{m}}(t)\right|^2 < \infty$ uniformly t, then the latter row is bounded by

$$\frac{g}{\varepsilon} \int_0^t d\tau \sum_{\substack{\boldsymbol{m}\in\mathcal{N}\\ m\leq E}} \left(\sum_{n>E+2} n \left|p_{n,+,\boldsymbol{m}}(\tau/\varepsilon)\right|^2 \right)^{\frac{1}{2}} \leq \frac{g}{\varepsilon} Ct \tag{6.35}$$

which is the bound we stated. As anticipated, the other summands in (6.26) can be estimated by essentially the same argument, yielding the claim.

To end the proof we illustrate an attempt to improve the previous estimate exploiting the oscillating phase by means of the Riemann-Lebesgue lemma. Notice that the sequence

$$\sum_{n>E+2}^{N} \sum_{\substack{\boldsymbol{m}\in\mathcal{N}\\ m\leq E}} p_{n,+,\boldsymbol{m}}(\tau/\varepsilon) \Gamma_n^- \left|n,+\right\rangle \left\langle \boldsymbol{m}\right|$$

is Cauchy in $C([0,t];\mathcal{B}(\mathcal{H}))$ and, being the integral continuous in that topology, we can move the integral inside the summation getting

$$\begin{aligned}
&\left\| e^{-iH_{\mathrm{JC}}\frac{t}{\varepsilon}} \frac{g}{2\varepsilon} \sum_{\substack{n>E+2\\ \boldsymbol{m}\in\mathcal{N}\\ m\leq E}} \sqrt{n}\cos\underline{\theta}_n \sin\underline{\theta}_{n-2} \int_0^t d\tau\, p_{n,+,\boldsymbol{m}}(\tau/\varepsilon) e^{iE_{(n-2,+)}\frac{\tau}{\varepsilon}} \left|n-2,+\right\rangle \left\langle \boldsymbol{m}\right| \right\| \\
&\qquad\leq g \sum_{\substack{n>E+2\\ \boldsymbol{m}\in\mathcal{N}\\ m\leq E}} \sqrt{n} \left| \frac{1}{\varepsilon}\int_0^t d\tau\, p_{n,+,\boldsymbol{m}}(\tau/\varepsilon) e^{iE_{(n-2,+)}\frac{\tau}{\varepsilon}} \right| \|\left|n-2,+\right\rangle\left\langle\boldsymbol{m}\right|\|. \qquad (6.36)
\end{aligned}$$

Then, the term inside the absolute value can be integrated by parts obtaining

$$\begin{aligned}
&\frac{1}{\varepsilon}\int_0^t d\tau\, p_{n,+,\boldsymbol{m}}(\tau/\varepsilon) e^{iE_{(n-2,+)}\frac{\tau}{\varepsilon}} \\
&\qquad= \left[\frac{p_{n,+,\boldsymbol{m}}(\tau)e^{iE_{(n-2,+)}\tau}}{iE_{(n-2,+)}}\right]_0^{\frac{t}{\varepsilon}} + i\frac{1}{E_{(n-2,+)}}\int_0^{\frac{t}{\varepsilon}} d\tau\, \frac{d\,p_{n,+,\boldsymbol{m}}}{d\tau}(\tau)\, e^{iE_{(n-2,+)}\tau}.
\end{aligned}$$

Therefore (6.36) is bounded by

$$\begin{aligned}
&g\sum_{\substack{n>E+2\\ \boldsymbol{m}\in\mathcal{N}\\ m\leq E}} \frac{\sqrt{n}}{\left|E_{(n-2,+)}\right|}\left(\left|p_{n,+,\boldsymbol{m}}(t/\varepsilon)\right| + \left|p_{n,+,\boldsymbol{m}}(0)\right| + \left|\int_0^{\frac{t}{\varepsilon}} d\tau\, \frac{d\,p_{n,+,\boldsymbol{m}}}{d\tau}(\tau)\, e^{iE_{(n-2,+)}\tau}\right|\right) \\
&\qquad\leq\; g\sum_{\substack{n>E+2\\ \boldsymbol{m}\in\mathcal{N}\\ m\leq E}} \frac{\sqrt{n}}{\left|E_{(n-2,+)}\right|}\left(\left|p_{n,+,\boldsymbol{m}}(t/\varepsilon)\right| + \left|p_{n,+,\boldsymbol{m}}(0)\right| + \left\|\frac{d}{dt}\left(p_{n,+,\boldsymbol{m}}\right)\right\|_\infty \frac{t}{\varepsilon}\right).
\end{aligned}$$

Since $\left|E_{(n-2,+)}\right| \sim n$, to bound the last line is sufficient to prove that $\sum n^\alpha \left|p_{n,+,\boldsymbol{m}}(t)\right|^2 < \infty$ for some $\alpha > 0$, which is satisfied because $\sqrt{n}\,p_{n,+,\boldsymbol{m}} \in l^2(\mathbb{N})$, and $\left\|\frac{d}{dt}\left(p_{n,+,\boldsymbol{m}}\right)\right\|_\infty \leq n^{-(1/2+\delta)}$ for some $\delta > 0$.

However, one can perform another integration by parts to obtain

$$\begin{aligned}
&\frac{1}{\varepsilon}\int_0^t d\tau\, p_{n,+,\boldsymbol{m}}(\tau/\varepsilon) e^{iE_{(n-2,+)}\frac{\tau}{\varepsilon}} = \\
&\qquad\qquad \left[\frac{p_{n,+,\boldsymbol{m}}(\tau)e^{iE_{(n-2,+)}\tau}}{iE_{(n-2,+)}}\right]_0^{\frac{t}{\varepsilon}} + i\left[\frac{\frac{d}{d\tau}\left(p_{n,+,\boldsymbol{m}}\right)(\tau)e^{iE_{(n-2,+)}\tau}}{iE^2_{(n-2,+)}}\right]_0^{\frac{t}{\varepsilon}} \\
&\qquad\qquad - \frac{1}{E^2_{(n-2,+)}}\int_0^{\frac{t}{\varepsilon}} d\tau\, \frac{d^2\,p_{n,+,\boldsymbol{m}}}{d\tau^2}(\tau) e^{iE_{(n-2,+)}\tau}.
\end{aligned}$$

Then (6.36) is bounded by

$$g \sum_{\substack{n>E+2 \\ \boldsymbol{m}\in\mathcal{N} \\ m\leq E}} \frac{\sqrt{n}}{\left|E_{(n-2,+)}\right|} \left(|p_{n,+,\boldsymbol{m}}(t/\varepsilon)| + |p_{n,+,\boldsymbol{m}}(0)|\right)$$
$$+ \frac{\sqrt{n}}{E^2_{(n-2,+)}} \left(\left| \frac{d\,p_{n,+,\boldsymbol{m}}}{dt}(t/\varepsilon) \right| + \left| \frac{d\,p_{n,+,\boldsymbol{m}}}{dt}(0) \right| + \left\| \frac{d^2\,p_{n,+,\boldsymbol{m}}}{dt^2} \right\|_\infty \frac{t}{\varepsilon} \right). \quad (6.37)$$

Observe that to have summability is now sufficient that $\sum n^\alpha \left|p_{n,+,\boldsymbol{m}}(t)\right|^2 < \infty$ for some $\alpha > 0$ and $\left\|\frac{d}{dt}(p_{n,+,\boldsymbol{m}})\right\|_\infty, \|\frac{d^2}{dt^2}(p_{n,+,\boldsymbol{m}})\|_\infty < \infty$. Those are weaker conditions that are satisfied as we have seen in Sect.6.2.3. In conclusion for (6.37) we get an estimate for the first summand in (6.26), namely

$$C_1 g + C_2 \frac{g}{\varepsilon} t \leq \max\{C_1\varepsilon, C_2\} \frac{g}{\varepsilon}(1+t).$$

The latter estimate is not better than (6.35) since the bound we obtained for $\|\frac{d^2}{dt^2}(p_{n,+,\boldsymbol{m}})\|_\infty$ is $O(1)$ as $\varepsilon \to 0$ and $O(1)$ as $g \to 0$ (see (6.33)). Therefore, to render useful this last argument we need to understand if the bound on $\|\frac{d^2}{dt^2}(p_{n,+,\boldsymbol{m}})\|_\infty$ could be improved to $O(g^\alpha)$ or $O(\varepsilon^\beta)$ for some $\alpha, \beta > 0$. It is not clear if this kind of bound can be achieved on the second time derivative or on higher derivatives.

Appendix 6.A

Proposition 6.4. *Let $\boldsymbol{n} \in \mathcal{N}$ and $E_{\boldsymbol{n}}$ defined as in* (5.13)

$$E_{\boldsymbol{n}}(g) = \omega(n+1) + \nu\frac{\omega+\Omega}{2}\sqrt{\varepsilon^2 + \frac{4g^2(n+1)}{(\omega+\Omega)^2}}.$$

Then

(a) *If $g = o(\varepsilon)$, i.e. $g/\varepsilon \to 0$*

$$E_{\boldsymbol{n}} = \omega(n+1) + \nu\frac{\omega+\Omega}{2}\varepsilon + \nu\frac{n+1}{\omega+\Omega}\frac{g^2}{\varepsilon} + \varepsilon \cdot o\left(\frac{g^2}{\varepsilon^2}\right) \quad (6.38)$$

(b) *If $g = \varepsilon^\alpha$ with $0 \leq \alpha < 1$, i.e. $\varepsilon/g \to 0$*

$$E_{\boldsymbol{n}} = \omega(n+1) + \nu\sqrt{n+1}g + \nu\frac{(\omega+\Omega)^2}{8\sqrt{n+1}}\frac{\varepsilon^2}{g} + g \cdot o\left(\frac{\varepsilon^2}{g^2}\right) \quad (6.39)$$

Proof. $E(x) = \sqrt{1+x} = 1 + \frac{1}{2}x + \sum_{n=2}^\infty c_n x^n$ for $|x| \leq 1$ with

$$c_n = (-1)^{n-1}\frac{(2n)!}{(2n-1)4^n(n!)^2}\left(= (-1)^{n-1}\frac{1}{2^n}\frac{1\cdot 3\cdot 5\cdots(2n-3)}{n!}\right).$$

Observe that

$$\begin{aligned} c_{n+1}x^{n+1} &= (-1)^{n+1-1}\frac{(2(n+1))!}{(2(n+1)-1)4^{n+1}(n+1)!(n+1)!}x^{n+1} \\ &= (-1)\frac{(2n-1)2(n+1)(2n+1)}{(2n+1)4(n+1)(n+1)}xc_nx^n \end{aligned}$$

so

$$c_nx^n + c_{n+1}x^{n+1} = c_nx^n(1-\frac{2n-1}{2n+2}x) \quad \begin{cases} <0 & \text{if} \quad c_n<0 \Leftrightarrow n=2k \\ >0 & \text{if} \quad c_n>0 \Leftrightarrow n=2k+1 \end{cases}.$$

Then

$$E(x) = 1 + \sum_{n=1}^{2k+1} c_nx^n + \sum_{m=2k+2}^{\infty} c_mx^m < 1 + \sum_{n=1}^{2k+1} c_nx^n, \qquad \forall k \in \mathbb{N},\ |x| \le 1$$

$$E(x) = 1 + \frac{1}{2}x + \sum_{n=2}^{2k} c_nx^n + \sum_{m=2k+1}^{\infty} c_mx^m > 1 + \frac{1}{2}x + \sum_{n=2}^{2k} c_nx^n, \qquad \forall k \in \mathbb{N},\ |x| \le 1$$

□

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