Universidad Complutense de Madrid

Facultad de Ciencias Físicas
Departamento de Física Teórica II
(Métodos Matemáticos de la Física)

Classical and Quantum Formulations of $\mathbb{S}^1 \times \mathbb{S}^2$ and $\mathbb{S}^3$ Gowdy Models Coupled with Matter

Exploring the Mathematical Aspects of
Gravity and Quantum Field Theory

Daniel Gómez Vergel

Instituto de Estructura de la Materia, CSIC

Research Advisors:
Dr. Jesús Fernando Barbero González[1]
Dr. Eduardo Jesús Sánchez Villaseñor[2]

[1]Instituto de Estructura de la Materia, CSIC
[2]Universidad Carlos III de Madrid

Contents

Introduction

Quantizing gravity

Despite the remarkable successes of some of the main approaches to quantum gravity, we still do not have a satisfactory theory unifying general relativity (GR) and quantum field theory (QFT). A suitable quantization of gravitation is, thus, the most important unsolved problem of modern theoretical physics. The relentless search for a final theory is motivated by the hope that it will let us address the fundamental questions in cosmology and astrophysics, in particular, those related to the physics of the primitive universe and the generic problem of the appearance of singularities in physically relevant situations such as the collapse of compact objects and the formation process of black holes.

Both GR and QFT are incomplete on their own. On one hand, the singularity theorems of GR state that, under certain energy conditions satisfied by matter, singularities are expected generic features of cosmological and collapse solutions [1]. The prediction of infinite energy densities and the consequent divergent curvature of the spacetime clearly indicates that the theory is being applied beyond its domain of validity. On the other hand, QFT has the problem of yielding infinities whenever the amplitudes for multiply-connected Feynman diagrams are calculated. When possible, these infinities are subtracted away by absorbing them into the free parameters of the theory through a renormalization process. In this context, quantum gravity is expected to provide a natural ultraviolet cutoff at the Planck length, $L_P \sim 10^{-35} m$, solving in part the problem of the divergencies. Concerning the foundations of quantum theory, it is necessary to probe new interpretations avoiding the instrumentalism of the standard Dirac-von Neumann postulates, based upon the artificial distinction between the quantum system under study and the external classical observer who measures it [2]. This is specially so in the context of quantum cosmology, where one faces the problem of correctly interpreting the wave function of the universe. The *measurement problem* in quantum mechanics deserves special attention. Recall that, given a physical system in a (possibly mixed) state ρ, the *result state* of an ideal measurement of a quantum observable A, with respect to a set of measured values in a Borel set $\Delta \in \mathrm{Bor}(\mathbb{R})$, is described by the density operator

$$\rho \mapsto \rho_{A,\Delta} = \frac{1}{\mathrm{Tr}(\rho E^A(\Delta))} \sum_{\alpha \in \Delta} E^A(\{\alpha\})\, \rho E^A(\{\alpha\})\,,$$

where E^A is the unique spectral measure associated with A. This transition is nonlocal, stochastic and irreversible, and may come into conflict with the deterministic evolution of closed systems. In this respect, some authors have put forward the idea that the reduction of the wave packet may be related to GR, concretely, to the existence of an initial singularity [3].

In view of the highly successful description of electromagnetic and nuclear forces provided by the $SU(3) \times SU(2) \times U(1)$ standard model, it is quite natural to attempt a quantization of the gravitational field following the same strategy that for the rest of interactions. To do this, one starts by assuming a concrete topology for the spacetime and splitting its metric $g_{\mu\nu}$ in the form

$$g_{\mu\nu} = g_{\mu\nu}^{\text{back}} + G_N h_{\mu\nu} \, ,$$

where $g_{\mu\nu}^{\text{back}}$ is taken to be a background metric and $h_{\mu\nu}$ is the dynamical field which measures the deviation of the physical metric from the background. G_N denotes the Newton constant. Quantum gravity is then seen as a theory of small quantum fluctuations around $g_{\mu\nu}^{\text{back}}$. Note that, in this context, the use of a background field is strictly necessary in order to apply the usual quantum field perturbative techniques, providing a fiducial causal structure used to discuss important items as micro-causality. In particular, when $g_{\mu\nu}^{\text{back}}$ is chosen to be the flat metric, one can use the well-known representation theory of the Poincaré group to show that the quanta of the $h_{\mu\nu}$ field are massless particles with spin two. These are the so-called *gravitons*, which interact with each other and with matter according to the Einstein-Hilbert Lagrangian or its possible extensions. Detailed calculations lead to conclude, however, that Einstein's GR is perturbatively non-renormalizable at two loops for pure gravity, and at one loop for gravity coupled to matter [4]. Because of this, it is generally agreed that the quantization procedure introduced above cannot provide a mathematically consistent and predictive *fundamental* theory valid to arbitrarily small distances. Indeed, in a non-renormalizable theory the number of basic parameters tends to infinity at high energies. From this point of view, GR is rather an effective theory valid only at low energies. There are proposals to overcome this non-renormalizability problem by adding additional high power terms of the Riemannian curvature to the original Lagrangian, but then some problematic issues related to unitarity arise.

Nevertheless, there are examples of field theories which *do* exist as fundamental theories despite their non-renormalizability. In the so-called *asymptotic safety scenario*, S. Weinberg pointed out the possibility that quantum gravity could be formulated in a nonperturbative way by invoking a non-Gaussian ultraviolet fixed point –in contrast with the standard perturbative renormalizations based upon Gaussian fixed points at which all couplings parameterizing the general action functional vanish. In this case, the theory would be asymptotically safe given the absence of unphysical singularities at high energies [5]. This issue is under investigation at the present moment, although most of the physicists focus their attention on two different research programs, namely, (super) string theory and loop quantum gravity (LQG). The main aim of the first approach is to perform a unification of all known fundamental interactions, including gravity, in terms of excitations of one-dimensional objects called *strings* that evolve in a certain background metric space. Although the theory includes GR in its low-energy regime, so far it has not been possible to recover univocally the correct 4-dimensional standard model. Major efforts are devoted to this issue and also to probing the nonperturbative aspects of the theory. Despite these serious difficulties, string theory has successfully explained the Bekenstein-Hawking area law for a limited class of objects, the so-called BPS-type extremal black holes, with the correct prefactor 1/4 relating entropy and area [6]. The theory has also been successful describing the emission of Hawking radiation. Furthermore, string theory is expected to make the self-interacting Feynman diagrams finite order-by-order, solving in this way the non-renormalizability problem of quantum gravity.

A leading alternative to string theory is LQG, a mathematically consistent, non-perturbative, generally-covariant and background-independent canonical quantization of GR which describes gravity as a theory of $SU(2)$ connections and holonomies. This formulation differs substantially from the previous approach, in the sense that it tries to preserve the profound implications that GR has for the notions of space, time and causality. In fact, Einstein's GR is taken here as the basic starting point; although high-energy corrections to Einstein's equation may appear after quantization, they are not expected to modify the elegant description of gravitation in terms of a curvature of the spacetime geometry at large scales. As the main achievement of the theory, LQG has provided the correct entropy for a wide variety of black holes, including the Schwarzschild and Kerr types. However, there is a quantization ambiguity due to the so-called Barbero-Immirzi parameter appearing in the eigenvalues of the area operator. To recover the right pre-factor 1/4, one has to properly fix this parameter for each class of black hole. An effective equi-spacing of the degeneracy spectrum of microscopic black holes has also been shown to exist [7]. This is in (surprising) agreement with some solid results by Bekenstein, who inferred that the horizon area spectra of a black hole far away from extremality must be necessarily discrete and equally spaced in the context of any consistent quantum theory of gravity [8]. Future investigations will try to extend these results to the macroscopic limit [9]. In addition, there are some relevant results concerning the resolution of classical singularities such as the one corresponding to the Schwarzschild metric [10]. Despite these remarkable successes, however, the theory has not been able to recover the classical GR at its low-energy limit, and a definite formulation of the dynamics (related to the quantization of the Hamiltonian constraint) is not yet available. Because of this, some issues such as Hawking radiation are not well understood.

Finally, we must mention another promising nonperturbative formulation of quantum gravity, the so-called causal dynamical triangulation (CDT) approach, whose aim is to give a rigorous mathematical meaning to the Lorentzian path integral corresponding to gravity (consisting of the usual Einstein-Hilbert action with a cosmological term) by restricting it to geometries with a well defined causal structure (even at the Planck length). Large fluctuations in curvature are allowed at short scale, but in such a way that the resulting large scale geometry is nondegenerate. Concretely, the picture of the spacetime which emerges is as follows: At sub-Planckian scales, spacetime is fractal with dimension two, whereas a smooth classical geometry of effective (spectral) dimensionality equal to four is recovered at large scales [11].

It is clear that quantum gravity differs substantially from the majority of research branches in theoretical physics due to the absence of the experimental data necessary to sift through the broad range of proposals. Indeed, the Planck energy $E_P \sim 10^{28} eV$, at which quantum gravity effects become relevant, is beyond the experimental range of any available (or conceivable) particle accelerator; in fact, these effects may only be probed in the very early age of our universe –the so-called Planck epoch– or in some violent astrophysical collapse processes. Given the obvious technical difficulties to access to this energy regime, it is not possible to subject the different tentative theories to a rigorous validation/falsation process in the traditional way. The feasibility of a quantum gravity formulation is rather settled by demanding that any reasonable theory predicts some of the well established semiclassical results already mentioned such as the Bekenstein-Hawking entropy, the Hawking radiation, or the quantization and equally-spacing (adiabatic invariance) of the horizon area of black holes. The mathematical consistency of the theory is also taken into account, as well as the successful attainment of concrete desired objectives, as the unification of all known fundamental forces in the case of string theory.

Two-Killing vector symmetry reductions

Along this thesis, we will adopt a somehow modest point of view. We will restrict ourselves to the study of some symmetry reductions of GR which are especially useful to gain valuable insights into the behavior of gravity in its quantum regime. In this context, Bianchi models and two-Killing vector reductions of GR have received a lot of attention owing to their applications in astrophysics and cosmology. Two-Killing vector reductions, in particular, have been widely considered as appealing testing grounds for quantum gravity owing to the fact that they still have local degrees of freedom[1] as well as (restricted) diffeomorphism invariance, two of the features of the gravitational theory that lie at the heart of the difficulties encountered in its quantization process. They often admit an exact quantization, being possible to make concrete predictions, at least in a qualitative way, about the relevant features that a full theory of quantum gravity should have (whatever it might be). In fact, these models have proved to be privileged frameworks to discuss some fundamental aspects of quantum theory. For instance,

[1]These models are usually referred to as *midi-superspace* models (see [12] and references therein), in contrast with the so-called *mini-superspace* models, like Bianchi types, which have a finite number of degrees of freedom.

Group $\left(G^{(2)}\right)$	Manifold $\left({}^{(3)}\Sigma\right)$	Action	Name of the model
$U(1)\times U(1)$	$\mathbb{R}^2\times\mathbb{S}^1$	Not free	
	$\mathbb{R}\times\mathbb{T}^2$	Free	Schmidt model
	$\mathbb{T}^3$	Free	$\mathbb{T}^3$ Gowdy model
	$\mathbb{S}^1\times\mathbb{S}^2$	Not free	$\mathbb{S}^1\times\mathbb{S}^2$ Gowdy model
	$\mathbb{S}^3$	Not free	$\mathbb{S}^3$ Gowdy model
$\mathbb{R}\times U(1)$	$\mathbb{R}^3$	Not free	Cylindrical gravitational waves
	$\mathbb{R}\times\mathbb{S}^2$	Free	Cylindrical wormhole
	$\mathbb{R}\times\mathbb{T}^2$	Free	
$\mathbb{R}^2$	$\mathbb{R}^3$	Free	
	$\mathbb{R}^2\times\mathbb{S}^1$	Free	

Table 1: Spatial topologies compatible with the abelian biparametric Lie group $G^{(2)}$, whith a smooth, effective and proper action on the spatial sections of a globally hyperbolic spacetime $({}^{(4)}\mathcal{M}\simeq\mathbb{R}\times{}^{(3)}\Sigma,{}^{(4)}g_{ab})$. The action of the group, unique up to automorphisms of $G^{(2)}$ and diffeomorphisms of ${}^{(3)}\Sigma$, can be free or have degenerate orbits.

one can analyze the need for quantum evolution to be unitary in order for physical predictions to be consistent with causality, and how this condition can be relaxed in some definite sense within the Heisenberg picture [13]. They also provide a natural framework to apply the so-called algebraic formulation of quantum theory, consisting in defining an appropriate $*$-algebra of quantum observables for each system, in order to facilitate the construction and analysis of the different Hilbert space representations for the models.

When the Killing fields commute and are hypersurface orthogonal, the resulting models –said to be *linearly polarized*– become specially simple and solvable. These reductions differ from each other in the action of the isometry group and the corresponding compatible spatial topologies (see *Table 1* and [14]). The so-called linear Einstein-Rosen waves [15], which describe the propagation of linearly polarized wave-like modes in a spacetime with noncompact spatial slices, deserve particular attention. Here, the symmetry group is $\mathbb{R}\times U(1)$ and the spacetime is topologically $\mathbb{R}^4$. The quantization of this system coupled to massless scalar fields has been rigorously analyzed recently, and has provided several interesting features relevant for quantum gravity [16]. In this context, the introduction of matter is a way to produce quantum test particles with controllable wave functions in order to explore the quantized spacetime geometry. A suitable gauge fixing procedure yields a time-independent Hamiltonian which is a nontrivial bounded function of the free Hamiltonian corresponding to two uncoupled massless and axially symmetric scalar fields evolving in the same fixed (1+2)-dimensional Minkowskian space. It has its origin in the boundary terms of the Einstein-Hilbert action needed to have a well-defined variational principle. This fact allows one to *exactly* quantize the model by using the standard techniques of QFT in curved backgrounds, even though the system is nonlinear and self-interacting. In particular, the quantum unitary evolution operator can be obtained in closed form in a straightforward way and used for a number of purposes leading to physical applications such as the discussion of the existence of large quantum gravity effects [17] or the study of the microcausality of the system [16]. Specifically, the field commutator can be obtained from the two-point correlation functions, interpreted here as approximate probability amplitudes for a particle created at certain radial distance from the cylindrical symmetry axis at certain time to be detected somewhere else at a different instant of time. One then observes purely quantum gravitational effects such as an enhancement of the probability of finding the field quanta very close to the symmetry axis. The probability amplitude is also high along lines that can be interpreted as approximate null geodesics of an emergent axially symmetric Minkowskian geometry, which provides a concrete example of how classical behavior can be recovered from a quantum gravity model [16].

Structure of the thesis

We will focus on the so-called linearly polarized Gowdy models [18] coupled to massless scalar fields. From the physical point of view, their most salient feature is the fact that they describe cosmological models with initial, or initial and final, singularities. Here, the isometry group is $U(1) \times U(1)$ and the spatial manifold is restricted to have the topology of a 3-torus $\mathbb{T}^3$, a 3-handle $\mathbb{S}^1 \times \mathbb{S}^2$, a 3-sphere $\mathbb{S}^3$, or that of the lens spaces $L(p,q)$ –that can be studied by imposing discrete symmetries on the $\mathbb{S}^3$ case [19]. The exact quantization of the linearly polarized $\mathbb{T}^3$ Gowdy model in the vacuum has been profusely analyzed in the past [20]. Its dynamics is governed by a quadratic nonautonomous Hamiltonian obtained through a deparameterization process. The gravitational local degrees of freedom can be interpreted as those corresponding to a massless scalar field in a fiducial background with initial singularity, so that the standard techniques of QFT in curved spacetimes can be applied in order to construct the quantum theory. The fact that the linear symplectic transformations describing the classical time evolution cannot be unitarily implemented in the physical Hilbert space when the system is written in terms of its original variables was initially interpreted as a serious obstacle for the feasibility of the model [21]. This problem should come as no surprise, however, since a generic feature of the quantization of infinite-dimensional linear symplectic dynamical systems is precisely the impossibility of defining the unitary quantum counterpart of *all* linear symplectic transformations on the phase space [22].[2] These transformations are characterized by $*$-automorphisms defined on the corresponding abstract $*$-algebra of quantum observables. Note that the lack of a unitary operator

[2]Consider, for example, the generic impossibility of making sense of the unitary quantum evolution operator when dealing with scalar fields propagating in the Minkowskian spacetime from initial to final Cauchy surfaces that are not level surfaces of some Minkowskian time [23].

implementing the quantum time evolution of the system comes into conflict with the axiomatic structure of quantum theory itself. In case of not rejecting the model for this reason, one must carefully analyze the viability of a suitable probabilistic interpretation for it, as discussed in [24]. Nevertheless, it is possible to overcome this problem just by performing a suitable time-dependent redefinition of the field [25]. Furthermore, by demanding the unitarity of the dynamics and the invariance under an extra $U(1)$ symmetry generated by a residual global constraint, the existence of a unique (up to unitary equivalence) Fock representation can be proved for the system [26].

The purpose of this thesis is twofold. First, we will generalize and extend the existing literature devoted to the vacuum 3-torus model to the remaining more complicated topologies, the 3-handle and the 3-sphere, allowing also the coupling of gravity to matter, concretely, to massless scalar fields. These topologies are less known than the 3-torus one but equally relevant in cosmology owing to the fact that they display both initial and final singularities. For this reason, they become specially useful test beds for issues related to canonical quantization in cyclic universes. Here, as in the case of linear Einstein-Rosen waves, the addition of matter is a useful way to probe the quantized geometry, much in the same way as test particles are introduced in classical GR in order to analyze the spacetime geometry. Second, concerning the canonical quantization of the resulting gauge systems, we will confirm and clarify several relevant results found in the literature devoted to the vacuum 3-torus case. This will be done by placing particular emphasis on mathematical issues such as the rigorous application of symplectic geometry to nonautonomous Hamiltonian systems or the algebraic formulation of quantum theory in terms of suitable $*$-algebras of observables.

The text is structured as follows. *Chapter 1* will be devoted to the Lagrangian and Hamiltonian formulations of the $\mathbb{S}^1 \times \mathbb{S}^2$ and $\mathbb{S}^3$ Gowdy models, whose treatment in previous literature has suffered from an obvious lack of rigor.[3] This will be done by applying modern differential-geometric techniques to analytical mechanics. In contrast with the 3-torus case, the existence of degenerate orbits under the action of the isometry group will force us to carefully consider the regularity conditions that the dynamical variables must verify. A Geroch symmetry reduction, and a subsequent conformal transformation, will allow us to interpret these models as (1+2)-dimensional gravity coupled to a set of massless scalar fields with axial symmetry. Some details concerning this reduction will vary depending on the topologies and will be commented separately for each case. Among several issues, we will explain how the topology of the spatial slices affects the definition of the constraints, and also how the coupling of massless scalar fields is realized in the different topologies. A careful application of the Dirac-Bergmann theory of constrained systems [28 − 30] yields a reduced phase space description of these systems in terms of coisotropic (or first class constrained) manifolds. This is the case

[3] The Hamiltonian analysis for these models in the vacuum has only been addressed in a partial way in [27], without providing the detailed phase space description necessary to understand several relevant geometrical issues.

when the Poisson algebra of the constraints is a proper Lie algebra. An appropriate partial gauge-fixing (*deparameterization*) process will allow us to characterize the dynamics through nonautonomous Hamiltonian systems, mathematically described as cosymplectic or contact manifolds. Within this Hamiltonian setting, we will understand in detail the mechanisms leading to the appearance of initial and final singularities. It is important to highlight the fact that for these models, at variance with the 3-torus case, there are no extra constraints after the deparameterization process. This will obviously simplify the construction of a Hilbert space representation of the canonical commutation relations within the quantization process. In particular, it will not be necessary to distinguish between kinematical and physical Hilbert spaces.

In *Chapter 2*, we will proceed to perform an exact Fock-type canonical quantization of the deparameterized models. Both gravitational and matter local degrees of freedom will be encoded in massless scalar fields evolving in the same fixed background metric conformally equivalent to the Einstein static (1+2)-dimensional universe, topologically $(0,\pi)\times\mathbb{S}^2$. This fact will allow us to treat these fields in a unified way in the construction of the quantum theory by applying the usual techniques of QFT in curved spacetimes. The appropriate starting point is the covariant formulation of the reduced phase-space in terms of smooth real solutions to the Klein-Gordon equation of motion. This approach is completely equivalent to the usual canonical one, but proves specially useful in this context in order to discuss some quantization issues such as the existence of (in principle) many nonunitarily equivalent Fock space representations for the canonical commutation relations, each of them characterized by $SO(3)$-invariant complex structures on the covariant phase space. These invariant complex structures will be parameterized by pairs $(\rho_\ell,\nu_\ell)\in(0,+\infty)\times\mathbb{R}$, $\ell\in\mathbb{N}_0$. A first result will be the impossibility to characterize the dynamics through a unitary evolution operator when the system is described in terms of its original variables. This feature will be proved to be insensitive to the election of the $SO(3)$-invariant complex structure used to quantize the system. Then, we will be forced to introduce new dynamical variables in order to properly describe the system. Concretely, with the aim of overcoming the non-unitarity obstruction we will perform a re-scaling of the fields similar to the one employed in the 3-torus case. This redefinition will be dictated *precisely* by the conformal factor that relates the Gowdy metrics to the Einstein metric. In this way, we will provide a suitable geometrical interpretation of the techniques previously employed in the literature devoted to the 3-torus topology: The singular behavior introduced by the conformal factor will be translated into the behavior of a singular and time-dependent potential term for the re-scaled fields. This potential term will be sufficiently well-behaved as a function of time –in spite of being singular at some instants– to allow the unitary implementation of the dynamics. Moreover, we will be able to fully characterize all $SO(3)$-invariant complex structures for which the time evolution is unitary in terms of the asymptotic behavior of the pairs (ρ_ℓ,ν_ℓ) for large values of ℓ. In addition, we will prove that the many different $SO(3)$-invariant Fock representations of this type are unitarily equivalent. It is important to remark in this respect that, in absence of extra constraints as in the 3-torus model, we will use the $SO(3)$ symmetry associated to the background metric in order to select a preferred class of complex structures such that the Fock quantization is unique (up to unitary equivalence). The simplicity of the arguments used to prove these results will convince the reader of the usefulness of the employed formalism.

Finally, *Chapter 3* will be devoted to the functional Schrödinger representation of these models. Here, quantum states are characterized by square integrable functionals belonging to a L^2-space constructed from an appropriate distributional extension of the classical configuration space –in this case, it is given by the space of tempered distributions on the 2-sphere $\mathbb{S}^2$– endowed with a time-dependent Gaussian measure whose support will be analyzed in detail. By virtue of the interrelation between measure theory and representation of canonical commutation relations, the momentum operators will differ from the usual ones in terms of derivatives by the appearance of linear multiplicative terms which depend on the configuration observables. We will check that, as a consequence of the unitary implementability of time evolution, the representations corresponding to different values of the time parameter are unitarily equivalent and, hence, their associated measures are mutually absolutely continuous. We will end this chapter by developing a general procedure to obtain the evolution operator for the systems under study, written explicitly *in closed form* in terms of the basic field and momentum observables. This analysis will be (implicitly) based upon the theory of adiabatic invariants developed by Lewis in the context of the study of classical and quantum systems with time-dependent harmonic-oscillator-type Hamiltonians [31].

To conclude, we will probe the existence of suitable semiclassical states for the Gowdy cosmologies and discuss several possible applications of our study, as well as some open problems to be tackled in the future.

The appendices, far for providing merely incidental details on these subjects, will give additional information on several results attained in the main body of the thesis, going deeply into the relevant mathematical aspects of the text.

In *Appendix A*, the reader will find a generalization of the Geroch symmetry reduction procedure with respect to a space-like hypersurface-orthogonal Killing vector field in presence of a (symmetric) massless scalar field minimally coupled to (1+3)-dimensional gravity. After a suitable conformal transformation, 4-dimensional Einstein-Klein-Gordon equations turn out to be equivalent to (1+2)-dimensional gravity coupled to two massless scalar fields, one of them proportional to the original scalar field, and the other being given by the logarithm of the norm of the Killing vector field.

In *Appendix B*, we will summarize the main proposals and results of symplectic geometry when applied to analytical mechanics, fixing the notation and conventions used throughout the thesis. We will pay special attention to the nonautonomous (i.e., time-dependent) Hamiltonian systems, in terms of which we describe the dynamics of the

Gowdy models after deparameterization.

Appendix C presents the general framework of the mathematical description of (classical and quantum) physical theories in terms of C^*-algebras. The main point here is to introduce the concepts of observables and states, and how these can be realized respectively as self-adjoint bounded operators and vectors (or density matrices) in Hilbert spaces. The reader is strongly advised to revisit these topics, particularly the usual Dirac-von Neumann axiomatic structure of quantum mechanics, from this algebraic point of view.

It is clear that, in the quest for a suitable quantization of systems of infinitely many time-dependent harmonic oscillators, like those describing the Gowdy cosmologies, the understanding of the special features of the single quantum oscillator is particularly advisable. In *Appendix D*, we reformulate the study of the unitary implementation of the dynamics for a single one-dimensional harmonic oscillator with nonconstant frequency, paying special attention to the search of semiclassical states and closed expressions for the evolution operators.

Finally, *Appendix E* summarizes the theory of symmetric/antisymmetric Fock spaces, in particular, the definition of the creation and annihilation operators and their canonical commutation/anticommutation relations.

Throughout the text, with the exception of the *Appendix B*, we will use the Penrose abstract index convention with tangent space indices belonging to the beginning of the Latin alphabet [32]. Lorentzian spacetime metrics will have signature $(-+++)$ and the conventions for the curvature tensors will be those of reference [33].

References

1 S. W. Hawking and G. F. R. Ellis, *The Large Scale Structure of spacetime*, Cambridge University Press (1973).

2 To initiate himself into different approaches to quantum mechanics, the reader can consult, among many others: H. Everett, Rev. Mod. Phys. **29**, 454 (1957); J. B. Hartle, Am. J. Phys. **36**, 704 (1968); B. S. De Witt, Physics Today **23**, 30 (1970); B. S. De Witt and N. Graham, eds., *The Many Worlds Interpretations of Quantum Mechanics*, Princeton University Press, Princeton (1973); C. Rovelli, Int. J. of Theor. Phys. **35**, 1637 (1996).

3 S. W. Hawking and R. Penrose, *The Nature of Space and Time*, Princeton University Press (1996).

4 G. 't Hooft and M. Veltman, Annales de l'institut Henri Poincaré (A) Physique Théorique **20**, 69-94 (1974).

5 S. Weinberg, "Ultraviolet divergencies in quantum theories of gravitation", in S. W. Hawking and W. Israel, eds., *General Relativity: An Einstein Centenary*

Survey, Cambridge University Press (1979); J. Gomis and S. Weinberg, Nucl. Phys. B **469**, 473-487 (1996).

6 A. Strominger and C. Vafa, Phys. Lett. B **379**, 99 (1996).

7 A. Corichi, J. Diaz-Polo, and E. Fernandez-Borja, Phys. Rev. Lett. **98**, 181301 (2007); Class. Quant. Grav. **24**, 243 (2007).

8 J. D. Bekenstein, Lett. Nuovo Cimento **11**, 467 (1974). V. F. Mukhanov, JETP Letters **44**, 63 (1986); J. D. Bekenstein, "Classical Properties, Thermodynamics and Heuristic Quantization", in *Cosmology and Gravitation*, M. Novello, ed., Atlantisciences, France (2000).

9 J. F. Barbero G. and E. J. S. Villaseñor, Physical Review D **77**, 121502(R) (2008).

10 Martin Bojowald, Living Rev. Relativity **11**, 4 (2008). R Gambini and J. Pullin, Phys. Rev. Lett. **101**, 161301 (2008).

11 J. Ambjorn, J. Jurkiewicz, and R. Loll, Phys. Rev. D **72** (2005) 064014; Phys. Rev. Lett. **95**, 171301 (2005).

12 C. G. Torre, Int. J. Theor. Phys. **38**, 1081-1102 (1999).

13 T. Jacobson, in *Conceptual Problems of Quantum Gravity*, edited by A. Ashtekar and J. Stachel, Birkhäuser, Boston (1991).

14 B. K. Berger, P. T. Chruściel, and V. Moncrief, Ann. Phys. **237**, 322 (1995).

15 A. Einstein and N. Rosen, J. Franklin Inst. **223**, 43 (1937). A. Ashtekar and M. Pierri, J. Math. Phys. **37**, 6250 (1996).

16 J. F. Barbero G., I. Garay, and E. J. S. Villaseñor, Physical Review D **74** 044004 (2006); Physical Review Letters **95** 051301 (2005).

17 A. Ashtekar, Phys. Rev. Lett. **77**, 4864 (1996). M. E. Angulo and G. A. Mena Marugán, Int. J. Mod. Phys. D **9**, 669-686 (2000). J. F. Barbero G., I. Garay, and E. J. S. Villaseñor, Class. Quant. Grav. **25**, 205013 (2008).

18 R. H. Gowdy, Phys. Rev. Lett. **27**, 826 (1971); Ann. Phys. **83**, 203 (1974).

19 P. S. Mostert, Ann. of Math. **65**, 447 (1957); **66**, 589 (1957).

20 C. W. Misner, Phys. Rev. D **8**, 3271 (1973). B. K. Berger, Ann. Phys. **83**, 458 (1974); Phys. Rev. D **11**, 2770 (1975). G. A. Mena Marugán, Phys. Rev. D **56**, 908 (1997). M. Pierri, Int. J. Mod. Phys. D **11**, 135 (2002).

21 A. Corichi, J. Cortez, and H. Quevedo, Int. J. Mod. Phys. D **11**, 1451 (2002).

22 D. Shale, Trans. Am. Math. Soc. **103**, 149 (1962).

23 C. G. Torre and M. Varadarajan, Class. Quant. Grav. **16**, 2651 (1999).

24 C. G. Torre, Phys. Rev. D **66**, 084017 (2002).

25 A. Corichi, J. Cortez, and G. A. Mena Marugán, Phys. Rev. D **73**, 041502 and 084020 (2006).

26 A. Corichi, J. Cortez, G. A. Mena Marugán, and J. M. Velhinho, Class. Quant. Grav. **23**, 6301 (2006). J. Cortez, G. A. Mena Marugán, and J. M. Velhinho, Phys. Rev. D **75**, 084027 (2007).

27 J. L. Hanquin and J. Demaret, J. Phys. A: Math. Gen. **16**, L5 (1983).

28 M. J. Gotay, J. M. Nester, and G. Hinds, J. Math. Phys. **19**, 23882399 (1978).

29 D. Chinea, M. de León, and J. C. Marrero, J. Math. Phys. **35**, 3410-3447 (1994).

30 M. Henneaux and C. Teitelboim, *Quantization of Gauge Systems.* Princeton University Press, 1994.

31 H. R. Lewis Jr., Phys. Rev. Lett. **18**, 510 (1967); J. Math. Phys. **9**, 1976-1986 (1968).

32 R. Penrose and W. Rindler, *Spinors and spacetime, Vol. 1: Two-Spinor Calculus and Relativistic Fields*, Cambridge University Press (1984).

33 R. M. Wald, *General Relativity*, The University of Chicago Press, Chicago and London (1984).

Chapter 1
Hamiltonian Formulation

J. F. Barbero G., D. G. Vergel, and E. J. S. Villaseñor
Classical and Quantum Gravity 24, 5945 (2007)

Consider a smooth, effective, and proper action[1] of the biparametric Lie Group

$$G^{(2)} := U(1) \times U(1) = \big\{(g_1, g_2) = (e^{ix_1}, e^{ix_2}) \,|\, x_1, x_2 \in \mathbb{R}(\mathrm{mod}\, 2\pi)\big\}$$

on a compact, connected, and oriented 3-manifold ${}^{(3)}\Sigma$. This manifold is then restricted to have the topology of a 3-torus $\mathbb{T}^3$, a 3-handle $\mathbb{S}^1 \times \mathbb{S}^2$, a 3-sphere $\mathbb{S}^3$, or that of the lens spaces $L(p, q)$. Moreover, the action of the group is unique up to automorphisms of $G^{(2)}$ and diffeomorphisms of ${}^{(3)}\Sigma$ [2, 3]. Next, we construct a 4-manifold ${}^{(4)}\mathcal{M}$, diffeomorphic to $\mathbb{R} \times {}^{(3)}\Sigma$, such that $({}^{(4)}\mathcal{M}, {}^{(4)}g_{ab})$ is a globally hyperbolic spacetime endowed with a Lorentzian metric ${}^{(4)}g_{ab}$. We further require $G^{(2)}$ to act by isometries on the spatial slices of ${}^{(4)}\mathcal{M}$, obtaining in this way the so-called *Gowdy models*. We will focus on the *linearly polarized cases*, where the isometry group is generated by pairs of mutually orthogonal, commuting, spacelike, and globally defined hypersurface-orthogonal Killing vector fields (ξ^a, σ^a).

Most of the work on these models, after the initial papers by Gowdy, has profusely analyzed the 3-torus spatial topology; in fact, this is by far the preferred choice to discuss quantization issues. Here, we will focus our attention on the other possible *closed* (compact and without boundary) topologies, the 3-handle and the 3-sphere. The lens spaces $L(p, q)$ can be studied by imposing discrete symmetries on the 3-sphere case and, in fact, the arguments presented for $\mathbb{S}^3$ remain valid for them. Specifically, the nonexistence of additional qualitative phenomena in the lens spaces with respect to the $\mathbb{S}^3$ models has its origin in the fact that the covering $\mathbb{S}^3 \to L(p, q)$ is the projection map of the quotient of $\mathbb{S}^3$ by a subgroup of the isometry group $G^{(2)}$.

[1]Let G be a Lie group and $\mathcal{M}$ a manifold. The (left) action of G on $\mathcal{M}$ is a differentiable map $\sigma : G \times \mathcal{M} \to \mathcal{M}$ which satisfies (i) $\sigma(e, p) = p$ for any $p \in \mathcal{M}$ and (ii) $\sigma(g_1, \sigma(g_2, p)) = \sigma(g_1 \cdot g_2, p)$. Here, e denotes the unit element of the group. The action is said to be (i) *smooth*, if the σ mapping is C^∞; (ii) *proper*, if the mapping $G \times \mathcal{M} \to \mathcal{M} \times \mathcal{M}$ given by $(g, p) \mapsto (\sigma(g, p), p)$ is proper, i.e., inverses of compact sets are compact; (iii) *effective* if the unit element $e \in G$ is the unique element that defines the trivial action on $\mathcal{M}$, i.e., $\sigma(g, p) = p\,,\ \forall\, p \in \mathcal{M} \Rightarrow g = e$ (see [1] for more details).

1.1 $\mathbb{S}^1\times\mathbb{S}^2$ Gowdy models coupled to massless scalars

Let us start by considering the 3-handle ${}^{(3)}\Sigma = \mathbb{S}^1\times\mathbb{S}^2$, whose points can be parameterized in the form $(e^{i\xi}, e^{i\sigma}\sin\theta, \cos\theta)$, with $\theta\in[0,\pi]$, $\xi,\sigma\in\mathbb{R}(\mathrm{mod}\,2\pi)$. We define the following (left) $G^{(2)}$-group action

$$(g_1,g_2)\cdot(e^{i\xi}, e^{i\sigma}\sin\theta, \cos\theta) = (e^{x_1}, e^{x_2})\cdot(e^{i\xi}, e^{i\sigma}\sin\theta, \cos\theta) = (e^{i(x_1+\xi)}, e^{i(x_2+\sigma)}\sin\theta, \cos\theta)\,.$$

The action of the two $U(1)$ commuting subgroup factors of $G^{(2)}$, $(g_1,g_2)=(e^{ix},1)$ and $(g_1,g_2)=(1,e^{ix})$, $x\in\mathbb{R}(\mathrm{mod}\,2\pi)$, is respectively given by

$$\begin{aligned}(e^{ix},1)\cdot(e^{i\xi}, e^{i\sigma}\sin\theta, \cos\theta) &= (e^{i(x+\xi)}, e^{i\sigma}\sin\theta, \cos\theta)\,,\\ (1,e^{ix})\cdot(e^{i\xi}, e^{i\sigma}\sin\theta, \cos\theta) &= (e^{i\xi}, e^{i(x+\sigma)}\sin\theta, \cos\theta)\,.\end{aligned}$$

The corresponding tangent vectors at each point of ${}^{(3)}\Sigma$, obtained by differentiating the previous expressions with respect to x at $x=0$, are

$$(ie^{i\xi},0,0)\,,\quad (0, ie^{i\sigma}\sin\theta, 0)\,.$$

It is straightforward to verify that both fields commute. As we can see, the first one is never zero but the latter vanishes at $\theta=0$ and $\theta=\pi$. This corresponds to the circles $(e^{i\xi},0,1)$ and $(e^{i\xi},0,-1)$.

Consider now the 4-manifold ${}^{(4)}\mathcal{M}\simeq\mathbb{R}\times\mathbb{S}^1\times\mathbb{S}^2$; let t be a global coordinate on $\mathbb{R}$. We want to introduce three smooth (almost everywhere nonvanishing) vector fields θ^a, σ^a, and ξ^a, tangent to the embedded submanifolds $\{t\}\times\mathbb{S}^1\times\mathbb{S}^2$. In order to do this, let us fix $t_0\in\mathbb{R}$ and define on $\{t_0\}\times\mathbb{S}^1\times\mathbb{S}^2$ the coordinate vector fields $(\partial/\partial\theta)^a$, $(\partial/\partial\sigma)^a$, and $(\partial/\partial\xi)^a$. We then extend these fields to the entire ${}^{(4)}\mathcal{M}$ space by Lie dragging them along a smooth vector field t^a defined as the tangent vector to a smooth congruence of curves transverse to the slices $\{t\}\times\mathbb{S}^1\times\mathbb{S}^2$. In particular, we can simply take $t^a:=(\partial/\partial t)^a$. By definition, the σ^a field is defined to be zero in the two aforementioned submanifolds each diffeomorphic to $\mathbb{R}\times\mathbb{S}^1$; by removing them, we obtain a 4-manifold ${}^{(4)}\tilde{\mathcal{M}}$ for which the 4-tuple $(t^a,\theta^a,\sigma^a,\xi^a)$ defines a parallelization. Once we have introduced these vector fields on ${}^{(4)}\mathcal{M}$ as *background* objects, we restrict ourselves to working with 4-metrics ${}^{(4)}g_{ab}$ satisfying the following conditions:

1. The action of the group $G^{(2)}$ on ${}^{(4)}\mathcal{M}$ given by $(g_1,g_2)\cdot(t,p)=(t,(g_1,g_2)\cdot p)$, $t\in\mathbb{R}$, $p\in\mathbb{T}^3$, with $(g_1,g_2)\cdot p$ defined above, is an action by isometries, i.e., ξ^a and σ^a are linearly independent Killing vector fields on ${}^{(4)}\tilde{\mathcal{M}}$, so that $\mathcal{L}_\xi{}^{(4)}g_{ab}=0$, $\mathcal{L}_\sigma{}^{(4)}g_{ab}=0$.

2. t is a global time function, i.e., ${}^{(4)}g^{ab}(\mathrm{d}t)_b$ is a timelike vector field. From now on, we will consider the manifold ${}^{(4)}\mathcal{M}$ to be endowed with a time orientation such that this vector field is past-directed.

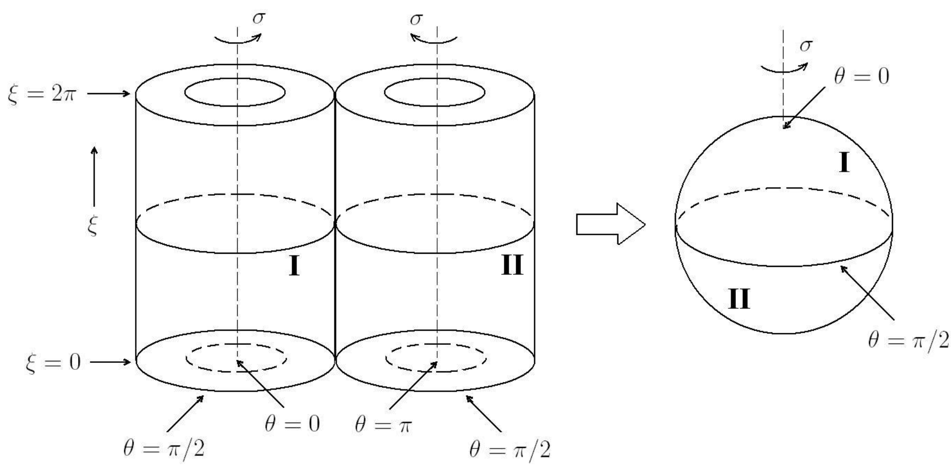

Figure 1.1: Cylindrical coordinates-patches on the 3-handle $\mathbb{S}^1 \times \mathbb{S}^2$, which has been sliced along the surface $\theta = \pi/2$. As a result, we obtain two solid tori that have been further sliced at $\xi = 0$ and rendered as solid cylinders. Each section of constant value of ξ consists of two discs, I and II (one in each cylinder), being identified at their edges to form a 2-sphere.

3. $\{t\} \times \mathbb{S}^1 \times \mathbb{S}^2$ are spacelike hypersurfaces for all $t \in \mathbb{R}$.
4. ξ^a and σ^a are hypersurface orthogonal. This defines the so called linearly polarized case. This condition means that the twists of the two fields vanish, which will ultimately allow us to simplify the field equations and describe the system as a simple theory of scalar fields.

Two simple but important results that can be proved at this point as a consequence of the first are the following:

i) If ξ^a and σ^a are Killing vectors and $[\xi, \sigma]^a = 0$, then $\mathcal{L}_\sigma({}^{(4)}g_{ab} - \xi_a\xi_b/\lambda_\xi) = 0$, where $\lambda_\xi := {}^{(4)}g_{ab}\xi^a\xi^b := \xi_a\xi^a > 0$.

ii) Furthermore, if we define the vector X^a orthogonal to ξ^a as $X^a := \sigma^a - \xi^a(\xi^b\sigma_b)/\lambda_\xi$, it satisfies $[\xi, X]^a = 0$ and also $\mathcal{L}_X({}^{(4)}g_{ab} - \xi_a\xi_b/\lambda_\xi) = 0$. This means that, without loss of generality, we can work with everywhere orthogonal and commuting Killing vector fields ξ^a and σ^a. In fact, we impose:

5. $(\theta^a, \sigma^a, \xi^a)$ are mutually ${}^{(4)}g$-orthogonal vector fields.

Let us consider now the Einstein-Klein-Gordon equations

$$ {}^{(4)}R_{ab} = 8\pi G_N (\mathrm{d}\phi)_a(\mathrm{d}\phi)_b\,, \quad {}^{(4)}g^{ab}\,{}^{(4)}\nabla_a{}^{(4)}\nabla_b\phi = 0\,, \tag{1.1} $$

corresponding to (1+3)-dimensional gravity minimally coupled to a zero rest mass scalar field ϕ symmetric under the diffeomorphisms generated by the Killing fields ($\mathcal{L}_\xi\phi =$

$\mathcal{L}_\sigma\phi = 0$, $\mathcal{L}_\xi {}^{(4)}g_{ab} = \mathcal{L}_\sigma {}^{(4)}g_{ab} = 0$). Here ${}^{(4)}R_{ab}$ and ${}^{(4)}\nabla_a$ denote the Ricci tensor and the Levi-Civita connection associated with ${}^{(4)}g_{ab}$, respectively. The exterior derivative of the scalar field ϕ is denoted by $(\mathrm{d}\phi)_a$ and G_N is the Newton constant. In order to get a simplified, lower dimensional description, we will perform a Geroch symmetry reduction with respect to the nonvanishing Killing vector field ξ^a on the 3-manifold ${}^{(3)}\mathcal{M} := {}^{(4)}\mathcal{M}/U(1) \simeq \mathbb{R}\times\mathbb{S}^2$. In the present situation, the hypersurface orthogonality of ξ^a allows us to view ${}^{(3)}\mathcal{M}$ as one of the embedded submanifolds everywhere orthogonal to the closed orbits of ξ^a, endowed with the induced metric

$${}^{(3)}g_{ab} := {}^{(4)}g_{ab} - \lambda_\xi^{-1}\xi_a\xi_b\,.$$

In the linearly polarized case, the twists of the Killing fields vanish and the field equations can be written as those corresponding to a set of massless scalar fields coupled to (1+2)-gravity by performing the conformal transformation $g_{ab} := \lambda_\xi {}^{(3)}g_{ab}$. The system (1.1) is then equivalent to (see the *Theorem A.2.1* in *appendix A* for more details)

$$R_{ab} = \frac{1}{2}\sum_i (\mathrm{d}\phi_i)_a(\mathrm{d}\phi_i)_b\,,\quad g^{ab}\nabla_a\nabla_b\phi_i = 0\,,\quad \mathcal{L}_\sigma g_{ab} = 0\,,\quad \mathcal{L}_\sigma\phi_i = 0\,, \tag{1.2}$$

where R_{ab} and ∇_a denote, respectively, the Ricci tensor and the Levi-Civita connection associated with g_{ab} –all of them being three dimensional objects on ${}^{(3)}\mathcal{M}$–, and we have defined[2] $\phi_1 := \log\lambda_\xi$, $\phi_2 := \sqrt{16\pi G_N}\phi$. Recall that we still have the additional symmetry generated by the remaining Killing vector field σ^a, which vanishes at $\theta = 0, \pi$. Let us consider the corresponding space of orbits ${}^{(2)}\mathcal{M} := {}^{(3)}\mathcal{M}/U(1) \simeq \mathbb{R}\times[0,\pi]$. The induced 2-metric of signature $(-+)$ on ${}^{(2)}\mathcal{M}$ can be written

$$s_{ab} = g_{ab} - \tau^{-2}\sigma_a\sigma_b\,,$$

where $\tau^2 := g_{ab}\sigma^a\sigma^b \geq 0$ is the area density of the symmetry $G^{(2)}$-group orbits, which vanishes at $\theta = 0, \pi$. In the following, we will use the notation $\tau = +\sqrt{\tau^2}$. The global time function t induces a foliation over ${}^{(2)}\mathcal{M}$. Let n^a be the g-unit and future-directed ($g^{ab}n_a(\mathrm{d}t)_b > 0$) vector field normal to this foliation, and let $\hat{\theta}^a$ be the g-unit spacelike vector field tangent to the slices of constant t, such that

$$\theta^a = e^{\gamma/2}\hat{\theta}^a$$

for some extra field γ. If we choose the congruence of curves with t^a tangent to ${}^{(2)}\mathcal{M}$, then the congruence is transverse to the foliation, and we can express

$$t^a = e^{\gamma/2}(Nn^a + N^\theta\hat{\theta}^a)\,, \tag{1.3}$$

where $N > 0$ and N^θ are proportional to the usual lapse and shift functions. As we will see, the unusual factor $e^{\gamma/2}$ will allow us to obtain a proper gauge algebra and simplify

[2]It is completely straightforward to couple any number N of massless scalar fields; in practice this can be done by supposing that the index i runs from 1 to $N+1$. The subindex $i = 1$ will always label the gravitational scalar that encodes the local gravitational degrees of freedom.

later calculations. We require N, N^θ, and γ to be smooth real-valued fields on ${}^{(3)}\mathcal{M}$. The expression of the metric in terms of the vector fields introduced above is

$$g_{ab} = -n_a n_b + \hat{\theta}_a \hat{\theta}_b + \tau^{-2}\sigma_a \sigma_b \,,$$

where the indices are raised or lowered with the g_{ab} metric. Using equation (1.3) and taking into account the orthogonality conditions

$$\begin{aligned} g_{ab}n^a n^b &= -1\,, & g_{ab}n^a\sigma^b &= 0\,,\\ g_{ab}\sigma^a\sigma^b &= \tau^2\,, & g_{ab}n^a\hat{\theta}^b &= 0\,,\\ g_{ab}\hat{\theta}^a\hat{\theta}^b &= +1\,, & g_{ab}\hat{\theta}^a\sigma^b &= 0\,, \end{aligned} \tag{1.4}$$

the metric may be expressed as

$$g_{ab} = e^\gamma\Big(\big(N^{\theta 2} - N^2\big)\,(\mathrm{d}t)_a(\mathrm{d}t)_b + 2N^\theta(\mathrm{d}t)_{(a}(\mathrm{d}\theta)_{b)} + (\mathrm{d}\theta)_a(\mathrm{d}\theta)_b\Big) + \tau^2(\mathrm{d}\sigma)_a(\mathrm{d}\sigma)_b\,. \tag{1.5}$$

The fact that the vectors $(t^a, \theta^a, \sigma^a)$ commute everywhere translates into necessary conditions that the vectors n^a and θ^a and the scalars N, N^θ, and γ must satisfy. As a consequence of the invariance property $\mathcal{L}_\sigma g_{ab} = 0$, the Lie derivative of relations (1.4) with respect to the Killing field σ^a yields

$$g_{ab}(\mathcal{L}_\sigma n)^a n^b = 0\,, \qquad g_{ab}(\mathcal{L}_\sigma n)^a\sigma^b = 0\,, \tag{1.6}$$

$$\mathcal{L}_\sigma\tau^2 = 0\,, \qquad g_{ab}(\mathcal{L}_\sigma n)^a\hat{\theta}^b + g_{ab}n^a(\mathcal{L}_\sigma\hat{\theta})^b = 0\,, \tag{1.7}$$

$$g_{ab}(\mathcal{L}_\sigma\hat{\theta})^a\hat{\theta}^b = 0\,, \qquad g_{ab}(\mathcal{L}_\sigma\hat{\theta})^a\sigma^b = 0\,. \tag{1.8}$$

Equations (1.6) and (1.8) imply that the unique nonvanishing terms of $(\mathcal{L}_\sigma n)^a$ y $(\mathcal{L}_\sigma\hat{\theta})^a$ lie on the $\hat{\theta}^a$ and n^a directions, respectively. They are related by

$$(\mathcal{L}_\sigma n)^a = \alpha\hat{\theta}^a\,, \quad (\mathcal{L}_\sigma\theta)^a = \alpha n^a\,, \tag{1.9}$$

where α is an extra scalar field. The commutation relations $[t,\sigma]^a = 0 = [\theta,\sigma]^a$ lead to

$$\begin{aligned} &\mathcal{L}_X N + \alpha N^\theta + \tfrac{1}{2}N\mathcal{L}_X\gamma = 0\,, && \mathcal{L}_X N^\theta + \alpha N + \frac{1}{2}N^\theta\mathcal{L}_X\gamma = 0\,,\\ &\alpha = 0\,, && \mathcal{L}_X\gamma = 0\,, \end{aligned}$$

so that the fields N, N^θ and γ are constant along the orbits defined by the remaining Killing vector field σ^a,

$$\mathcal{L}_\sigma N = 0\,, \quad \mathcal{L}_\sigma N^\theta = 0\,, \quad \mathcal{L}_\sigma\gamma = 0\,. \tag{1.10}$$

Note that the scalars ϕ_i are also constant on the orbits of σ^a, the matter scalar ϕ_2 because we have imposed this from the start and the gravitational scalar ϕ_1 due to the fact that the two Killings ξ^a and σ^a commute: $\mathcal{L}_\sigma\lambda_\xi = 0$. Therefore, we will end up with an essentially two dimensional model with fields depending only on coordinates t

and θ. In what follows, we will simply denote $\mathcal{L}_t$ with a dot; however, for the moment we will keep the notation for the Lie derivative along θ^a, $\mathcal{L}_\theta$, having in mind that we will later introduce a more convenient smooth derivative for smooth axially symmetric functions. From equation (1.9), we get for $\alpha = 0$

$$(\mathcal{L}_\sigma n)^a = 0\,, \quad (\mathcal{L}_\sigma \hat{\theta})^a = 0\,. \tag{1.11}$$

Finally, from the commutation relation $[\theta, t]^a = 0$ we obtain

$$\frac{1}{2}(\mathcal{L}_\theta \gamma)(N n^a + N^\theta \hat{\theta}^a) - \frac{1}{2}\dot{\gamma}\hat{\theta}^a + N e^{\gamma/2}[\hat{\theta}, n]^a + (\mathcal{L}_\theta N) n^a + (\mathcal{L}_\theta N^\theta)\hat{\theta}^a = 0\,.$$

This last equation can be projected in the directions defined by the vectors n^a, $\hat{\theta}^a$, and σ^a/τ to give

$$\frac{1}{2}N(\mathcal{L}_\theta \gamma) + \mathcal{L}_\theta N + N e^{\gamma/2} n^a n^b \nabla_a \hat{\theta}_b = 0\,, \tag{1.12}$$

$$\frac{1}{2}N^\theta \mathcal{L}_\theta \gamma + \mathcal{L}_\theta N^\theta - \frac{1}{2}\dot{\gamma} + N e^{\gamma/2}\hat{\theta}^a \hat{\theta}^b \nabla_a n_b = 0\,, \tag{1.13}$$

$$\hat{\theta}^a \sigma^b \nabla_a n_b = 0\,. \tag{1.14}$$

1.1.1 Lagrangian formulation

The set of equations (1.2) can be derived from a (1+2)-dimensional Einstein-Hilbert action corresponding to gravity minimally coupled to massless scalars

$$\begin{aligned} {}^{(3)}S(g_{ab}, \phi_i) &= \frac{1}{16\pi G_3}\int_{(t_0,t_1)\times\mathbb{S}^2} {}^{(3)}\mathbf{e}\,|g|^{1/2}\left(R - \frac{1}{2}\sum_i g^{ab}(\mathrm{d}\phi_i)_a(\mathrm{d}\phi_i)_b\right) \\ &+ \frac{1}{8\pi G_3}\int_{\{t_0\}\times\mathbb{S}^2}^{\{t_1\}\times\mathbb{S}^2} {}^{(2)}\mathbf{e}\,|h|^{1/2}K\,. \end{aligned} \tag{1.15}$$

Here, R denotes the Ricci scalar associated with g_{ab}. K and h_{ab} are, respectively, the trace of the second fundamental form K_{ab} and the induced 2-metric on the hypersurfaces diffeomorphic to $\{t\}\times\mathbb{S}^2$. In terms of the n^a vector field, $K_{ab} = h_a{}^c \nabla_c n_b$. G_3 denotes the Newton constant per unit length in the direction of the ξ-symmetric orbits. We have restricted the integration region to a closed interval $[t_0, t_1]$. The action is written with the help of a fiducial (i.e., non dynamical) volume form ${}^{(3)}\mathbf{e}$ compatible with the canonical volume form ${}^{(3)}\boldsymbol{\epsilon}$ defined by the 3-metric g_{ab}. This is given by ${}^{(3)}\boldsymbol{\epsilon} = \sqrt{|g|}\,{}^{(3)}\mathbf{e}$. The notation adopted here is such that in any basis where the nonvanishing components of ${}^{(3)}\boldsymbol{\epsilon}$ have the values ± 1, the scalar $|g|^{1/2}$ coincides with the square root of the determinant of the matrix of the metric $g_{\mu\nu}$ in that basis. The volume form ${}^{(3)}\boldsymbol{\epsilon}$ induces a 2-form ${}^{(2)}\boldsymbol{\epsilon}_{ab} = {}^{(3)}\boldsymbol{\epsilon}_{abc} n^c$ on each slice $\{t\}\times\mathbb{S}^2$ which agrees with the volume associated with the 2-metric h_{ab}. We have also introduced a fixed volume 2-form ${}^{(2)}\mathbf{e}$ on $\{t\}\times\mathbb{S}^2$ such that ${}^{(2)}\boldsymbol{\epsilon} = \sqrt{|h|}\,{}^{(2)}\mathbf{e}$. It satisfies $\sqrt{|g|}\,{}^{(3)}\mathbf{e}_{abc}n^c = \sqrt{|h|}\,{}^{(2)}\mathbf{e}_{ab}$. We require that both ${}^{(3)}\mathbf{e}$ and ${}^{(2)}\mathbf{e}$ be time-independent, i.e., $\mathcal{L}_t{}^{(3)}\mathbf{e} = 0 = \mathcal{L}_t{}^{(2)}\mathbf{e}$. We also demand them to be invariant under the action of the remaining Killing vector field. In particular, given the (1+2)-dimensional splitting of $\mathbb{R}\times\mathbb{S}^2$, it is natural to choose ${}^{(3)}\mathbf{e} = \mathrm{d}t\wedge{}^{(2)}\mathbf{e}$, with ${}^{(2)}\mathbf{e}$ being the fiducial 2-form associated with a round metric on $\mathbb{S}^2$ such that ${}^{(2)}\mathbf{e}_{ab}\theta^a\sigma^b = Ne^{\gamma}\tau/|g|^{1/2} = \sin\theta$, i.e., ${}^{(2)}\mathbf{e} = \sin\theta\mathrm{d}\theta\wedge\mathrm{d}\sigma$. The last integral which appears in (1.15) is notation for the integral over the final $\{t_1\}\times\mathbb{S}^2$-hypersurface minus the integral over the initial $\{t_0\}\times\mathbb{S}^2$-hypersurface. This boundary term is necessary in order to ensure that the variational principle is well defined [4]. We have the Codazzi relation

$$R = {}^{(2)}R + K_{ab}K^{ab} - K^2 + 2\nabla_a(n^aK - n^b\nabla_b n^a)$$

where ${}^{(2)}R$ denotes the Ricci scalar associated with h_{ab}. Making use of Stokes' theorem,

$$\int_{\mathrm{int}(\mathcal{U})}{}^{(3)}\mathbf{e}|g|^{1/2}\nabla_a A^a = \int_{\partial\mathcal{U}}{}^{(2)}\mathbf{e}|h|^{1/2}\eta_a A^a\,,$$

with $\mathcal{U}$ being a compact and oriented manifold and η^a the exterior normal unit vector to its boundary (in our case, $\eta^a = n^a$ on $\{t_1\}\times\mathbb{S}^2$ and $\eta^a = -n^a$ on $\{t_0\}\times\mathbb{S}^2$), and taking into account that $n_a n^b\nabla_b n^a = 0$, we get

$$\begin{aligned}{}^{(3)}S(g_{ab},\phi_i) = \frac{1}{16\pi G_3}\int_{t_0}^{t_1}\mathrm{d}t\int_{\mathbb{S}^2}{}^{(2)}\mathbf{e}\,|g|^{1/2}\Big(&{}^{(2)}R + K_{ab}K^{ab} - K^2\\ &-\frac{1}{2}\sum_i g^{ab}(\mathrm{d}\phi_i)_a(\mathrm{d}\phi_i)_b\Big).\end{aligned} \tag{1.16}$$

The matrix of the h_{ab} metric induced on $\{t\}\times\mathbb{S}^2$ takes the expression

$$\begin{bmatrix} h_{\theta\theta} & h_{\theta\sigma}\\ h_{\sigma\theta} & h_{\sigma\sigma}\end{bmatrix} = \begin{bmatrix} e^{\gamma} & 0\\ 0 & \tau^2\end{bmatrix}, \tag{1.17}$$

so that the unique nonvanishing Christoffel symbols are $\Gamma^{\theta}_{\theta\theta} = \frac{1}{2}\mathcal{L}_\theta\gamma$, $\Gamma^{\theta}_{\sigma\sigma} = -e^{-\gamma}\tau\mathcal{L}_\theta\tau$, and $\Gamma^{\sigma}_{\theta\sigma} = \tau^{-1}\mathcal{L}_\theta\tau$. Hence, the Ricci scalar is given by

$${}^{(2)}R = \tau^{-1}e^{-\gamma}\left((\mathcal{L}_\theta\tau)\mathcal{L}_\theta\gamma - 2\mathcal{L}_\theta^2\tau\right), \tag{1.18}$$

where $\mathcal{L}_\theta^2 := \mathcal{L}_\theta\circ\mathcal{L}_\theta$. Next, we proceed to calculate the components of the extrinsic curvature $K_{ab} = h_a{}^c\nabla_c n_b$. On one hand,

$$\begin{aligned}\hat\theta^a\hat\theta^b K_{ab} &= \hat\theta^a\hat\theta^b h_a^{\ c}\nabla_c n_b = \hat\theta^a\hat\theta^b\left(\hat\theta_a\hat\theta^c + \tau^{-2}\sigma_a\sigma^c\right)\nabla_c n_b = \hat\theta^a\hat\theta^b\nabla_a n_b\\ &= \frac{e^{-\gamma/2}}{2N}\left(\dot\gamma - 2\mathcal{L}_\theta N^\theta - N^\theta\mathcal{L}_\theta\gamma\right),\end{aligned}$$

where we have used the equations (1.11) and (1.13). Similarly,

$$\begin{aligned}\sigma^a\sigma^b K_{ab} &= \sigma^a\sigma^b h_a^{\ c}\nabla_c n_b = \sigma^a\sigma^b\left(\hat\theta_a\hat\theta^c + \tau^{-2}\sigma_a\sigma^c\right)\nabla_c n_b = \sigma^a\sigma^b\nabla_a n_b\\ &= \sigma^b n^a\nabla_a\sigma_b = \tau n^a\nabla_a\tau = \frac{\tau}{N}\left(e^{-\gamma/2}t^a - N^\theta\hat\theta^a\right)\nabla_a\tau\\ &= \frac{\tau e^{-\gamma/2}}{N}\left(\dot\tau - N^\theta\mathcal{L}_\theta\tau\right),\end{aligned}$$

where we have used the relations (1.3) and (1.11), as well as

$$\hat\theta^a X^b K_{ab} = \hat\theta^a X^b h_a^{\ c}\nabla_c n_b = \hat\theta^a X^b\left(\hat\theta_a\hat\theta^c + \tau^{-2}X_a X^c\right)\nabla_c n_b = \hat\theta^a X^b\nabla_a n_b = 0\,,$$

which follows from (1.11) and (1.14). Hence, we finally obtain

$$K_{ab} = \frac{e^{-\gamma/2}}{2N}\left(\dot\gamma - N^\theta\mathcal{L}_\theta\gamma - 2\mathcal{L}_\theta N^\theta\right)\hat\theta_a\hat\theta_b + \frac{e^{-\gamma/2}}{N\tau^3}\left(\dot\tau - N^\theta\mathcal{L}_\theta\tau\right)\sigma_a\sigma_b\,,$$

with trace $K = h^{ab}K_{ab}$. From this expression, we easily get

$$K_{ab}K^{ab} - K^2 = -\frac{e^{-\gamma}}{N^2\tau}\left(\dot\gamma - N^\theta\mathcal{L}_\theta\gamma - 2\mathcal{L}_\theta N^\theta\right)\left(\dot\tau - N^\theta\mathcal{L}_\theta\tau\right). \tag{1.19}$$

For the scalar fields ϕ_i, we have

$$\begin{aligned}g^{ab}\left(\nabla_a\phi_i\right)\nabla_b\phi_i &= \left(-n^a n^b + \hat\theta^a\hat\theta^b + \tau^{-2}X^a X^b\right)\nabla_a\phi_i\nabla_b\phi_i\\ &= \Big(-\frac{e^{-\gamma}}{N^2}\left(t^a - N^\theta e^{\gamma/2}\hat\theta^a\right)\left(t^b - N^\theta e^{\gamma/2}\hat\theta^b\right) + \hat\theta^a\hat\theta^b\\ &+ \tau^{-2}X^a X^b\Big)\left(\nabla_a\phi_i\right)\nabla_b\phi_i\\ &= -\frac{e^{-\gamma}}{N^2}\left(\dot\phi_i^2 - 2N^\theta\dot\phi_i\mathcal{L}_\theta\phi_i + \left((N^\theta)^2 - N^2\right)\left(\mathcal{L}_\theta\phi_i\right)^2\right).\end{aligned} \tag{1.20}$$

Substituting (1.18), (1.19) and (1.20) in the action (1.16), we finally get

$$\begin{aligned}{}^{(3)}S(N, N^\theta, \gamma, \tau, \phi_i) &= \frac{1}{16\pi G_3}\int_{t_0}^{t_1}\mathrm{d}t\int_{\mathbb{S}^2}{}^{(2)}\mathbf{e}\,|g|^{1/2}e^{-\gamma}\Bigg\{\frac{1}{\tau}\left((\mathcal{L}_\theta\gamma)\mathcal{L}_\theta\tau - 2\mathcal{L}_\theta^2\tau\right)\\ &- \frac{1}{\tau N^2}\left(\dot\gamma - 2\mathcal{L}_\theta N^\theta - N^\theta\mathcal{L}_\theta\gamma\right)\left(\dot\tau - N^\theta\mathcal{L}_\theta\tau\right)\\ &+ \frac{1}{2N^2}\sum_i\left[\dot\phi_i^2 - 2N^\theta\dot\phi_i\mathcal{L}_\theta\phi_i + \left((N^\theta)^2 - N^2\right)\left(\mathcal{L}_\theta\phi_i\right)^2\right]\Bigg\}.\end{aligned} \tag{1.21}$$

1.1.2 Regularity of the metric

From a classical point of view, the final outcome of the Hamiltonian analysis of the system that we will discuss in the following is a set of equations whose solutions allow us to reconstruct a four dimensional spacetime metric and a set of scalar fields satisfying the coupled Einstein-Klein-Gordon equations. This means that, once we decide the functional space to which this metric belongs, the objects that appear during the dimensional reduction, gauge fixing and so on may be subject to some regularity conditions. In the 3-torus case these are simple smoothness requirements but in the present case, due to the existence of a symmetry axis, these are more complicated. The regularity conditions that the metric components for an axially symmetric metric must verify can be deduced as in [3, 5]. Given an 4-dimensional axisymmetric spacetime with polar coordinates (t, z, r, φ) in a neighborhood of the axis, any regular symmetric tensor field M_{ab} must take the form

$$[M_{\mu\nu}] = \begin{bmatrix} A & B & rD & r^2F \\ B & C & rE & r^2G \\ rD & rE & H + r^2J & r^3K \\ r^2F & r^2G & r^3K & r^2(H - r^2J) \end{bmatrix}, \tag{1.22}$$

where $A, B, \ldots, K$ are functions of t, z and r^2. By using the coordinates (t, θ, σ, ξ), we can write the original 4-metric ${}^{(4)}g_{ab}$ for the Gowdy $\mathbb{S}^1 \times \mathbb{S}^2$ models as

$$\begin{aligned} {}^{(4)}g_{ab} &= e^{(\gamma-\phi_1)}\Big((N^{\theta 2} - N^2)(\mathrm{d}t)_a(\mathrm{d}t)_b + 2N^\theta(\mathrm{d}t)_{(a}(\mathrm{d}\theta)_{b)} + (\mathrm{d}\theta)_a(\mathrm{d}\theta)_b\Big) \qquad (1.23) \\ &+ \tau^2 e^{-\phi_1}(\mathrm{d}\sigma)_a(\mathrm{d}\sigma)_b + e^{\phi_1}(\mathrm{d}\xi)_a(\mathrm{d}\xi)_b\,. \end{aligned}$$

Identifying $t \leftrightarrow t$, $z \leftrightarrow \xi$, $r \leftrightarrow \theta$ and $\varphi \leftrightarrow \sigma$, we easily obtain the following regularity conditions for the metric (here we impose analyticity; otherwise we need only to know the asymptotic behavior for small values of $\sin\theta$)

$$e^{(\gamma-\phi_1)}(N^{\theta 2} - N^2) = A(t, \cos\theta)\,, \tag{1.24}$$
$$e^{(\gamma-\phi_1)}N^\theta = B(t, \cos\theta)\sin\theta\,, \tag{1.25}$$
$$e^{\phi_1} = C(t, \cos\theta)\,, \tag{1.26}$$
$$e^{\gamma-\phi_1} = D(t, \cos\theta) + E(t, \cos\theta)\sin^2\theta\,, \tag{1.27}$$
$$\tau^2 e^{-\phi_1} = \sin^2\theta\big(D(t, \cos\theta) - E(t, \cos\theta)\sin^2\theta\big)\,, \tag{1.28}$$

where A, B, C, D, E are analytic in their arguments. Here, $C > 0$ and $D(t, \cos\theta) \pm E(t, \cos\theta)\sin^2\theta > 0$, so that $D > 0$. Finally, $0 < N^2 = N^{\theta^2} - e^{-(\gamma-\phi_g)}A(t, \cos\theta)$, which implies $\big(B^2(t, \cos\theta) - A(t, \cos\theta)E(t, \cos\theta)\big)\sin^2\theta > A(t, \cos\theta)D(t, \cos\theta)$. The conditions for the fields themselves (dropping the t dependence) become

$$\phi_i = \hat{\phi}_i(\cos\theta)\,, \tag{1.29}$$
$$\gamma = \hat{\gamma}(\cos\theta)\,, \tag{1.30}$$
$$N^\theta = \hat{N}^\theta(\cos\theta)\sin\theta\,, \tag{1.31}$$
$$N = \hat{N}(\cos\theta)\,, \tag{1.32}$$
$$\tau = \hat{T}(\cos\theta)\sin\theta\,, \tag{1.33}$$
$$\tau^2 e^{-\gamma} = \frac{D(\cos\theta) - E(\cos\theta)\sin^2\theta}{D(\cos\theta) + E(\cos\theta)\sin^2\theta}\sin^2\theta\,, \tag{1.34}$$

where $\hat{\phi}_i, \hat{\gamma}, \hat{N}^\theta, \hat{N}, \hat{T} : [-1,1] \to \mathbb{R}$ ($\hat{N} > 0$) can be written as functions of A, B, C, D, E. They must be differentiable functions in $(-1,1)$ with definite right and left derivatives at ± 1. This is, they must be C^∞ functions in $(-1,1)$ with bounded derivatives. Note that the singular dependence of all relevant fields has been factored out ($\sin\theta$ is *not* a smooth function on the sphere). The functions defined on $\mathbb{S}^2$ as $\hat{\phi}_i \circ \cos\theta, \hat{\gamma}\circ\cos\theta, \hat{N}^\theta \circ \cos\theta, \hat{N}\circ\cos\theta, \hat{T}\circ\cos\theta$, which are analytic on the sphere and invariant under rotations around its symmetry axis, will be considered as the basic fields to describe our system. In what follows, they will be simply referred to as $\hat{\phi}_i, \hat{\gamma}, \hat{N}^\theta, \hat{N}, \hat{T}$ (without the $\circ\cos\theta$ that will only be used if the possibility of confusion arises), and collectively as the *hat*-fields.

Note that condition (1.34) implies that the values of the fields $\hat{T}$ and $\hat{\gamma}$ at the poles of the sphere are not independent of each other, but are related by the relations

$$\hat{T}(\pm 1) = e^{\hat{\gamma}(\pm 1)/2}\,. \tag{1.35}$$

As we will see, these *polar constraints* are necessary ingredients to ensure the consistency of the models as they guarantee the differentiability of the other constraints present in them.

Now, we proceed to rewrite the action (1.21) as the integral of a smooth function on the sphere. This will contain essentially the *hat*-fields, some suitable smooth derivative of them, and smooth functions of $\cos\theta$. Indeed, given a smooth and axially symmetric function on $\mathbb{S}^2$, its $\mathcal{L}_\theta$-derivative cannot necessarily be extended as a smooth function on the sphere. For a concrete example, consider the function $\cos\theta$ itself, whose derivative is given by $\mathcal{L}_\theta \cos\theta = -\sin\theta$. We can, however, define a smooth derivative f' for any smooth axially symmetric function as the extension of

$$f' := -\frac{1}{\sin\theta}\partial_\theta f \tag{1.36}$$

to $\mathbb{S}^2$. This is formally done by considering f as a function of $\cos\theta$ and differentiating. In particular, $f'' = -(\cos\theta/\sin^3\theta)\partial_\theta f + (1/\sin^2\theta)\partial^2_\theta f$. In the following, the *prime* symbol will always refer to this derivative. Taking this into account, we get the action

$$\frac{1}{16\pi G_3}\int_{t_0}^{t_1}\mathrm{d}t\int_{\mathbb{S}^2}{}^{(2)}\mathbf{e}\Big\{\hat{N}[(\hat{\gamma}'\hat{T}'-2\hat{T}'')\sin^2\theta+(6\hat{T}'-\hat{\gamma}'\hat{T})\cos\theta+2\hat{T}]$$
$$+\frac{1}{\hat{N}}[\hat{N}^\theta\hat{T}\cos\theta-\dot{\hat{T}}-\hat{N}^\theta\hat{T}'\sin^2\theta]\,[\dot{\hat{\gamma}}+(2\hat{N}^{\theta\prime}+\hat{N}^\theta\hat{\gamma}')\sin^2\theta-2\hat{N}^\theta\cos\theta]$$
$$+\frac{\hat{T}}{2\hat{N}}\sum_i\Big(\dot{\hat{\phi}}_i^{\,2}+2\hat{N}^\theta\dot{\hat{\phi}}_i\,\hat{\phi}_i'\sin^2\theta+(\hat{N}^{\theta 2}\sin^2\theta-\hat{N}^2)\hat{\phi}_i'^2\sin^2\theta\Big)\Big\}.$$

From now on, we will use units such that $16\pi G_3=1$. In order to express the action in its canonical form we must obtain the corresponding canonically conjugate momenta through a Legendre transformation,

$$\Pi:=p_{\hat{N}}=0\,,\quad \Pi_\theta:=p_{\hat{N}^\theta}=0\,,\tag{1.37}$$
$$p_{\hat{\gamma}}=\frac{1}{\hat{N}}\Big(\hat{N}^\theta\hat{T}\cos\theta-\dot{\hat{T}}-\hat{N}^\theta\hat{T}'\sin^2\theta\Big)\,,\tag{1.38}$$
$$p_{\hat{T}}=-\frac{1}{\hat{N}}\Big(\dot{\hat{\gamma}}+(2\hat{N}^{\theta\prime}+\hat{N}^\theta\hat{\gamma}')\sin^2\theta-2\hat{N}^\theta\cos\theta\Big)\,,\tag{1.39}$$
$$p_{\hat{\phi}_i}=\frac{\hat{T}}{\hat{N}}\Big(\dot{\hat{\phi}}_i+\hat{N}^\theta\hat{\phi}_i'\sin^2\theta\Big)\,.\tag{1.40}$$

We see that the Lagrangian function is singular, which prevents solving for *all* the generalized velocities in terms of momenta. This can certainly be done for $\dot{\hat{\gamma}}$, $\dot{\hat{T}}$ and $\dot{\hat{\phi}}_i$, but not for $\dot{\hat{N}}$ and $\dot{\hat{N}}^\theta$. The Hamiltonian formalism of the model therefore requires the application of the Dirac-Bergmann algorithm for constrained systems.[3] Introducing the Lagrange multipliers λ and λ^θ to enforce the primary constraints (1.37), we obtain the action

$$\int_{t_0}^{t_1}\mathrm{d}t\left(\int_{\mathbb{S}^2}{}^{(2)}\mathbf{e}\left(\dot{\hat{N}}p_{\hat{N}}+\dot{\hat{N}}^\theta p_{\hat{N}^\theta}+\dot{\hat{\gamma}}p_{\hat{\gamma}}+\dot{\hat{T}}p_{\hat{T}}+\sum_i\dot{\hat{\phi}}_i p_{\hat{\phi}_i}\right)-H[\lambda,\lambda^\theta,\hat{N},\hat{N}^\theta]\right),\tag{1.41}$$

with the Hamiltonian function

$$H[\lambda,\lambda^\theta,\hat{N},\hat{N}^\theta]:=\int_{\mathbb{S}^2}{}^{(2)}\mathbf{e}\Big(\lambda\Pi+\lambda^\theta\Pi_\theta+\hat{N}C+\hat{N}^\theta C_\theta\Big)\,,\tag{1.42}$$

where

$$C:=-p_{\hat{\gamma}}p_{\hat{T}}+(2\hat{T}''-\hat{\gamma}'\hat{T}')\sin^2\theta+(\hat{\gamma}'\hat{T}-6\hat{T}')\cos\theta-2\hat{T}$$
$$+\frac{1}{2}\sum_i\left(\frac{p^2_{\hat{\phi}_i}}{\hat{T}}+\hat{T}\hat{\phi}_i'^2\sin^2\theta\right),\tag{1.43}$$
$$C_\theta:=\Big(2p_{\hat{\gamma}}'-\hat{\gamma}'p_{\hat{\gamma}}-\hat{T}'p_{\hat{T}}-\sum_i\hat{\phi}_i'p_{\hat{\phi}_i}\Big)\sin^2\theta+\Big(\hat{T}p_{\hat{T}}-2p_{\hat{\gamma}}\Big)\cos\theta\,.\tag{1.44}$$

[3]For more details on the treatment of constrained Hamiltonian system, the reader can consult the *appendix B*.

The variation of the action with respect to the Lagrange multipliers λ and λ^θ provides the primary constraints (1.37). In order to guarantee the consistency of the dynamics of the system, these constraints must be preserved under the time evolution of the system (intuitively speaking, their Poisson brackets with the Hamiltonian must vanish). This leads us to impose the *secondary constraints*

$$C = 0\,, \quad C_\theta = 0\,. \tag{1.45}$$

It is easy to check that, by imposing again the consistency of the secondary constraints, one does not obtain additional (tertiary) constraints. Therefore, the dynamical variables are restricted to belong to a constraint surface in the canonical phase space of the system, coordinatized by $(\hat{N}, p_{\hat{N}}; \hat{N}^\theta, p_{\hat{N}^\theta}; \hat{\gamma}, p_{\hat{\gamma}}; \hat{T}, p_{\hat{T}}; \hat{\phi}_i, p_{\hat{\phi}_i})$. This surface is globally defined by the constraints $\Pi = 0 = \Pi_\theta$ and $C = 0 = C_\theta$. The Hamiltonian of the system is identically zero on it. Note, however, that the equations of motion of $\hat{N}$ and $\hat{N}^\theta$ are, respectively, $\dot{\hat{N}} = \lambda$ and $\dot{\hat{N}}^\theta = \lambda^\theta$, with λ and λ^θ being unspecified time-dependent functions. As a consequence, the dynamical trajectories of $\hat{N}$ and $\hat{N}^\theta$ are completely arbitrary. Moreover, the Hamilton equations corresponding to the canonical pairs $(\hat{\gamma}, p_{\hat{\gamma}}; \hat{T}, p_{\hat{T}}; \hat{\phi}_i, p_{\hat{\phi}_i})$ are not affected by the term $\big(\lambda\Pi + \lambda^\theta \Pi_\theta\big)$ appearing in the Hamiltonian (1.42). Thus, with respect to the dynamical variables $\hat{\gamma}, \hat{T}, \hat{\phi}_i$, the action (1.41) is completely equivalent to [6]

$$S := \int_{t_0}^{t_1} \mathrm{d}t \left(\int_{\mathbb{S}^2} {}^{(2)}\mathbf{e} \left(\dot{\hat{\gamma}} p_{\hat{\gamma}} + \dot{\hat{T}} p_{\hat{T}} + \sum_i \dot{\hat{\phi}}_i p_{\hat{\phi}_i} \right) - H[\hat{N}, \hat{N}^\theta] \right). \tag{1.46}$$

Here, the terms proportional to λ and λ^θ have been dropped and $\hat{N}$ and $\hat{N}^\theta$ are simply treated as Lagrange multipliers. The new Hamiltonian is given by

$$H[\hat{N}, \hat{N}^\theta] = \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e} \left(\hat{N} C + \hat{N}^\theta C_\theta \right). \tag{1.47}$$

The canonical phase space of the system, denoted by Γ, is now coordinatized by the conjugated pairs $(\hat{\gamma}, p_{\hat{\gamma}}; \hat{T}, p_{\hat{T}}; \hat{\phi}_i, p_{\hat{\phi}_i})$ and endowed with the standard (weakly) symplectic form

$$\omega := \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e} \left(\delta\hat{\gamma} \wedge \delta p_{\hat{\gamma}} + \delta\hat{T} \wedge \delta p_{\hat{T}} + \sum_i \delta\hat{\phi}_i \wedge \delta p_{\hat{\phi}_i} \right). \tag{1.48}$$

Now we proceed to analyze the gauge transformations generated by the constraints. For this aim, we have to smear the constraints to obtain well defined functions on the phase space,

$$C[\hat{N}_g] := \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e} \hat{N}_g C\,, \quad C_\theta[\hat{N}_g^\theta] := \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e} \hat{N}_g^\theta C_\theta\,. \tag{1.49}$$

It is straightforward to check that the polar constraints (1.35) guarantee the differentiability of (1.49) without further restrictions on $\hat{N}_g$ and $\hat{N}_g^\theta$. Indeed, consider the exterior derivative of $C[\hat{N}_g]$,

$$\delta C[\hat{N}_g] = \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e} \sum_{\chi} \frac{\delta C[\hat{N}_g]}{\delta \chi(s)} \delta\chi(s) \,,$$

with the sum extended over all canonical coordinates of Γ and $\delta/\delta\chi$ denoting a functional derivative. Integrating by parts, we encounter the surface term $-2\hat{N}_g \cos\theta\delta\hat{T} + \hat{N}_g\hat{T}\cos\theta\delta\hat{\gamma}\big]_{\theta=0}^{\pi}$, which vanishes by virtue of (1.35). The differentiability of $C_\theta[\hat{N}_g^\theta]$ is trivially verified, since the corresponding surface term is proportional to $\sin\theta$ evaluated at $\theta = 0, \pi$. We then have the gauge transformations[4]

$$\begin{aligned}
\{\hat{\gamma}, C[\hat{N}_g]\} &= -\hat{N}_g p_{\hat{T}} \,, \\
\{\hat{T}, C[\hat{N}_g]\} &= -\hat{N}_g p_{\hat{\gamma}} \,, \\
\{\hat{\phi}_i, C[\hat{N}_g]\} &= \frac{\hat{N}^g}{\hat{T}} p_{\hat{\phi}_i} \,, \\
\{p_{\hat{\gamma}}, C[\hat{N}_g]\} &= \hat{N}_g'(\hat{T}\cos\theta - \hat{T}'\sin^2\theta) + \hat{N}_g(\hat{T} + 3\hat{T}'\cos\theta - \hat{T}''\sin^2\theta) \,, \\
\{p_{\hat{T}}, C[\hat{N}_g]\} &= \hat{N}_g'(2\cos\theta - \hat{\gamma}'\sin^2\theta) + \hat{N}_g(\hat{\gamma}'\cos\theta - \hat{\gamma}''\sin^2\theta) - 2\hat{N}_g''\sin^2\theta \\
&\quad + \frac{\hat{N}_g}{2}\sum_i \left(\frac{p_{\hat{\phi}_i}^2}{\hat{T}^2} - \sin^2\theta\hat{\phi}_i'^2\right) , \\
\{p_{\hat{\phi}_i}, C[\hat{N}_g]\} &= \hat{N}_g'\hat{T}\hat{\phi}_i'\sin^2\theta + \hat{N}_g[(\hat{T}'\hat{\phi}_i' + \hat{T}\hat{\phi}_i'')\sin^2\theta - 2\hat{T}\hat{\phi}_i'\cos\theta] \,,
\end{aligned}$$

and

$$\begin{aligned}
\{\hat{\gamma}, C_\theta[\hat{N}_g^\theta]\} &= -2\hat{N}_g^{\theta\prime}\sin^2\theta + \hat{N}_g^\theta(2\cos\theta - \hat{\gamma}'\sin^2\theta) \,, \\
\{\hat{T}, C_\theta[\hat{N}_g^\theta]\} &= \hat{N}_g^\theta(\hat{T}\cos\theta - \hat{T}'\sin^2\theta) \,, \\
\{\hat{\phi}_i, C_\theta[\hat{N}_g^\theta]\} &= -\hat{N}_g^\theta\hat{\phi}_i'\sin^2\theta \,, \\
\{p_{\hat{\gamma}}, C_\theta[\hat{N}_g^\theta]\} &= \hat{N}_g^\theta(2p_{\hat{\gamma}}\cos\theta - p_{\hat{\gamma}}'\sin^2\theta) - \hat{N}_g^{\theta\prime}p_{\hat{\gamma}}\sin^2\theta \,, \\
\{p_{\hat{T}}, C_\theta[\hat{N}_g^\theta]\} &= \hat{N}_g^\theta(p_{\hat{T}}\cos\theta - p_{\hat{T}}'\sin^2\theta) - \hat{N}_g^{\theta\prime}p_{\hat{T}}\sin^2\theta \,, \\
\{p_{\hat{\phi}_i}, C_\theta[\hat{N}_g^\theta]\} &= \hat{N}_g^\theta(2p_{\hat{\phi}_i}\cos\theta - p_{\hat{\phi}_i}'\sin^2\theta) - \hat{N}_g^{\theta\prime}p_{\hat{\phi}_i}\sin^2\theta \,.
\end{aligned}$$

Finally, we must check the stability of the polar constraints (1.35), $(\hat{T}e^{-\hat{\gamma}/2})(\pm 1) = 1$. To this end, we compute

$$\begin{aligned}
\{\hat{T}e^{-\hat{\gamma}/2}, C[\hat{N}_g]\} &= 8\pi G_3\hat{N}_g e^{-\hat{\gamma}/2}\left(\hat{T}p_{\hat{T}} - 2p_{\hat{\gamma}}\right) , \\
\{\hat{T}e^{-\hat{\gamma}/2}, C_\theta[\hat{N}_g^\theta]\} &= e^{-\hat{\gamma}/2}\left(\hat{T}\hat{N}_g^{\theta\prime} + \hat{N}_g^\theta\left(\frac{1}{2}\hat{T}\hat{\gamma}' - \hat{T}'\right)\right)\sin^2\theta \,.
\end{aligned}$$

[4]The following identities become very useful in this context: Given a canonical pair (φ, p_φ) and a smooth axially symmetric function F on the sphere, we have $\int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\,\{\varphi', p_\varphi\}F = -F'$ and $\int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\,\{\varphi'', p_\varphi\}F = F''$.

The first expression vanishes at the poles as a consequence of the constraint (1.44) for $\theta = 0,\, \pi$ ($\sin\theta = 0$ and $|\cos\theta| = 1$) whereas the second vanishes because of the $\sin^2\theta$ factor. We then conclude that there are no secondary constraints coming from the stability of the polar constraints.

1.1.3 Deparameterization

The dynamical variables are restricted to belong to a constraint surface $\Gamma_c \subset \Gamma$ globally defined by the constraints $C = 0$, $C_\theta = 0$. A straightforward calculation shows that these constraints are first class in Dirac's terminology, or equivalently that Γ_c is a coisotropic submanifold of Γ. Indeed, the Poisson algebra of the constraints is a proper Lie algebra

$$\begin{aligned}
\{C[\hat{N}_g], C[\hat{M}_g]\} &= C_\theta[\hat{M}_g \hat{N}_g' - \hat{N}_g \hat{M}_g'] \,, \\
\{C[\hat{N}_g], C_\theta[\hat{M}_g^\theta]\} &= C[(\hat{M}_g^\theta \hat{N}_g' - \hat{N}_g \hat{M}_g^{\theta\prime}) \sin^2\theta + \hat{N}_g \hat{M}_g^\theta \cos\theta] \,, \\
\{C_\theta[\hat{N}_g^\theta], C_\theta[\hat{M}_g^\theta]\} &= C_\theta[(\hat{M}_g^\theta \hat{N}_g^{\theta\prime} - \hat{N}_g^\theta \hat{M}_g^{\theta\prime}) \sin^2\theta] \,.
\end{aligned}$$

Note that, as a consequence of the introduction of the suitable exponential factor $e^{\gamma/2}$ in (1.3) we have a *closed* gauge algebra [7, 8], i.e., with structure *constants*.

Motion along the directions defined by the weighted constraints corresponds then to *gauge transformations*, i.e., transformations that do not affect the physical state of the system. Due to this fact, we would like to isolate the true physical degrees of freedom of the model. As is well known, there are several possible ways to do this. The first one is to eliminate the variables representing the gauge degrees of freedom by introducing the so-called *reduced phase space* of the system, that is, the (quotient) space of orbits of the gauge diffeomorphisms. Each point on the reduced phase space is an equivalence class of points on the constraint surface Γ_c, where two points are regarded as equivalent if they differ by a symplectic transformation generated by the (weighted) constraints. The successful implementation of the reduction allows us not only to label gauge orbits but also provides us with important mathematical structures (topological, symplectic, etc) from the ones present in the initial phase space. The second way is to fix a gauge, by choosing a global cross-section of Γ intersecting the gauge orbits once and only once. Here, we will see that a *partial* gauge fixing procedure (*deparameterization*) provides another interesting way to deal with the system, allowing us to describe it as a nonautonomous –i.e., time-dependent– quadratic Hamiltonian system [9, 10, 11].

The Hamiltonian vector fields associated with the weighted constraints $C[\hat{N}_g]$ and $C_\theta[\hat{N}_g^\theta]$ are tangential to Γ_c and define the degenerate directions of the pull-back of ω to this submanifold. The deparameterization procedure is based on the choice of one of these Hamiltonian vector fields to define an evolution vector field E_{H_R} associated with some reduced Hamiltonian H_R of a generically nonautonomous system. As shown in this section, we will be able to impose gauge fixing conditions in such a way that just one of the first class constraints, say $\mathcal{C}$, is not fixed. This will be used to define dynamics. Let $\iota : \Gamma_G \to \Gamma$ denote the embedding of the gauge fixed surface given by the first class constraints (1.45) and the gauge fixing conditions; the pull-back of the symplectic form to this surface, $\iota^*\omega$, has just one degenerate direction defined by a Hamiltonian vector field E_{H_R}. Select then a suitable phase space variable T such that $E_{H_R}(T) = 1$. The level surfaces of T are all diffeomorphic to a manifold Γ_R and transverse to E_{H_R}, defining a foliation of Γ_G with T as global time function. In this case, $\iota^*\omega = -\mathrm{d}T \wedge \mathrm{d}H_R + \omega_R$ and $E_{H_R} = \partial_T + X_{H_R}$, where ω_R is a weakly nondegenerate form, and the triplet $(\Gamma_R, \omega_R, H_R(T))$ defines a nonautonomous Hamiltonian system, mathematically characterized by a cosymplectic manifold (see the *appendix B*).

We begin by choosing gauge fixing conditions similar to those employed in the 3-torus case [12],

$$\hat{T}' = 0\,, \quad p'_{\hat{\gamma}} = 0\,. \tag{1.50}$$

They mean that both $\hat{T}$ and $p_{\hat{\gamma}}$ take the same value irrespective of θ, but we do not specify which one. Note that conditions of the type $\hat{T} = T$, $p_{\hat{\gamma}} = p$, with $T, p \in \mathbb{R}$, not only would tell us that $\hat{T}$ and $p_{\hat{\gamma}}$ are independent of θ, but also assign a fixed value to them, thus removing additional degrees of freedom. With our choice, there is still a dynamical mode in $\hat{T}$ which may vary in the evolution but is constant on every spatial slice in the (1+3)-decomposition. It will be eventually identified with a certain function of the time parameter. A convenient way to discuss the gauge fixing procedure is to describe the family of gauge conditions (1.50) by introducing an orthonormal basis of weight functions on the subspace of axially symmetric functions on $\mathbb{S}^2$,

$$Y_n := \left(\frac{2n+1}{4\pi}\right)^{1/2} \mathscr{P}_n(\cos\theta)\,, \;\; n \in \mathbb{N}_0\,, \tag{1.51}$$

where $\mathscr{P}_n$ are the Legendre polynomials. By expanding now

$$\hat{T} = \sum_{n=0}^{\infty} \hat{T}_n Y_n\,, \quad p_{\hat{\gamma}} = \sum_{n=0}^{\infty} p_{\hat{\gamma}_n} Y_n\,,$$

with

$$\hat{T}_n = \left(\frac{2n+1}{4\pi}\right)^{1/2} \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\, \mathscr{P}_n(\cos\theta)\hat{T}\,, \quad p_{\hat{\gamma}_n} = \left(\frac{2n+1}{4\pi}\right)^{1/2} \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\, \mathscr{P}_n(\cos\theta) p_{\hat{\gamma}}\,,$$

the previous gauge fixing conditions (1.50) become

$$\hat{T}_n = 0 = p_{\hat{\gamma}_n}\,, \;\; \forall\, n \in \mathbb{N}\,. \tag{1.52}$$

In order to see if this is a good gauge fixation –and, alternatively, find out if some gauge freedom is left– we compute

$$\{\hat{T}_n, C[Y_m]\} \approx -\sqrt{\frac{(2n+1)(2m+1)}{(4\pi)^3}}\, p_{\hat{\gamma}0} \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\, \mathscr{P}_n(\cos\theta)\mathscr{P}_m(\cos\theta) = \frac{1}{\sqrt{4\pi}} p_{\hat{\gamma}0}\delta_{nm}$$

$$\{\hat{T}_n, C_\theta[Y_m]\} \approx \frac{\hat{T}_0}{4\pi}\sqrt{\frac{(2n+1)(2m+1)}{4\pi}} \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\, \cos\theta\mathscr{P}_n(\cos\theta)\mathscr{P}_m(\cos\theta)$$

$$= \begin{cases} -\dfrac{(m+1)\hat{T}_0}{\sqrt{4\pi(2m+1)(2m+3)}} & \text{if } n = m+1 \\ -\dfrac{m\hat{T}_0}{\sqrt{4\pi(2m+1)(2m-1)}} & \text{if } n = m-1 \\ 0 \quad \text{otherwise} \end{cases}$$

$$\{p_{\hat{\gamma}_n}, C[Y_m]\} \approx \hat{T}_0\sqrt{\frac{(2n+1)(2m+1)}{(4\pi)^3}} \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\, \mathscr{P}_n(\cos\theta)\big(\mathscr{P}_m(\cos\theta) + \cos\theta\mathscr{P}'_m(\cos\theta)\big)$$

$$= \begin{cases} 0 & \text{if } m = 0 \text{ or } m < n \\ -\hat{T}_0\dfrac{n+1}{\sqrt{4\pi}} & \text{if } m = n \\ \star & \text{otherwise} \end{cases}$$

$$\{p_{\hat{\gamma}_n}, C_\theta[Y_m]\} \approx p_{\hat{\gamma}_0}\sqrt{\frac{(2n+1)(2m+1)}{(4\pi)^3}} \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\, \mathscr{P}_n(\cos\theta)\big(\mathscr{P}_m(\cos\theta) - \sin^2\theta\mathscr{P}'_m(\cos\theta)\big)$$

$$= \begin{cases} 0 & \text{if } m = 0 \text{ or } m < n-1 \\ * & \text{otherwise} \end{cases}$$

where $n \in \mathbb{N}$ and $m \in \mathbb{N}_0$. The symbol $\approx$ denotes equality on the hypersurface defined by the gauge fixing conditions and the constraints, the so-called gauge-fixing surface $\Gamma_G \subset \Gamma_c$. The $\star$ and $*$ symbols denote terms (computable in closed form but with somewhat complicated expressions) that are not needed in the following discussion. It is convenient to display the previous results in a table form as below.

	$\hat{T}_1 = 0$	$p_{\hat{\gamma}_1} = 0$	$\hat{T}_2 = 0$	$p_{\hat{\gamma}_2} = 0$	$\dots$
$C[Y_0]$	0	0	0	0	$\dots$
$C_\theta[Y_0]$	$\frac{\hat{T}_0}{2\sqrt{3\pi}}$	0	0	0	$\dots$
$C[Y_1]$	$-\frac{p_{\hat{\gamma}_0}}{2\sqrt{\pi}}$	$\frac{\hat{T}_0}{\sqrt{\pi}}$	0	0	$\dots$
$C_\theta[Y_1]$	0	$*$	$\frac{\hat{T}_0}{\sqrt{15\pi}}$	0	$\dots$
$C[Y_2]$	0	$\star$	$-\frac{p_{\hat{\gamma}_0}}{2\sqrt{\pi}}$	$\frac{3\hat{T}_0}{\sqrt{4\pi}}$	$\dots$
$C_\theta[Y_2]$	$\frac{\hat{T}_0}{\sqrt{15\pi}}$	$*$	0	$*$	$\dots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$

One must also check if the polar constraints are gauge fixed by conditions (1.52). To this end, we compute

$$\{\hat{T}_n, \hat{T}e^{-\hat{\gamma}/2}\} \approx 0\,,$$
$$\{p_{\hat{\gamma}_n}, \hat{T}e^{-\hat{\gamma}/2}\} \approx \frac{1}{2}\hat{T}e^{-\hat{\gamma}/2}\sqrt{\frac{2n+1}{4\pi}}\mathscr{P}_n(\cos\theta)\,.$$

The last Poisson bracket is different from zero at the poles ($\theta = 0, \pi$) for all values of $n \in \mathbb{N}$. Therefore, the only constraint that is not gauge-fixed by the conditions introduced above, as long as $p_{\hat{\gamma}_0} \neq 0$ and $\hat{T}_0 \neq 0$, is $C[1]$,

$$\int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\left(-p_{\hat{\gamma}}p_{\hat{T}} + \hat{\gamma}'\hat{T}\cos\theta - 2\hat{T} + \frac{1}{2}\sum_i\left(\frac{p^2_{\hat{\phi}_i}}{\hat{T}} + \hat{T}\hat{\phi}_i'^2\sin^2\theta\right)\right) \approx 0\,. \tag{1.53}$$

This is in contrast with the situation for the 3-torus case, where one is left with two constraints instead of just one. The final description of our system is then considerably simpler that in the $\mathbb{T}^3$ case. This fact will obviously facilitate the canonical quantization of these models, as well. We now pullback every relevant geometric object to the submanifold Γ_G defined by the gauge fixing conditions with the aim of eliminating some of the variables in our model. Denoting by $\iota : \Gamma_G \to \Gamma$ the immersion map, the pullback of the (weakly) symplectic form (1.48) becomes

$$\iota^*\omega = \mathrm{d}\hat{\gamma}_0 \wedge \mathrm{d}p_{\hat{\gamma}_0} + \mathrm{d}\hat{T}_0 \wedge \mathrm{d}p_{\hat{T}_0} + \sum_i \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\,\delta\phi_i \wedge \delta p_{\phi_i}\,. \tag{1.54}$$

The pullback of the constraint (1.53) is

$$\begin{aligned}\mathcal{C} \;:=\; & -p_{\hat{\gamma}_0}p_{\hat{T}_0} + \hat{T}_0\Big(4\sqrt{\pi}\Big(\log\frac{\hat{T}_0}{\sqrt{4\pi}} - 1\Big) - \hat{\gamma}_0\Big) \\ + \; & \frac{1}{2}\sum_i \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\left(\frac{\sqrt{4\pi}}{\hat{T}_0}p^2_{\hat{\phi}_i} + \frac{\hat{T}_0}{\sqrt{4\pi}}\hat{\phi}_i'^2\sin^2\theta\right) \approx 0\,.\end{aligned} \tag{1.55}$$

The gauge transformations generated by this constraint in the variables $\hat{T}_0$ and $p_{\hat{\gamma}_0}$ are

$$\{\hat{T}_0, \mathcal{C}\} = -p_{\hat{\gamma}_0}\,, \quad \{p_{\hat{\gamma}_0}, \mathcal{C}\} = \hat{T}_0\,,$$

so if we parameterize the gauge orbits with $s \in (0, \pi)$ we see that on them we have $\hat{T}_0 = p\sin s$ and $p_{\hat{\gamma}_0} = -p\cos s$, $p \neq 0$. This suggests that a notable simplification of our models will occur if we introduce (a series of) canonical transformations substituting $\hat{T}_0$ and $p_{\hat{\gamma}_0}$ for new canonical variables. First, consider [12]

$$\begin{aligned}\hat{T}_0 &= P\sin T\,, & p_{\hat{T}_0} &= \frac{p_T}{P}\cos T - Q\sin T\,,\\ \hat{\gamma}_0 &= -Q\cos T - \frac{p_T}{P}\sin T\,, & p_{\hat{\gamma}_0} &= -P\cos T\,,\end{aligned} \tag{1.56}$$

where (Q, P) and (T, p_T) denote canonically conjugate pairs. It is straightforward to check that this is indeed a canonical transformation, i.e., (1.54) coincides with $\mathrm{d}Q \wedge \mathrm{d}P + \mathrm{d}T \wedge \mathrm{d}p_T + \sum_i \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\, \delta\phi_i \wedge \delta p_{\phi_i}$. It is possible to write the remaining constraint $\mathcal{C}$ in a more pleasant form by performing a further canonical transformation (here, again, $(\tilde{Q}, \tilde{P})$ and $(\varphi_i, p_{\varphi_i})$ are canonical pairs)

$$\begin{aligned} \tilde{Q} &:= PQ + \frac{1}{2}\sum_i \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\, p_{\hat{\phi}_i}\hat{\phi}_i\,, & \tilde{P} &:= \log P\,, \\ \varphi_i &= (4\pi)^{-1/4}\sqrt{P}\hat{\phi}_i\,, & p_{\varphi_i} &= (4\pi)^{1/4}\frac{p_{\hat{\phi}_i}}{\sqrt{P}}\,, \end{aligned} \tag{1.57}$$

giving

$$\mathcal{C} = p_T + 4\sqrt{\pi}e^{\tilde{P}}\Big(\log\frac{\sin T}{\sqrt{4\pi}} + \tilde{P} - 1\Big)\sin T + \frac{1}{2}\sum_i \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\left(\frac{p_{\varphi_i}^2}{\sin T} + \varphi_i'^2 \sin T \sin^2\theta\right) \approx 0\,. \tag{1.58}$$

The 2-form (1.54) then becomes

$$\iota^*\omega = \mathrm{d}\tilde{Q} \wedge \mathrm{d}\tilde{P} + \sum_i \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\, \delta\varphi_i \wedge \delta p_{\varphi_i} + \mathrm{d}T \wedge \mathrm{d}p_T\,. \tag{1.59}$$

Expressions (1.58) and (1.59), in particular, the linearity of the first one in the momentum p_T, allow us to interpret the 4-tuple $((0,\pi) \times \Gamma_R, \mathrm{d}t, \omega_R, H_R)$ as a nonautonomous Hamiltonian system with $T = t$ as the time parameter [13]. The resulting phase space Γ_R is coordinatized by the canonical pairs $(\tilde{Q}, \tilde{P}; \varphi_i, p_{\varphi_i})$ and is endowed with the (weakly) symplectic form

$$\omega_R := \mathrm{d}\tilde{Q} \wedge \mathrm{d}\tilde{P} + \sum_i \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\, \delta\varphi_i \wedge \delta p_{\varphi_i}\,. \tag{1.60}$$

Here, the canonical pair $(\tilde{Q}, \tilde{P})$ describes a global degree of freedom. The dynamics is given by the time-dependent Hamiltonian $H_R(t) : \Gamma_R \to \mathbb{R}$

$$H_R(t) = 4\sqrt{\pi}e^{\tilde{P}}\Big(\log\frac{\sin t}{\sqrt{4\pi}} + \tilde{P} - 1\Big)\sin t + \frac{1}{2}\sum_i \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e}\left(\frac{p_{\varphi_i}^2}{\sin t} + \varphi_i'^2 \sin t \sin^2\theta\right). \tag{1.61}$$

Note that from the point of view of the phase-space description of the dynamics developed here, we are able to understand in very simple terms the appearance of both initial and final singularities in the spacetime metrics of these models. The singularities that must be present as a consequence of the Hawking-Penrose theorems [14] can be understood as coming from the behavior of the Hamiltonian, which is singular whenever $\sin t = 0$. This means that if we pick the initial time $t_0 \in (0, \pi)$ in order to write the Cauchy data we meet a past singularity at $t = 0$ and a future singularity at $t = \pi$. The evolution vector field corresponding to (1.61) is

$$\begin{aligned} E_{H_R} &= \frac{\partial}{\partial t} + 4\sqrt{\pi} e^{\tilde{P}} (\log \frac{\sin t}{\sqrt{4\pi}} + \tilde{P}) \sin t \frac{\partial}{\partial \tilde{Q}} \\ &\quad + \sum_i \int_{\mathbb{S}^2} {}^{(2)}\mathbf{e} \left(\frac{p_{\varphi_i}}{\sin t} \frac{\delta}{\delta \varphi_i} + (\sin^2 \theta \varphi_i')' \sin t \frac{\delta}{\delta p_{\varphi_i}} \right) . \end{aligned} \tag{1.62}$$

It is possible to recover the original 4-dimensional spacetime from this 3-dimensional formulation. The fact that the gauge fixing conditions (1.52) defining the deparameterization must be preserved under the dynamics generated by the Hamiltonian $H[\hat{N}, \hat{N}^\theta]$ (i.e., $\{\hat{T}_n, H[\hat{N}, \hat{N}^\theta]\} \approx 0$ and $\{p_{\hat{\gamma}_n}, H[\hat{N}, \hat{N}^\theta]\} \approx 0$, for all $n \in \mathbb{N}$) forces $\hat{N}$ to be θ-independent and $\hat{N}^\theta$ to be zero. A suitable redefinition of the time parameter allows us to express the metric g_{ab} found after the deparameterization as

$$g_{ab} = e^\gamma \Big(-(\mathrm{d}t)_a (\mathrm{d}t)_b + (\mathrm{d}\theta)_a (\mathrm{d}\theta)_b \Big) + \frac{P^2}{4\pi} \sin^2 t \sin^2 \theta (\mathrm{d}\sigma)_a (\mathrm{d}\sigma)_b \,, \tag{1.63}$$

defined on $(0, \pi) \times \mathbb{S}^2$, with singular behavior at $t = 0, \pi$. Once we integrate the Hamiltonian equations corresponding to (1.61), undo the canonical transformation defined above, and solve the constraints in order to obtain the γ function, we uniquely determine the 3-metric (1.63) and, thereby, the original 4-metric.

Finally, we point out the possibility of reinterpreting the dynamics of these models as simple massless scalar field theories in conformally stationary backgrounds. This will allow us to use well-known techniques of quantum field theory in curved backgrounds in order to quantize the systems. Let us start by giving a simple way to solve equations (1.2). Given a specific solution $(\mathring{g}_{ab}, \mathring{\phi}_i)$, whenever condition $\mathcal{L}_\sigma \phi_i = 0$ is satisfied the following equivalence

$$g^{ab} \nabla_a \nabla_b \phi_i = 0 \;\Leftrightarrow\; \mathring{g}^{ab} \mathring{\nabla}_a \mathring{\nabla}_b \phi_i = 0$$

holds. On can solve the last equation in some convenient background $\mathring{g}_{ab}$ and then use equation $R_{ab} = \frac{1}{2} \sum_i (\mathrm{d}\phi_i)_a (\mathrm{d}\phi_i)_b$ just to give integrability conditions allowing us to recover g_{ab}. In the 3-handle case, the metric found after deparameterization is given by (1.63); a possible (non unique) choice for $(\mathring{g}_{ab}, \mathring{\phi}_i)$ is in this case

$$\begin{aligned} \mathring{g}_{ab} &= \sin^2 t \Big(-(\mathrm{d}t)_a (\mathrm{d}t)_a + (\mathrm{d}\theta)_a (\mathrm{d}\theta)_b + \sin^2 \theta (\mathrm{d}\sigma)_a (\mathrm{d}\sigma)_b \Big) \,, \\ \mathring{\phi}_1 &= \log \sin(t/2) - \log \cos(t/2) \,, \quad \mathring{\phi}_i = 0 \,, \;\; i \neq 1 \,. \end{aligned}$$

It is important to notice that even though the metric $\mathring{g}_{ab}$ is not stationary, it is conformal to the Einstein static metric on $(0, \pi) \times \mathbb{S}^2$. The scalar field dynamics generated by the nonautonomous Hamiltonian (1.61) corresponds exactly to the one defined by the Klein-Gordon equations on the background given by $\mathring{g}_{ab}$.

1.2 $\mathbb{S}^3$ Gowdy models coupled to massless scalars

Let us now consider the case where the spatial slices have the topology of a 3-sphere $\mathbb{S}^3$, described as $\mathbb{S}^3 = \{(z_1, z_2) \in \mathbb{C}^2 : |z_1|^2 + |z_2|^2 = 1\}$. A useful parametrization of $\mathbb{S}^3$, in terms of the so-called Hopf coordinates, is $z_1 = e^{i\sigma}\sin(\theta/2)$, $z_2 = e^{i\xi}\cos(\theta/2)$, with $\theta \in [0, \pi]$, $\xi, \sigma \in \mathbb{R}(\mathrm{mod}\, 2\pi)$. We define the following action of $G^{(2)}$ on $\mathbb{S}^3$

$$\begin{aligned}(g_1, g_2) \cdot (z_1, z_2) = (e^{ix_1}, e^{ix_2}) \cdot (z_1, z_2) &= (e^{ix_1} z_1, e^{ix_2} z_2)\\ &= (e^{i(x_1+\sigma)}\sin(\theta/2), e^{i(x_2+\xi)}\cos(\theta/2))\,.\end{aligned}$$

The action of the two $U(1)$ subgroup factors is

$$(e^{ix}, 1) \cdot (z_1, z_2) = (e^{ix} z_1, z_2)\,, \quad (1, e^{ix}) \cdot (z_1, z_2) = (z_1, e^{ix} z_2)\,.$$

The corresponding tangent vectors at each point of $\mathbb{S}^3$, obtained by differentiating the previous expressions with respect to x at $x = 0$, are now

$$(iz_1, 0)\,, \quad (0, iz_2).$$

These are commuting vector fields. As we can see, they vanish respectively at $z_1 = 0$ and $z_2 = 0$, i.e., at the circles $(0, e^{i\xi})$ and $(e^{i\sigma}, 0)$. We proceed now to construct a spacetime $({}^{(4)}\mathcal{M} \simeq \mathbb{R} \times \mathbb{S}^3, {}^{(4)}g_{ab})$ in the same way as in the 3-handle models. Here, however, we face the fact that the Killing vectors fields $\xi^a = (\partial/\partial\xi)^a$ and $\sigma^a = (\partial/\partial\sigma)^a$ vanish alternatively in two different circles when trying to perform a Geroch reduction. Consider in particular, the Killing field ξ^a which vanishes at (the one-dimensional submanifold of $\mathbb{S}^3$) $\theta = \pi$ and is nonzero at $\theta = 0$. Let ${}^{(4)}\tilde{\mathcal{M}}$ be the space ${}^{(4)}\mathcal{M}$ with the submanifold where ξ^a vanishes (diffeomorphic to $\mathbb{R} \times \mathbb{S}^1$) removed. This substraction does not affect the (1+3)-dimensional Einstein-Hilbert action for gravity coupled to matter, since we have removed a zero-measure set. Of course, one must take into account the fact that the fields in the new integration region cannot be completely arbitrary but should be subject to some restrictions (regularity conditions) reflecting the fact that they should extend to the full ${}^{(4)}\mathcal{M}$ in a smooth way. By performing a Geroch reduction on ${}^{(4)}\tilde{\mathcal{M}}/U(1)$ with respect to ξ^a, we obtain an action of the form (1.15) where the 2-dimensional spatial sections are now diffeomorphic to the open disc $D(0; \pi)$.

As in the 3-handle case, we are going to use $(t^a, \theta^a, \sigma^a)$ as coordinate vector fields. We will write now $\theta^a = f\hat{\theta}^a$ and $t^a = (Nn^a + N^\theta\hat{\theta}^a)f$. Here, the scalars $f > 0$, $N > 0$, and N^θ are supposed to be smooth fields on $\mathbb{R}\times D(0; \pi)$ subject to some regularity conditions that we must specify. Note that we write f instead of $e^\gamma/2$ foreseing the vanishing of this function at the disc boundary. Again, $(N, N^\theta, \gamma, \phi_i)$ are constant on the orbits of the remaining Killing field σ^a and, hence, they only depend on the coordinates (t, θ). The commutation relations verified by $(t^a, \theta^a, \sigma^a)$ yield

$$N\mathcal{L}_\theta f + f\mathcal{L}_\theta N + Nf^2 n^a n^b \nabla_a \hat{\theta}_b = 0\,, \tag{1.64}$$

$$N^\theta \mathcal{L}_\theta f + f\mathcal{L}_\theta N^\theta - \mathcal{L}_t f + Nf^2 \hat{\theta}^a \hat{\theta}^b \nabla_a n_b = 0\,, \tag{1.65}$$

$$\hat{\theta}^a \sigma^b \nabla_a n_b = 0\,. \tag{1.66}$$

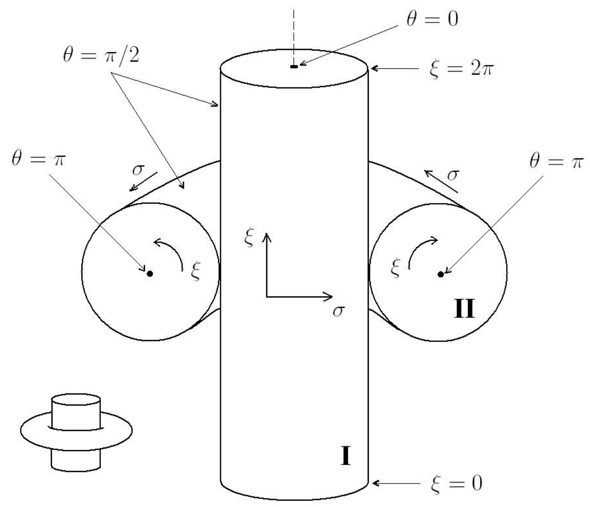

Figure 1.2: Cylindrical coordinates-patches on the 3-sphere $\mathbb{S}^3$, which has been sliced along the surface $\theta = \pi/2$. One of the resulting solid toroids (number I) has been further sliced at $\xi = 0$ and rendered as a solid cylinder. The half of toroid II has been cut away to display the behavior of the coordinates. The complete figure is showed in the lower left. For any fixed value of $\theta \in (0, \pi)$, the coordinates (σ, ξ) parameterize a 2-torus. In the degenerate cases corresponding to $\theta = 0$ and $\theta = \pi$ these coordinates describe circles.

Using the coordinates system (t, θ, σ, ξ) we can write the original 4-metric ${}^{(4)}g_{ab}$ as

$$\begin{aligned} {}^{(4)}g_{ab} &= \frac{f^2}{\lambda_\xi}\big((N^{\theta 2} - N^2)(\mathrm{d}t)_a(\mathrm{d}t)_b + 2N^\theta(\mathrm{d}t)_{(a}(\mathrm{d}\theta)_{b)} + (\mathrm{d}\theta)_a(\mathrm{d}\theta)_b\big) \\ &+ \frac{\tau^2}{\lambda_\xi}(\mathrm{d}\sigma)_a(\mathrm{d}\sigma)_b + \lambda_\xi(\mathrm{d}\xi)_a(\mathrm{d}\xi)_b\,. \end{aligned} \tag{1.67}$$

Next, we impose the regularity conditions to be satisfied by this metric. At $\theta = 0$, where σ^a vanishes, the regularity conditions should be of the same type as the ones that we have already used in the $\mathbb{S}^1 \times \mathbb{S}^2$ case. It suffices to use the expression (1.22) and identify $t \leftrightarrow t$, $z \leftrightarrow \xi$, $r \leftrightarrow 2\sin(\theta/2)$, and $\varphi \leftrightarrow \sigma$. Here, however, we also have to impose regularity conditions when we approach the boundary of the the filled torus that we obtained by removing the circle where the Killing ξ^a vanishes. In this case, we must simply identify $t \leftrightarrow t$, $z \leftrightarrow \sigma$, $r \leftrightarrow 2\cos(\theta/2)$, and $\varphi \leftrightarrow \xi$. Note that we use the functions $\sin(\theta/2)$ and $\cos(\theta/2)$ because they alternatively vanish on the circles where the Killings themselves become zero; in addition, they have the dependence of a regular scalar function in terms of the *radial* coordinates θ or $\pi - \theta$ on the circles where the

Killing fields do not vanish. According to this, we find

$$\frac{f^2}{\lambda_\xi}(N^{\theta 2}-N^2)=A(t,\cos\theta)\,, \tag{1.68}$$

$$\frac{f^2}{\lambda_\xi}N^\theta=B(t,\cos\theta)\sin\theta\,, \tag{1.69}$$

$$\lambda_\xi=4\cos^2(\theta/2)\big(F(t,\cos\theta)-G(t,\cos\theta)\cos^2(\theta/2)\big)\,, \tag{1.70}$$

$$\begin{aligned}\frac{f^2}{\lambda_\xi}&=D(t,\cos\theta)+E(t,\cos\theta)\sin^2(\theta/2)\\ &=F(t,\cos\theta)+G(t,\cos\theta)\cos^2(\theta/2)\,,\end{aligned} \tag{1.71}$$

$$\frac{\tau^2}{\lambda_\xi}=4\sin^2(\theta/2)\big(D(t,\cos\theta)-E(t,\cos\theta)\sin^2(\theta/2)\big)\,, \tag{1.72}$$

where A, B, D, E, F, and G are analytic in their arguments. The cosine dependence of these functions is dictated by regularity at certain submanifolds diffeomorphic to $\mathbb{R}\times\mathbb{S}^1$. This will prove to be very important because we will be able to describe the system in terms of these fields, and having $\cos\theta$ as their argument they can be interpreted as functions on $\mathbb{S}^2$ as in the 3-handle case. Note that they are not independent because they are constrained to satisfy (1.71). In addition, $D(t,\cos\theta)\pm E(t,\cos\theta)\sin^2\theta>0$ and $F(t,\cos\theta)\pm G(t,\cos\theta)\sin^2\theta>0$, so that $D>0$ and $F>0$; finally, $B^2(t,\cos\theta)-A(t,\cos\theta)\big(D(t,\cos\theta)+E(t,\cos\theta)\sin^2\theta\big)>0$. The conditions that the fields themselves must satisfy (dropping the t-dependence) are

$$\lambda_\xi=e^{\phi_1}=e^{\hat\phi_1(\cos\theta)}\cos^2(\theta/2)\,, \tag{1.73}$$

$$\phi_2=\hat\phi_2(\cos\theta)\,, \tag{1.74}$$

$$f=\cos(\theta/2)e^{\hat\gamma(\cos\theta)/2}\,, \tag{1.75}$$

$$N^\theta=\hat N^\theta(\cos\theta)\sin\theta\,, \tag{1.76}$$

$$N=\hat N(\cos\theta)\,, \tag{1.77}$$

$$\tau=\hat T(\cos\theta)\sin\theta\,, \tag{1.78}$$

$$\hat T^2e^{-\hat\gamma}=\frac{D(\cos\theta)-E(\cos\theta)\sin^2(\theta/2)}{D(\cos\theta)+E(\cos\theta)\sin^2(\theta/2)}\,, \tag{1.79}$$

$$e^{2\hat\phi_1-\hat\gamma}=4\frac{F(\cos\theta)-G(\cos\theta)\cos^2(\theta/2)}{F(\cos\theta)+G(\cos\theta)\cos^2(\theta/2)}\,, \tag{1.80}$$

where we have used $\sin\theta=2\sin(\theta/2)\cos(\theta/2)$. Here, as in the $\mathbb{S}^1\times\mathbb{S}^2$ case, we have that $\hat\phi_i,\hat\gamma,\hat N^\theta,\hat N,\hat T:[-1,1]\to\mathbb{R}$ ($\hat N>0$). They must be C^∞ in $(-1,1)$ with bounded derivative. Conditions (1.79) and (1.80) imply the *polar constraints* for the $\mathbb{S}^3$ models

$$\hat T(+1)e^{-\hat\gamma(+1)/2}=1\quad\text{and}\quad e^{2\hat\phi_1(-1)-\hat\gamma(-1)}=4\,.$$

Note that in this case the resulting conditions involve different pairs of objets at each pole $\theta=0$ or $\theta=\pi$. Our starting point is now the action (we take again units such that $16\pi G_3 = 1$)

$$
\begin{aligned}
{}^{(3)}S(N, N^\theta, f, \tau, \phi_i) \;=\; & \int_{(t_0,t_1)} \mathrm{d}t \int_{D(0;\pi)} {}^{(2)}\mathbf{e} \Bigg\{ \underbrace{\frac{2N}{f\sin\theta}\left((\mathcal{L}_\theta f)\mathcal{L}_\theta \tau - f\mathcal{L}_\theta^2 \tau\right)}_{(a)} \\
& \underbrace{- \frac{2}{Nf\sin\theta}\left(\dot{f} - f\mathcal{L}_\theta N^\theta - N^\theta \mathcal{L}_\theta f\right)\left(\dot{\tau} - N^\theta \mathcal{L}_\theta \tau\right)}_{(b)} \\
& \underbrace{+ \frac{\tau}{2N\sin\theta}\sum_{i\neq 1}\left[\dot{\phi}_i^2 - 2N^\theta \dot{\phi}_i \mathcal{L}_\theta \phi_i + \left((N^\theta)^2 - N^2\right)(\mathcal{L}_\theta \phi_i)^2\right]}_{(c)} \\
& \underbrace{+ \frac{\tau}{2N\lambda_\xi^2 \sin\theta}\left[\dot{\lambda}_\xi^2 - 2N^\theta \dot{\lambda}_\xi \mathcal{L}_\theta \lambda_\xi + \left((N^\theta)^2 - N^2\right)(\mathcal{L}_\theta \lambda_\xi)^2\right]}_{(d)} \Bigg\},
\end{aligned}
$$

where the Lagrangian can be easily deduced from (1.21) by substituting $\phi_1 \to \log\lambda_\xi$ and $\gamma \to 2\log f$. Here, as in the case of the 3-handle, we choose the fiducial volume element ${}^{(2)}\mathbf{e}$ to be compatible with the auxiliary round metric on the 2-sphere $\mathbb{S}^2$, i.e., ${}^{(2)}\mathbf{e} = \sin\theta \mathrm{d}\theta \wedge \mathrm{d}\sigma$, with ${}^{(2)}\mathbf{e}_{ab}\theta^a \sigma^b = Nf^2\tau/|g|^{1/2} = \sin\theta$. In terms of the fields $(\hat{N}, \hat{N}^\theta, \hat{\gamma}, \hat{T}, \hat{\phi}_i)$, and using again the prime derivative defined in (1.36), we have

$$
\begin{aligned}
(a) \;&=\; \hat{N}\Big[\Big(2 - \frac{\tan(\theta/2)}{\tan\theta}\Big)\hat{T} + \hat{T}' + (5\hat{T}' - \hat{\gamma}'\hat{T})\cos\theta + (\hat{\gamma}'\hat{T}' - 2\hat{T}'')\sin^2\theta\Big], \\
(b) \;&=\; \frac{1}{\hat{N}}\Big[\dot{\hat{T}} - \hat{N}^\theta \hat{T}\cos\theta + \hat{N}^\theta \hat{T}'\sin^2\theta\Big]\Big[\dot{\hat{\gamma}} + (2\hat{N}^{\theta\prime} + \hat{N}^\theta \hat{\gamma}')\sin^2\theta + (1 - 3\cos\theta)\hat{N}^\theta\Big], \\
(c) \;&=\; \frac{\hat{T}}{2\hat{N}}\sum_{i\neq 1}\Big[\dot{\hat{\phi}}_i^2 + 2\hat{N}^\theta \dot{\hat{\phi}}_i \hat{\phi}_i' \sin^2\theta + \big((\hat{N}^\theta)^2\sin^2\theta - \hat{N}^2\big)\hat{\phi}_i'^2 \sin^2\theta\Big], \\
(d) \;&=\; \frac{\hat{T}}{2\hat{N}}\Big[\dot{\hat{\phi}}_1^2 + 2\hat{N}^\theta \dot{\hat{\phi}}_1 \hat{\phi}_1' \sin^2\theta + \big((\hat{N}^\theta)^2\sin^2\theta - \hat{N}^2\big)\hat{\phi}_1'^2 \sin^2\theta \\
&\quad + 2(1-\cos\theta)\big(\hat{N}^\theta \dot{\hat{\phi}}_1 + \big((\hat{N}^\theta)^2\sin^2\theta - \hat{N}^2\big)\hat{\phi}_1'\big) + (1-\cos\theta)^2 \hat{N}^{\theta 2} - \tan^2(\theta/2)\hat{N}^2\Big].
\end{aligned}
$$

We can change the spatial integration region in the action from $D(0;\pi)$ to $\mathbb{S}^2$ because the Lagrangian can be written as a smooth function on the 2-sphere in terms of the *hat*-fields, that are smoothly extendable to $\mathbb{S}^2$. We arrive at this result after several nontrivial cancellations of terms that would diverge at the poles. Note, in particular, that the fist term in (a) and the last term in (d) involving $\tan(\theta/2)$ yield $(2 - \tan(\theta/2)/\tan\theta -$

$(1/2)\tan^2(\theta/2))\hat{T}=(3/2)\hat{T}$ when they are added. In this way,

$$
\begin{aligned}
{}^{(3)}S(\hat{N},\hat{N}^\theta,\hat{\gamma},\hat{T},\hat{\phi}_i) &= \int_{t_0}^{t_1}\mathrm{d}t\int_{\mathbb{S}^2}{}^{(2)}\mathbf{e}\bigg(\hat{N}[(\hat{\gamma}'\hat{T}'-2\hat{T}'')\sin^2\theta+(5\hat{T}'-\hat{\gamma}'\hat{T})\cos\theta+\hat{T}'+\frac{3}{2}\hat{T}] \\
&+\frac{1}{\hat{N}}[\hat{N}^\theta\hat{T}\cos\theta-\dot{\hat{T}}-\hat{N}^\theta\hat{T}'\sin^2\theta][\dot{\hat{\gamma}}+(2\hat{N}^{\theta\prime}+\hat{N}^\theta\hat{\gamma}')\sin^2\theta+(1-3\cos\theta)\hat{N}^\theta] \\
&+\frac{\hat{T}}{2\hat{N}}\sum_i\left[\dot{\hat{\phi}}_i^2+2\hat{N}^\theta\dot{\hat{\phi}}_i\,\hat{\phi}_i'\sin^2\theta+(\hat{N}^{\theta2}\sin^2\theta-\hat{N}^2)\hat{\phi}_i'^2\sin^2\theta\right] \\
&+\frac{\hat{T}}{2\hat{N}}[2(1-\cos\theta)(\hat{N}^\theta\dot{\hat{\phi}}_1+(\hat{N}^{\theta2}\sin^2\theta-\hat{N}^2)\hat{\phi}_1')+(1-\cos\theta)^2\hat{N}^{\theta2}]\bigg)\,. \qquad (1.81)
\end{aligned}
$$

The Hamiltonian of the system can be readily obtained by performing the Legendre transformation

$$
\begin{aligned}
&p_{\hat{N}}=0=p_{\hat{N}^\theta}\,,\\
&p_{\hat{\gamma}}=\frac{1}{\hat{N}}\Big(\hat{N}^\theta\hat{T}\cos\theta-\dot{\hat{T}}-\hat{N}^\theta\hat{T}'\sin^2\theta\Big)\,,\\
&p_{\hat{T}}=-\frac{1}{\hat{N}}\Big(\dot{\hat{\gamma}}+\big(2\hat{N}^{\theta\prime}+\hat{N}^\theta\hat{\gamma}'\big)\sin^2\theta+(1-3\cos\theta)\hat{N}^\theta\Big)\,,\\
&p_{\hat{\phi}_1}=\frac{\hat{T}}{\hat{N}}\Big(\dot{\hat{\phi}}_1+\hat{N}^\theta\hat{\phi}_1'+(1-\cos\theta)\hat{N}^\theta\Big)\,,\quad p_{\hat{\phi}_i}=\frac{\hat{T}}{\hat{N}}\Big(\dot{\hat{\phi}}_i+\hat{N}^\theta\hat{\phi}_i'\Big)\,,\ i\neq1\,.
\end{aligned}
$$

It is important to highlight that gravitational and matter modes (encoded by $\hat{\phi}_1$ and $\hat{\phi}_i$, $i\neq1$, respectively) cease to play a symmetric role in this particular description, at variance with the 3-handle case. This issue will be further discussed at the end of the section. The Hamiltonian is given by

$$
H=\int_{\mathbb{S}^2}{}^{(2)}\mathbf{e}\left(\hat{N}C+\hat{N}^\theta C_\theta\right),
$$

with

$$
\begin{aligned}
C &:= -p_{\hat{\gamma}}p_{\hat{T}}+\big(2\hat{T}''-\hat{\gamma}'\hat{T}'\big)\sin^2\theta+(\hat{\gamma}'\hat{T}-5\hat{T}')\cos\theta-\frac{3}{2}\hat{T}-\hat{T}'\\
&\quad+\frac{1}{2}\sum_i\left(\frac{p_{\hat{\phi}_i}^2}{\hat{T}}+\hat{T}\hat{\phi}_i'^2\sin^2\theta\right)+(1-\cos\theta)\hat{T}\hat{\phi}_1'\,,\\
C_\theta &= \Big(2p_{\hat{\gamma}}'-\hat{\gamma}'p_{\hat{\gamma}}-\hat{T}'p_{\hat{T}}-\sum_i\hat{\phi}_i'p_{\hat{\phi}_i}\Big)\sin^2\theta+\big(\hat{T}p_{\hat{T}}-p_{\hat{\gamma}}+p_{\hat{\phi}_1}\big)\cos\theta-p_{\hat{\gamma}}-p_{\hat{\phi}_1}\,.
\end{aligned}
$$

The two previous expressions, together with the conditions at the poles $\hat{T}(+1)e^{-\hat{\gamma}(+1)/2}=1$ and $e^{2\hat{\phi}_1(-1)-\hat{\gamma}(-1)}=4$, define the constraints of the system. As before, the polar constraints are necessary conditions to guarantee the differentiability of the (weighted) constraints $C[\hat{N}_g]$ and $C_\theta[\hat{N}_g^\theta]$. Concretely, it is straightforward to check that the surface term which appears when calculating the exterior derivative $\delta C[\hat{N}_g]$, namely, $-(1+\cos\theta)\hat{N}_g\delta\hat{T}+\hat{N}_g\hat{T}\cos\theta\delta\hat{\gamma}+(1-\cos\theta)\hat{N}_g\hat{T}\delta\hat{\phi}_1\big]_{\theta=0}^{\pi}$, vanishes by virtue of these constraints. The gauge transformations generated by $C[\hat{N}_g]$ and $C_\theta[\hat{N}_g^\theta]$ are

$$\begin{aligned}
&\{\hat{\gamma}, C[\hat{N}_g]\} = -\hat{N}_g p_{\hat{T}}\,,\\
&\{\hat{T}, C[\hat{N}_g]\} = -\hat{N}_g p_{\hat{\gamma}}\,,\\
&\{\hat{\phi}_i, C[\hat{N}_g]\} = \hat{N}_g \frac{p_{\hat{\phi}_i}}{\hat{T}}\,,\\
&\{p_{\hat{\gamma}}, C[\hat{N}_g]\} = \hat{N}_g'(\hat{T}\cos\theta-\hat{T}'\sin^2\theta)+\hat{N}_g(3\hat{T}'\cos\theta+\hat{T}-\hat{T}''\sin^2\theta),\\
&\{p_{\hat{T}}, C[\hat{N}_g]\} = \hat{N}_g\big[\frac{1}{2}-\hat{\phi}_1'+(\hat{\gamma}'+\hat{\phi}_1')\cos\theta-\hat{\gamma}''\sin^2\theta\big]+\hat{N}_g'(3\cos\theta-1-\hat{\gamma}'\sin^2\theta)\\
&\qquad\qquad -2\hat{N}_g''\sin^2\theta+\frac{\hat{N}_g}{2}\sum_i\left(\frac{p^2_{\hat{\phi}_i}}{\hat{T}^2}-\sin^2\theta\hat{\phi}_i'^2\right),\\
&\{p_{\hat{\phi}_1}, C[\hat{N}_g]\} = [\hat{N}_g\hat{T}(\hat{\phi}_2'\sin^2\theta+1-\cos\theta)]'\,,\\
&\{p_{\hat{\phi}_2}, C[\hat{N}_g]\} = (\hat{N}_g\hat{T}\hat{\phi}_2'\sin^2\theta)'\,,
\end{aligned}$$

and

$$\begin{aligned}
&\{\hat{\gamma}, C_\theta[\hat{N}_g^\theta]\} = -2\hat{N}_g^{\theta\prime}\sin^2\theta+\hat{N}_g^\theta(3\cos\theta-\hat{\gamma}'\sin^2\theta-1)\,,\\
&\{\hat{T}, C_\theta[\hat{N}_g^\theta]\} = \hat{N}_g^\theta(\hat{T}\cos\theta-\hat{T}'\sin^2\theta)\,,\\
&\{\hat{\phi}_1, C_\theta[\hat{N}_g^\theta]\} = \hat{N}_g^\theta(\cos\theta-1-\hat{\phi}_2'\sin^2\theta)\,,\\
&\{\hat{\phi}_2, C_\theta[\hat{N}_g^\theta]\} = -\hat{N}_g^\theta\hat{\phi}_2'\sin^2\theta\,,\\
&\{p_{\hat{\gamma}}, C_\theta[\hat{N}_g^\theta]\} = -(\hat{N}_g^\theta p_{\hat{\gamma}}\sin^2\theta)'\,,\\
&\{p_{\hat{T}}, C_\theta[\hat{N}_g^\theta]\} = \hat{N}_g^\theta(p_{\hat{T}}\cos\theta-p_{\hat{T}}'\sin^2\theta)-\hat{N}_g^{\theta\prime}p_{\hat{T}}\sin^2\theta\,,\\
&\{p_{\hat{\phi}_i}, C_\theta[\hat{N}_g^\theta]\} = -(\hat{N}_g^\theta p_{\hat{\phi}_i}\sin^2\theta)'\,.
\end{aligned}$$

The Poisson brackets of these constraints give exactly the same result that we obtained for the $\mathbb{S}^1\times\mathbb{S}^2$ topology and, hence, define a fist class constrained surface $\Gamma_c\subset\Gamma$. Here, (Γ,ω) denotes the canonical phase space of the system, coordinatized by the canonical pairs $(\hat{\gamma},p_{\hat{\gamma}};\hat{T},p_{\hat{T}};\hat{\phi}_i,p_{\hat{\phi}_i})$, endowed with the standard (weakly) symplectic form (1.48). We must check now the stability of the polar constraints. We do this by computing

$$\{\hat{T}e^{-\hat{\gamma}/2}, C[\hat{N}_g]\} = \frac{1}{2}\hat{N}_g e^{-\hat{\gamma}/2}(\hat{T}p_{\hat{T}}-2p_{\hat{\gamma}})\,, \tag{1.82}$$

$$\{\hat{T}e^{-\hat{\gamma}/2}, C_\theta[\hat{N}_g^\theta]\} = e^{-\hat{\gamma}/2}\left(\frac{1}{2}\hat{N}_g^\theta\hat{T}(1-\cos\theta)+(\hat{N}_g^{\theta\prime}\hat{T}-\hat{N}_g^\theta\hat{T}'+\frac{1}{2}\hat{N}_g^\theta\hat{T}\hat{\gamma}')\sin^2\theta\right), \tag{1.83}$$

$$\{e^{2\hat{\phi}_1-\hat{\gamma}}, C[\hat{N}_g]\} = \frac{\hat{N}^g}{\hat{T}}e^{2\hat{\phi}_1-\hat{\gamma}}(2p_{\hat{\phi}_1}+\hat{T}p_{\hat{T}})\,, \tag{1.84}$$

$$\{e^{2\hat{\phi}_1-\hat{\gamma}}, C_\theta[\hat{N}_g^\theta]\} = e^{2\hat{\phi}_1-\hat{\gamma}}\Big(-\hat{N}_g^\theta(1+\cos\theta)+(2\hat{N}_g^{\theta\prime}-2\hat{N}_g^\theta\hat{\phi}_2'+\hat{N}_g^\theta\hat{\gamma}')\sin^2\theta\Big)\,. \tag{1.85}$$

The constraint $C_\theta = 0$ at the poles $\theta = 0, \pi$ gives $\hat{T}(+1)p_{\hat{T}}(+1) - 2p_{\hat{\gamma}}(+1) = 0$, and $\hat{T}(-1)p_{\hat{T}}(-1) + 2p_{\hat{\phi}_1}(-1) = 0$, respectively. These relations guarantee that the Poisson bracket (1.82) vanishes at $\theta = 0$ and (1.84) vanishes at $\theta = \pi$. The vanishing of (1.83) at $\theta = 0$ is due to the presence of the factors $1 - \cos\theta$ and $\sin^2\theta$ and, finally, (1.85) is zero at $\theta = \pi$ due to the factors $1+\cos\theta$ and $\sin^2\theta$. As in the 3-handle case, we conclude that there are no secondary constraints coming from the stability of these polar constraints.

1.2.1 Deparameterization

The deparameterization process in this case follows closely the one developed for the $\mathbb{S}^1 \times \mathbb{S}^2$ topology. Particularly, the same gauge fixing conditions (1.50) work in this case too. It suffices to check if the polar constraints are gauge fixed. This only requires the computation of the Poisson bracket

$$\{p_{\hat{\gamma}n}, e^{2\hat{\phi}_1-\hat{\gamma}}\} = e^{2\hat{\phi}_1-\hat{\gamma}}\sqrt{\frac{2n+1}{4\pi}}\mathscr{P}_n(\cos\theta)\,,$$

which is different from zero at the poles. As we see, the situation now is completely analogous to the 3-handle case. The only constraint that is not gauge-fixed by the deparameterization conditions is $C[1]$. The pull-back of the symplectic form to the phase space hypersurface defined by the gauge fixing conditions is given again by (1.54). We are left only with the constraint

$$\begin{aligned}\mathcal{C} \;&:=\; -p_{\hat{\gamma}_0}p_{\hat{T}_0} + \hat{T}_0\left(\sqrt{4\pi}\log\frac{\hat{T}_0}{\sqrt{4\pi}} - \hat{\gamma}_0 - \sqrt{\pi}(2\log 2 + 3) + \hat{\phi}_{1_0}\right) \\ &+\; \frac{1}{2}\sum_i\int_{\mathbb{S}^2}{}^{(2)}\mathbf{e}\left(\frac{\sqrt{4\pi}p^2_{\hat{\phi}_i}}{\hat{T}_0} + \frac{\hat{T}_0}{\sqrt{4\pi}}\hat{\phi}_i'^2\right) \approx 0\,.\end{aligned} \tag{1.86}$$

The gauge transformations generated by this constraint on the variables $\hat{T}_0$ and $p_{\hat{\gamma}_0}$ are the same as for the three-handle and, hence, we can use the canonical transformations (1.56) and (1.57) introduced at the end of the previous section to rewrite (1.86) as

$$\begin{aligned}p_T \;&+\; (4\pi)^{1/4}e^{\tilde{P}/2}\varphi_{1_0}\sin T + 2\sqrt{\pi}e^{\tilde{P}}\left(\log\frac{\sin T}{\sqrt{4\pi}} + \tilde{P} - \log 2 - \frac{3}{2}\right)\sin T \\ &+\; \frac{1}{2}\sum_i\int_{\mathbb{S}^2}{}^{(2)}\mathbf{e}\left(\frac{p^2_{\varphi_i}}{\sin T} + \varphi_i'^2\sin T\sin^2\theta\right) \approx 0.\end{aligned} \tag{1.87}$$

Again, it is possible to interpret the dynamics as being described by a nonautonomous Hamiltonian system $((0,\pi)\times\Gamma_R, \mathrm{d}t, \omega_R, H_R)$, where Γ_R denotes the reduced phase space coordinatized by the canonical pairs $(\tilde{Q}, \tilde{P}; \varphi_i, p_{\varphi_i})$, endowed with the standard (weakly) symplectic form (1.60). The dynamics is given by the time-dependent Hamiltonian

$H_R(t):\Gamma_R\rightarrow\mathbb{R}$

$$\begin{aligned} H_R(t) &= (4\pi)^{1/4}e^{\tilde{P}/2}\varphi_{1_0}\sin t+2\sqrt{\pi}e^{\tilde{P}}\Big(\log\frac{\sin t}{\sqrt{4\pi}}+\tilde{P}-\log 2-\frac{3}{2}\Big)\sin t \\ &+ \frac{1}{2}\sum_i\int_{\mathbb{S}^2}{}^{(2)}\mathbf{e}\left(\frac{p^2_{\varphi_i}}{\sin t}+\varphi_i'^2\sin t\sin^2\theta\right). \end{aligned}$$

Both initial and final singularities show up in the same way as for the $\mathbb{S}^1\times\mathbb{S}^2$ topology. The corresponding evolution vector field is given by

$$\begin{aligned} E_{H_R} &= \frac{\partial}{\partial t}+\left[(4\pi)^{1/4}e^{\tilde{P}/2}\varphi_{1_0}\sin t+2\sqrt{\pi}e^{\tilde{P}}\sin t\left(\log\frac{\sin t}{\sqrt{4\pi}}+\tilde{P}-\log 2-\frac{1}{2}\right)\right]\frac{\partial}{\partial\tilde{Q}} \\ &- (4\pi)^{1/4}e^{\tilde{P}/2}\sin t\frac{\partial}{\partial p_{\varphi_{1_0}}}+\sum_i\int_{\mathbb{S}^2}{}^{(2)}\mathbf{e}\left(\frac{p_{\varphi_i}}{\sin t}\frac{\delta}{\delta\varphi_i}+(\sin^2\theta\varphi_i')'\sin t\frac{\delta}{\delta p_{\varphi_i}}\right). \end{aligned}$$

It is interesting at this point to compare the dynamics of this model and the 3-handle one. First of all, we see that the global mode has a different behavior now, in particular it couples to φ_{1_0} through the term $e^{\tilde{P}/2}\varphi_{1_0}\sin t$. As we see, the gravitational and matter modes apparently cease to play a symmetric role in this particular description, at variance with the other topologies. However, we will see next that it is possible to restore the symmetry between the gravitational and matter scalars.

We proceed as at the end of the section devoted to the $\mathbb{S}^1\times\mathbb{S}^2$ topology by introducing a convenient auxiliary set $(\mathring{g}_{ab},\mathring{\phi}_i)$ in terms of which we can solve the original Einstein-Klein-Gordon equations. After the deparameterization procedure, and imposing the consistency of the gauge fixing conditions under the dynamics generated by the Hamiltonian $H[\hat{N},\hat{N}^\theta]$, the 3-metric g_{ab} of the 3-sphere model can be written

$$g_{ab}=\cos^2(\theta/2)e^{\gamma}\Big(-(\mathrm{d}t)_a(\mathrm{d}t)_b+(\mathrm{d}\theta)_a(\mathrm{d}\theta)_b\Big)+\frac{P^2}{4\pi}\sin^2 t\sin^2\theta(\mathrm{d}\sigma)_a(\mathrm{d}\sigma)_b\,,$$

defined on $(0,\pi)\times D(0;\pi)$. In this case, a possible choice of $(\mathring{g}_{ab},\mathring{\phi}_i)$ is

$$\begin{aligned} \mathring{g}_{ab} &= \cos^2(\theta/2)e^{\mathring{\gamma}}\Big(-(\mathrm{d}t)_a(\mathrm{d}t)_b+(\mathrm{d}\theta)_a(\mathrm{d}\theta)_b\Big)+\sin^2 t\sin^2\theta(\mathrm{d}\sigma)_a(\mathrm{d}\sigma)_b\,, \\ \mathring{\phi}_1 &= \cos\theta\cos t\log(\tan(t/2))+\cos\theta+\log(\cos^2(\theta/2))+\log(2\sin t)\,, \\ \mathring{\phi}_i &= 0\,,\ \ i\neq 0\,, \end{aligned}$$

where

$$\begin{aligned} \mathring{\gamma} &:= \frac{\sin^2\theta}{4}\Big(\sin^2 t\log^2(\tan t/2)-2\cos t\log(\tan t/2)-1\Big)+\log\big(\sin^2 t\big) \\ &- \cos t\log(\tan(t/2))+\cos\theta\cos t\log(\tan(t/2))+\cos\theta-1. \end{aligned}$$

In fact, the concrete functional form of $\mathring{\gamma}$ is irrelevant here since whenever $\mathcal{L}_\sigma\phi_i=0$ we have the following equivalence in $(0,\pi)\times(\mathbb{S}^2-\{\theta=\pi\})$:

$$\mathring{g}^{ab}\mathring{\nabla}_a\mathring{\nabla}_b\phi_i=0\Leftrightarrow\breve{g}^{ab}\breve{\nabla}_a\breve{\nabla}_b\phi_i=0\,,$$

with

$$\breve{g}_{ab}=\sin^2t\Big(-(\mathrm{d}t)_a(\mathrm{d}t)_b+(\mathrm{d}\theta)_a(\mathrm{d}\theta)_b+\sin^2\theta(\mathrm{d}\sigma)_a(\mathrm{d}\sigma)_b\Big)\,.$$

Here, the metric $\breve{g}_{ab}$ coincides with that one found for the 3-handle case, conformal to the Einstein static metric on $(0,\pi)\times\mathbb{S}^2$, but restricted now to the manifold $(0,\pi)\times D(0;\pi)$ obtained by removing the pole $\theta=\pi$ from the 2-sphere. Note that the ϕ_1 field cannot be extended to the boundary of the disc, parameterized as $\theta=\pi$, because (1.73) forces it to behave as $\log(\cos^2(\theta/2))$ when $\theta\to\pi$. However, if we split ϕ_1 as $\phi_1=\phi_1^{\text{sing}}+\phi_1^{\text{reg}}$, with $\phi_1^{\text{sing}}:=\log(\cos^2(\theta/2))+\log(2\sin t)$ satisfying

$$\breve{g}^{ab}\breve{\nabla}_a\breve{\nabla}_b\phi_1^{\text{sing}}=0\,,$$

we guarantee that the gravitational degrees of freedom encoded by ϕ_1^{reg} still satisfy $\breve{g}^{ab}\breve{\nabla}_a\breve{\nabla}_b\phi_1^{\text{reg}}=0$ (just the same equation as the matter fields ϕ_i, $i\neq1$) and can be extended to $(0,\pi)\times\mathbb{S}^2$. Both regularized gravitational and matter fields, respectively ϕ_1^{reg} and ϕ_i, $i\neq1$, are then well behaved on $(0,\pi)\times\mathbb{S}^2$ and play a symmetric role just as in the description of the 3-handle topology. Within the Lagrangian formulation of the 3-sphere model, this can be attained by introducing an extra $\hat{T}$ field on the right-hand side of the regularity condition (1.73).

References

1 M. Nakahara, *Geometry, Topology and Physics*, Second Edition. Graduate Student Series in Physics, Taylor & Francis (2003).

2 P. S. Mostert, Ann. of Math. **65**, 447 (1957); **66**, 589 (1957).

3 P. T. Chruściel, Ann. Phys. **202**, 100 (1990).

4 S. W. Hawking and G. T. Horowitz, Class. Quant. Grav. **13**, 1487 (1996). S. W. Hawking and C. J. Hunter, Class. Quant. Grav. **13**, 2735 (1996).

5 O. Rinne and J. M. Stewart, Class. Quant. Grav. 22, 1143 (2005).

6 T. Thiemann, *Modern Canonical Quantum General Relativity* (Cambridge Monographs on Mathematical Physics), Cambridge University Press (2007).

7 J. D. Romano and C. G. Torre, Phys. Rev. D **53**, 5634 (1996).

8 A. Ashtekar, *Lectures on Non-perturbative Canonical Gravity*, Advanced series in Astrophysics and Cosmology, Vol. 6, World Scientific (1991).

9 C. W. Misner, Phys. Rev. D **8**, 3271 (1973).

10 B. K. Berger, Ann. Phys. **83**, 458 (1974).

11 M. Pierri, Int. J. Mod. Phys. D **11**, 135 (2002).

12 J. Cortez and G. A. Mena Marugán, Phys. Rev. D **72**, 064020 (2005).

13 D. Chinea, M. de León, and J.C. Marrero, "Locally conformal cosymplectic manifolds and time-dependent Hamiltonian systems", Comment. Math. Univ. Carolinae, 32, 2 (1991), 383-387.

14 S. W. Hawking and R. Penrose, Proc. Roy. Soc. Lond. A **267**, 529-48 (1970).

Chapter 2
Fock Space Quantization

J. F. Barbero G., D. G. Vergel, and E. J. S. Villaseñor
Classical and Quantum Gravity 25, 085002 (2008)

D. G. Vergel and E. J. S. Villaseñor
Classical and Quantum Gravity 25, 145008 (2008)

In this chapter, we will proceed to exactly quantize the classical theory developed in *Chapter 1* by promoting the canonical variables $(\tilde{Q}, \tilde{P}; \varphi_i, p_{\varphi_i})$ characterizing the global and local degrees of freedom to quantum operators $(\hat{\tilde{Q}}, \hat{\tilde{P}}; \hat{\varphi}_i, \hat{p}_{\varphi_i})$. Our starting point is given by the interpretation of the compact $\mathbb{S}^1 \times \mathbb{S}^2$ and $\mathbb{S}^3$ Gowdy models coupled to matter as scalar field theories in curved backgrounds conformally equivalent to the $(1+2)$-dimensional Einstein metric on $(0,\pi) \times \mathbb{S}^2$. Here, the corresponding conformal factor will be a simple function of t, specifically, $\sin t$. This description will be used to gain useful insights into the problem of the unitary implementability of the quantum time evolution for these models.

Let $\mathscr{H} = \mathscr{H}_0 \otimes \mathscr{H}_c = \mathscr{H}_0 \otimes (\otimes_i \mathscr{F}_i)$ be the Hilbert space of the system. The absence of extra constraints for the topologies under consideration was proved in the previous chapter. From here follows the unnecessary distinction between kinematical and physical Hilbert spaces.[1] This is in contrast with the 3-torus case, where an extra $U(1)$ symmetry generated by a residual global constraint still remains after deparameterization. The global modes $(\tilde{Q}, \tilde{P})$ can be quantized in a straightforward way in terms of standard position and momentum operators with dense domains in $\mathscr{H}_0 \cong L^2(\mathbb{R}, \mathrm{d}q)$, such that[2] $\hat{\tilde{Q}}\psi = q\psi$, $\hat{\tilde{P}}\psi = -i\partial_q\psi$, for $\psi = \psi(q) \in L^2(\mathbb{R})$. The Hilbert spaces for gravitational and matter modes, on the other hand, adopt the structure of symmetric Fock spaces $\mathscr{F}_i$ built from appropriate one-particle Hilbert spaces. As they are all isomorphic, and all massless scalar fields φ_i satisfy the same Euler-Lagrange equation, the same construction is valid for all of them. For this reason, we will omit the i-index in the following. The local degrees of freedom (φ, p_φ) are then promoted to operator-valued distributions on

[1] Nevertheless, in spite of the apparent simplicity of the phase space description after deparameterization given the absolute decoupling of gravitational and matter degrees of freedom, the full $(1+3)$-dimensional metric that solves the original Einstein-Klein-Gordon equations depends on both types of modes in a nontrivial way.

[2] In what follows, we will use units such that $\hbar = 1$.

$\mathbb{S}^2$ for each value of the time parameter t. They act as the identity over $\mathscr{H}_0$. Similarly, the $\hat{\mathring{Q}}$ and $\hat{\mathring{P}}$ operators act as the identity over $\mathscr{F}$.

2.1 Canonical and covariant phase spaces

The dynamics of the local degrees of freedom of both $\mathbb{S}^1 \times \mathbb{S}^2$ and $\mathbb{S}^3$ Gowdy models can be described after deparameterization by the same Euler-Lagrange equation in a fixed background metric conformal to the (1+2)-dimensional Einstein static metric on $(0, \pi) \times \mathbb{S}^2$,

$$\mathring{g}_{ab} = \sin^2 t \left(-(\mathrm{d}t)_a(\mathrm{d}t)_b + \gamma_{ab}\right), \tag{2.1}$$

where γ_{ab} denotes the round unit metric on the 2-sphere $\mathbb{S}^2$; in spherical coordinates $(\theta, \sigma) \in (0, \pi) \times (0, 2\pi)$ on $\mathbb{S}^2$, $\gamma_{ab} = (\mathrm{d}\theta)_a(\mathrm{d}\theta)_b + \sin^2\theta(\mathrm{d}\sigma)_a(\mathrm{d}\sigma)_b$. In addition, we must impose the invariance under the diffeomorphisms generated by the Killing vector field $\sigma^a = (\partial/\partial\sigma)^a$. The equation of motion can be derived, by imposing the additional symmetry condition $\mathcal{L}_\sigma\varphi = 0$ on the solutions, from the action

$$\begin{aligned} S(\varphi) &= -\frac{1}{2}\int_{[t_0,t_1]\times\mathbb{S}^2} |\mathring{g}|^{1/2}\mathring{g}^{ab}(\mathrm{d}\varphi)_a(\mathrm{d}\varphi)_b \\ &= \frac{1}{2}\int_{t_0}^{t_1}\mathrm{d}t\int_{\mathbb{S}^2}|\gamma|^{1/2}\sin t\left(\dot{\varphi}^2 + \varphi\,\Delta_{\mathbb{S}^2}\varphi\right), \end{aligned} \tag{2.2}$$

where $\Delta_{\mathbb{S}^2}$ denotes the Laplace-Beltrami operator on the round 2-sphere $\mathbb{S}^2$. The space of smooth and symmetric real solutions to the corresponding massless Klein-Gordon equation of motion has the structure of an infinite-dimensional $\mathbb{R}$-vector space

$$\begin{aligned} \mathcal{S} &:= \{\varphi \in C^\infty((0,\pi)\times\mathbb{S}^2;\mathbb{R}) \,|\, \mathring{g}^{ab}\mathring{\nabla}_a\mathring{\nabla}_b\varphi = 0;\ \mathcal{L}_\sigma\varphi = 0\} \\ &= \{\varphi \in C^\infty((0,\pi)\times\mathbb{S}^2;\mathbb{R}) \,|\, \ddot{\varphi} + \cot t\,\dot{\varphi} - \Delta_{\mathbb{S}^2}\varphi = 0;\ \mathcal{L}_\sigma\varphi = 0\}. \end{aligned} \tag{2.3}$$

The variational principle (2.2) gives rise to a natural (weakly) symplectic structure Ω on $\mathcal{S}$ defined by

$$\Omega(\varphi_1, \varphi_2) := \sin t \int_{\mathbb{S}^2} |\gamma|^{1/2}\imath_t^*\left(\varphi_2\dot{\varphi}_1 - \varphi_1\dot{\varphi}_2\right). \tag{2.4}$$

Here, $\imath_t : \mathbb{S}^2 \to (0,\pi)\times\mathbb{S}^2$ denotes the inclusion given by $\imath_t(s) = (t, s) \in (0,\pi)\times\mathbb{S}^2$. It is straightforward to show that Ω does not depend upon the choice of the value of time t used to define the embedding $\imath_t(\mathbb{S}^2) \subset \mathbb{R}\times\mathbb{S}^2$. We will refer to the infinite-dimensional linear symplectic space $\Gamma := (\mathcal{S}, \Omega)$ as the *covariant phase space* of the system [1]. We will denote the usual *canonical phase space* as $\Upsilon := (\mathbf{P}, \omega)$. Here, $\mathbf{P}$ is the space of smooth and symmetric Cauchy data $\mathbf{P} := \{(Q, P) \in C^\infty(\mathbb{S}^2;\mathbb{R}) \times C^\infty(\mathbb{S}^2;\mathbb{R}) \,|\, \mathcal{L}_\sigma Q = \mathcal{L}_\sigma P = 0\}$, endowed with the standard symplectic structure

$$\omega((Q_1, P_1), (Q_2, P_2)) := \int_{\mathbb{S}^2} |\gamma|^{1/2}(Q_2P_1 - Q_1P_2). \tag{2.5}$$

Given any value of t, it is possible to construct a symplectomorphism between the spaces Γ and Υ. The bijection $\mathfrak{I}_t : \Upsilon \to \Gamma$, that maps every Cauchy data (Q, P) to the unique solution $\varphi \in \mathcal{S}$ such that

$$\varphi(t,s) = Q(s) \quad \text{and} \quad (\sin t)\dot{\varphi}(t,s) = P(s) \tag{2.6}$$

is, irrespective of the value of t, a linear symplectomorphism, i.e., $\omega = \mathfrak{I}_t^*\Omega$.

Any vector $\varphi \in \Gamma$ is a smooth function on $\mathbb{R} \times \mathbb{S}^2$. Therefore, for each value of $t \in (0,\pi)$ we have $\iota_t^*\varphi \in C^\infty(\mathbb{S}^2;\mathbb{R})$. It is well known that any smooth *symmetric* function on $\mathbb{S}^2$ can be written in the form

$$(\iota_t^*\varphi)(s) = \varphi(t,s) = \sum_{\ell=0}^{\infty} A_\ell(t) Y_{\ell 0}(s)\,, \tag{2.7}$$

where $Y_{\ell 0}$ denote the spherical harmonics (1.51) that in standard spherical coordinates have the form

$$Y_{\ell 0}(s) = \left(\frac{2\ell+1}{4\pi}\right)^{1/2} \mathscr{P}_\ell(\cos\theta(s))$$

in terms of Legendre polynomials $\mathscr{P}_\ell$, satisfying the equations

$$\Delta_{\mathbb{S}^2} Y_{\ell 0} = -\ell(\ell+1) Y_{\ell 0}\,, \quad \mathcal{L}_\sigma Y_{\ell 0} = 0\,,$$

and verifying the $L^2(\mathbb{S}^2)$-orthogonality conditions[3]

$$\int_{\mathbb{S}^2} |\gamma|^{1/2} \bar{Y}_{\ell_1 0} Y_{\ell_2 0} = \delta(\ell_1,\ell_2)\,.$$

The coefficients $A_\ell(t)$ appearing in (2.7) are defined in terms of φ through

$$A_\ell(t) = \int_{\mathbb{S}^2} |\gamma|^{1/2} \bar{Y}_{\ell 0}\, \iota_t^*\varphi\,.$$

Given the reality of the field φ, it is clear that $\bar{A}_\ell(t) = A_\ell(t)$. From the fact that, for any fixed value of t and for all $n \in \mathbb{N}_0$, $\partial_t^n \varphi(t,\cdot)$ is a smooth function on $\mathbb{S}^2$, we have

$$\lim_{\ell\to+\infty} \frac{1}{\ell^p} \frac{\mathrm{d}^n A_\ell(t)}{\mathrm{d}t^n} = 0\,, \quad \forall\, p,n \in \mathbb{N}_0\,, \ \forall\, t \in (0,\pi)\,.$$

Then, it is clear that any $\varphi \in \Gamma$ can be expanded in the form

$$\varphi(t,s) = \sum_{\ell=0}^{\infty} \Big(a_\ell y_\ell(t) + \overline{a_\ell y_\ell(t)} \Big) Y_{\ell 0}(s)\,. \tag{2.8}$$

[3]The bar denotes complex conjugation and $\delta(\ell_1,\ell_2)$ is the Kronecker delta.

The massless Klein-Gordon equation defining $\mathcal{S}$ leads to the following equation for the complex functions $y_\ell(t)$

$$\ddot{y}_\ell + (\cot t)\dot{y}_\ell + \ell(\ell+1)y_\ell = 0\,. \tag{2.9}$$

We will always assume that, for each ℓ, the real and imaginary parts of y_ℓ, denoted u_ℓ and v_ℓ respectively, are two real linearly independent solutions of (2.9). The complex coefficients a_ℓ must satisfy the fall-off conditions

$$\lim_{\ell\to+\infty}\frac{1}{\ell^p}\left(a_\ell\frac{\mathrm{d}y_\ell}{\mathrm{d}t^n}(t)+\bar{a}_\ell\frac{\mathrm{d}\bar{y}_\ell}{\mathrm{d}t^n}(t)\right)=0\,,\quad \forall\, p,n\in\mathbb{N}_0\,,\ \ \forall\, t\,\in(0,\pi)\,.$$

From the point of view of the classical theory, these conditions are necessary to guarantee the smoothness of the solution to the field equations. However, we do not need to know them in detail to discuss the quantization of the models. In fact, they will be relaxed to the milder condition $\sum_\ell |a_\ell|^2 < +\infty$ when we introduce the one-particle Hilbert space. We will not make at this point any specific choice for the complex functions y_ℓ, but we will fix their normalization in the following way. Let us substitute first (2.8) in the symplectic structure (2.4). We find that

$$\Omega(\varphi_1,\varphi_2)=\sin t\sum_{\ell=0}^{\infty}\big(\bar{a}_\ell^{(1)}a_\ell^{(2)}-\bar{a}_\ell^{(2)}a_\ell^{(1)}\big)\big(y_\ell(t)\dot{\bar{y}}_\ell(t)-\dot{y}_\ell(t)\bar{y}_\ell(t)\big)\,.$$

By explicitly decomposing $y_\ell(t)=u_\ell(t)+iv_\ell(t)$ and writing

$$y_\ell(t)\dot{\bar{y}}_\ell(t)-\dot{y}_\ell(t)\bar{y}_\ell(t)=2i\det\begin{bmatrix}\dot{u}_\ell(t) & u_\ell(t)\\ \dot{v}_\ell(t) & v_\ell(t)\end{bmatrix}=:2iW(t;u_\ell,v_\ell)\,.$$

we have that, by virtue of the differential equation (2.9), the Wronskian W satisfies

$$\dot{W}+(\cot t)W=0\Rightarrow W(t;u_\ell,v_\ell)=\frac{c_\ell}{\sin t}\,,\quad c_\ell\in\mathbb{R}\,,$$

and hence the symplectic structure takes the simple expression

$$\Omega(\varphi_1,\varphi_2)=2i\sum_{\ell=0}^{\infty}c_\ell\big(\bar{a}_\ell^{(1)}a_\ell^{(2)}-\bar{a}_\ell^{(2)}a_\ell^{(1)}\big)\,. \tag{2.10}$$

Note that the time-independence of the symplectic structure is explicit now. In the following, we will choose the pair of functions (u_ℓ,v_ℓ) to be normalized in such a way that $c_\ell=1/2$, $\forall\,\ell\in\mathbb{N}_0$, i.e.,

$$W(t;u_\ell,v_\ell)=\frac{1}{2\sin t}\,,\quad \forall\,(u_\ell,v_\ell)\,,\ \ \ell\in\mathbb{N}_0\,. \tag{2.11}$$

It could appear that this condition is rather arbitrary but, as we will see, it is expedient to make this choice in order to ensure that the modes $(\varphi_\ell := y_\ell Y_{\ell 0})_{\ell\in\mathbb{N}_0}$ define an orthogonal basis of the one-particle Hilbert space used to construct the Fock space for the quantum theory. We also obtain in this way a very convenient expression for the symplectic structure Ω that will be our starting point for the quantization of the models. A concrete election satisfying (2.11) is given by

$$u_{0\ell}(t) = \frac{1}{\sqrt{2}}\mathscr{P}_\ell(\cos t), \quad v_{0\ell}(t) = \frac{1}{\sqrt{2}}\mathscr{Q}_\ell(\cos t)\,, \quad \ell \in \mathbb{N}_0\,, \tag{2.12}$$

with $\mathscr{P}_\ell$ and $\mathscr{Q}_\ell$ denoting the first and second class Legendre functions, respectively.

2.1.1 Classical dynamics

The classical time evolution from the embedding $\imath_{t_0}(\mathbb{S}^2) \subset (0,\pi) \times \mathbb{S}^2$ to $\imath_{t_1}(\mathbb{S}^2) \subset (0,\pi) \times \mathbb{S}^2$ is implemented on the canonical phase space Υ by the symplectic transformation $\tau_{(t_1,t_0)} : \Upsilon \to \Upsilon$ defined as

$$\tau_{(t_1,t_0)} := \mathfrak{J}_{t_1}^{-1} \circ \mathfrak{J}_{t_0} \tag{2.13}$$

in terms of the symplectic maps $\mathfrak{J}_t : \Upsilon \to \Gamma$ introduced in (2.6) and their inverses. The maps $\mathfrak{J}_t$ can be easily computed in terms of the Fourier coefficients a_ℓ of φ (2.8) as

$$a_\ell(t) = -i \sin t \dot{\bar{y}}_\ell(t) \int_{\mathbb{S}^2} |\gamma|^{1/2} Y_{\ell 0} Q + i \bar{y}_\ell(t) \int_{\mathbb{S}^2} |\gamma|^{1/2} Y_{\ell 0} P\,. \tag{2.14}$$

The operator $\tau_{(t_1,t_0)}$ acts as follows: (i) first, it takes initial Cauchy data on $\imath_{t_0}(\mathbb{S}^2)$, (ii) evolves them to the corresponding solution in $\mathcal{S}$, and (iii) finds the Cauchy data induced by this solution on $\imath_{t_1}(\mathbb{S}^2)$. On the other hand, time evolution can also be viewed as a symplectic transformation on the covariant phase space, $\mathcal{T}_{(t_1,t_0)} : \Gamma \to \Gamma$, defined by

$$\mathcal{T}_{(t_1,t_0)} := \mathfrak{J}_{t_1} \circ \tau_{(t_1,t_0)} \circ \mathfrak{J}_{t_1}^{-1} = \mathfrak{J}_{t_0} \circ \mathfrak{J}_{t_1}^{-1}\,, \tag{2.15}$$

that (i) takes a solution of $\mathcal{S}$, (ii) finds the induced Cauchy data on $\imath_{t_1}(\mathbb{S}^2)$, and (iii) takes those data as initial data on $\imath_{t_0}(\mathbb{S}^2)$, finding the unique solution of $\mathcal{S}$ which corresponds to these initial conditions. In our case, combining (2.6) and (2.14), it is straightforward to check that the action of the operator $\mathcal{T}_{(t_1,t_0)}$ is given by

$$(\mathcal{T}_{(t_1,t_0)}\varphi)(t,s) \;=\; \sum_{\ell=0}^{\infty} \Big(\mathfrak{a}_\ell(t_1,t_0) y_\ell(t) + \overline{\mathfrak{a}_\ell(t_1,t_0) y_\ell(t)} \Big) Y_{\ell 0}(s)\,, \tag{2.16}$$

where

$$\begin{aligned} \mathfrak{a}_\ell(t_1,t_0) \;&:=\; i\big(\sin t_1 \bar{y}_\ell(t_0) \dot{y}_\ell(t_1) - \sin t_0 y_\ell(t_1) \dot{\bar{y}}_\ell(t_0)\big) a_\ell \\ &+\; i\big(\sin t_1 \bar{y}_\ell(t_0) \dot{\bar{y}}_\ell(t_1) - \sin t_0 \bar{y}_\ell(t_1) \dot{\bar{y}}_\ell(t_0)\big) \bar{a}_\ell\,. \end{aligned} \tag{2.17}$$

In the next sections we will try to find out if this classical evolution can be unitarily implemented in a Fock quantization of the system.

2.2 Fock quantization

In the passage to the quantum theory, we have to introduce a Hilbert space for our system. This will have the structure of a symmetric Fock space $\mathscr{F}$ built from some appropriate one-particle Hilbert space. We will review in this section the Fock quantization techniques based on the covariant phase space description of the model, following the quantization steps discussed in section 2.3 of reference [2]. It is well known that for a system of a finite number of uncoupled quantum harmonic oscillators this procedure provides a quantum theory unitarily equivalent to the usual tensor product of one-particle Hilbert spaces. However, for the case of a system of infinitely many uncoupled quantum harmonic oscillators, the tensor product of infinite number of one-particle Hilbert spaces gives rise to nonseparable Hilbert spaces, as well as reducible representations of the canonical commutation relations. The Fock quantization process analyzed below provides a better approach to deal with the infinitely many degrees of freedom present in these models, for it avoids the aforementioned difficulties. As expected for scalar fields in nonstationary curved background spacetimes, the Fock representation obtained in this way is highly non-unique; this is a problem that will be discussed in detail.

In order to define the one-particle Hilbert space used to build the Fock space $\mathscr{F}$, let $\mathcal{S}_{\mathbb{C}} := \mathbb{C}\otimes\mathcal{S}$ denote the $\mathbb{C}$-vector space obtained by the complexification of the solution space $\mathcal{S}$ (2.3). The elements of $\mathcal{S}_{\mathbb{C}}$ are ordered pairs of objects $(\varphi_1,\varphi_2)\in\mathcal{S}\times\mathcal{S}$ that we will write in the form[4] $\Phi := \varphi_1 + i\varphi_2$ with the natural definition for their sum. Multiplication by complex scalars $\mathbb{C}\ni\lambda=\lambda_1+i\lambda_2$, $\lambda_1,\lambda_2\in\mathbb{R}$, is defined as

$$\lambda\Phi := (\lambda_1\varphi_1-\lambda_2\varphi_2)+i(\lambda_2\varphi_1+\lambda_1\varphi_2)\,.$$

We also introduce the conjugation $\bar{\ } : \mathcal{S}_{\mathbb{C}}\to\mathcal{S}_{\mathbb{C}} : (\varphi_1+i\varphi_2)\mapsto(\varphi_1-i\varphi_2)$. Every vector $\Phi\in\mathcal{S}_{\mathbb{C}}$ can be expanded with the help of the basis $(\varphi_\ell := y_\ell Y_{\ell 0}, \bar{\varphi}_\ell := \overline{y_\ell Y_{\ell 0}})_{\ell\in\mathbb{N}_0}$ introduced above as

$$\Phi=\sum_{\ell=0}^{\infty}\Big(a_\ell y_\ell Y_{\ell 0}+b_\ell\overline{y_\ell Y_{\ell 0}}\Big)\,,$$

with $a_\ell, b_\ell\in\mathbb{C}$. We extend the symplectic structure (2.4) to $\mathcal{S}_{\mathbb{C}}$ by complex linearity in each variable,

$$\Omega_{\mathbb{C}}(\Phi_1,\Phi_2) := i\sum_{\ell=0}^{\infty}\big(b_\ell^{(1)}a_\ell^{(2)}-b_\ell^{(2)}a_\ell^{(1)}\big)\,.$$

For each pair $\Phi_1,\Phi_2\in\mathcal{S}_{\mathbb{C}}$, consider now the sesquilinear map $\langle\cdot|\cdot\rangle : \mathcal{S}_{\mathbb{C}}\times\mathcal{S}_{\mathbb{C}}\to\mathbb{C}$ defined by

$$\langle\Phi_1|\Phi_2\rangle := -i\Omega_{\mathbb{C}}(\bar{\Phi}_1,\Phi_2)\,. \tag{2.18}$$

It is antilinear in the first argument and linear in the second, satisfying all the properties of an inner product on $\mathcal{S}_{\mathbb{C}}$ except that it fails to be positive definite. There are,

[4]Here, $i\in\mathbb{C}$ denotes the imaginary unit.

however, linear subspaces of $\mathcal{S}_{\mathbb{C}}$ where $\langle\cdot|\cdot\rangle$ is positive definite (and, hence, defines an inner product). Consider, in particular, the Lagrangian subspace

$$\mathcal{P} := \Big\{\Phi \in \mathcal{S}_{\mathbb{C}} \,\Big|\, \Phi = \sum_{\ell=0}^{\infty} a_\ell \varphi_\ell \Big\} . \tag{2.19}$$

Here, the restriction $\langle\cdot|\cdot\rangle|_{\mathcal{P}}$ defines an inner product given by

$$\langle \Phi_1 | \Phi_2 \rangle = \sum_{\ell=0}^{\infty} \bar{a}_\ell^{(1)} a_\ell^{(2)} \,, \quad \Phi_1, \Phi_2 \in \mathcal{P} \,. \tag{2.20}$$

The separable and infinite-dimensional *one-particle Hilbert space* $\mathscr{H}_{\mathcal{P}} \cong \ell^2(\mathbb{C})$ is then obtained by Cauchy completion of $(\mathcal{P}, \langle\cdot|\cdot\rangle|_{\mathcal{P}})$ with respect to the norm defined by the inner product $\langle\cdot|\cdot\rangle|_{\mathcal{P}}$,

$$\mathscr{H}_{\mathcal{P}} := \overline{(\mathcal{P}, \langle\cdot|\cdot\rangle|_{\mathcal{P}})}^{\langle\cdot|\cdot\rangle|_{\mathcal{P}}} = \Big\{\Phi = \sum_{\ell=0}^{\infty} a_\ell \varphi_\ell \;\Big|\; a_\ell \in \mathbb{C} \,, \sum_{\ell=0}^{\infty} |a_\ell|^2 < +\infty \Big\} .$$

Note that the set $(\varphi_\ell = y_\ell Y_{\ell 0})_{\ell \in \mathbb{N}_0}$ becomes an orthonormal basis of $\mathscr{H}_{\mathcal{P}}$, satisfying $\langle \varphi_{\ell_1} \,|\, \varphi_{\ell_2} \rangle|_{\mathcal{P}} = \delta(\ell_1, \ell_2)$. The Hilbert space of the quantum theory is finally given by the symmetric Fock space

$$\mathscr{F}_+(\mathscr{H}_{\mathcal{P}}) = \bigoplus_{n=0}^{\infty} \mathscr{P}_+^{(n)} \left(\mathscr{H}_{\mathcal{P}}^{\otimes n}\right) ,$$

where $\mathscr{H}_{\mathcal{P}}^{\otimes 0} := \mathbb{C}$ and $\mathscr{P}_+^{(n)}\left(\mathscr{H}_{\mathcal{P}}^{\otimes n}\right)$ denotes the n-fold symmetric tensor product of $\mathscr{H}_{\mathcal{P}}$ (see *appendix E*). Associated with the orthonormal modes $\varphi_\ell \in \mathscr{H}_{\mathcal{P}}$, we define the corresponding annihilation $\hat{a}_\ell := A(\varphi_\ell)$ and creation operators $\hat{a}_\ell^\dagger := C(\varphi_\ell)$, with nonvanishing commutation relations given by $[\hat{a}_{\ell_1}, \hat{a}_{\ell_2}^\dagger] = \delta(\ell_1, \ell_2)$. As usual, we will denote as $|0\rangle_{\mathcal{P}}$ the Fock vacuum $1 \oplus 0 \oplus 0 \oplus \cdots \in \mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$ whose only nonzero component is $1 \in \mathbb{C}$. The vacuum is in the domain of all finite products of creation and annihilation operators, and the vectors

$$|{}^1n_{\ell_1}\, {}^2n_{\ell_2} \,\cdots\, {}^kn_{\ell_k}\rangle := \frac{1}{\sqrt{{}^1n!\,{}^2n!\,\cdots\,{}^kn!}} (\hat{a}_{\ell_1}^\dagger)^{{}^1n} (\hat{a}_{\ell_1}^\dagger)^{{}^2n} \cdots (\hat{a}_{\ell_k}^\dagger)^{{}^kn} |0\rangle_{\mathcal{P}} \in \mathscr{F}_+(\mathscr{H}_{\mathcal{P}}) \,,$$

where $k \in \mathbb{N}_0$, $({}^1n, {}^2n, \ldots, {}^kn) \in \mathbb{N}^k$, and $\ell_i \neq \ell_j$ for $i \neq j$, provide a basis of $\mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$. The basis vectors are normalized according to

$$\begin{aligned} \langle\, {}^1n_{\ell_1} \cdots {}^kn_{\ell_k} \,|\, {}^1m_{\ell'_1} \cdots {}^rm_{\ell'_r} \rangle \;&=\; \delta(k,r) \sum_{\sigma \in \Pi_k} \delta({}^1n, {}^{\pi(1)}m) \cdots \delta({}^kn, {}^{\pi(k)}m) \\ &\qquad \times \delta(\ell_1, \ell'_{\pi(1)}) \cdots \delta(\ell_k, \ell'_{\pi(k)}) \,, \end{aligned}$$

where Π_k denotes the set of permutations σ of the k symbols $\{1, 2, \ldots, k\}$. The creation and annihilation operators satisfy

$$\hat{a}_\ell^\dagger |n_\ell\rangle = \sqrt{n+1}\, |(n+1)_\ell\rangle \,, \quad \hat{a}_\ell |n_\ell\rangle = \sqrt{n}\, |(n-1)_\ell\rangle \,.$$

Using the notation introduced above, the modes φ_ℓ of the one particle Hilbert space $\mathscr{H}_\mathcal{P}$ can now be considered as one-particle states that we will denote as $|1_\ell\rangle := a_\ell^\dagger|0\rangle_\mathcal{P} \in \mathscr{F}_+(\mathscr{H}_\mathcal{P})$.

Note that every choice (2.19) of the Lagrangian subspace $\mathcal{P}$ corresponds to the specification of a complex structure $J_\mathcal{P}$ on the space of solutions $\mathcal{S}$. Indeed, owing to the fact that $\mathcal{P}\cap\bar{\mathcal{P}} = \{0\}$, where $\bar{\mathcal{P}}$ is the complex conjugate space of $\mathcal{P}$, it follows that $\mathcal{S}_\mathbb{C} = \mathcal{P}\oplus\bar{\mathcal{P}}$ and, hence, any vector $\varphi \in \mathcal{S}$ can be uniquely decomposed as $\varphi = \Phi + \bar{\Phi}$, with $\Phi \in \mathcal{P}$, $\bar{\Phi} \in \bar{\mathcal{P}}$. Then, given $\mathcal{P}$ and $\bar{\mathcal{P}}$, we can define the complex structure $J_\mathcal{P} : \mathcal{S} \to \mathcal{S}$ by $J_\mathcal{P}\varphi := i(\Phi - \bar{\Phi})$. This map is a linear canonical transformation on $\Gamma = (\mathcal{S}, \Omega)$ –i.e., $J_\mathcal{P}$ on $\mathcal{S}$ is compatible with Ω–, with $J_\mathcal{P}^2 = J_\mathcal{P} \circ J_\mathcal{P} = -\mathrm{Id}_\mathcal{S}$.

Denote by $\mathcal{S}_{J_\mathcal{P}}$ the complex vector space $\mathcal{S}$ where, given any $\varphi \in \mathcal{S}$, the product by complex scalars $\mathbb{C} \ni z = x + iy$, $x, y \in \mathbb{R}$, is defined by the rule $z\cdot\varphi := x\varphi + yJ_\mathcal{P}\varphi$. We have that the formula

$$\mu_{J_\mathcal{P}}(\varphi_1, \varphi_2) := \frac{1}{2}\Omega(J_\mathcal{P}\varphi_1, \varphi_2) \tag{2.21}$$

defines a positive definite bilinear symmetric form on $\mathcal{S}$. We then conclude that the sesquilinear map

$$\langle\varphi_1|\varphi_2\rangle_{J_\mathcal{P}} := \mu_{J_\mathcal{P}}(\varphi_1, \varphi_2) - \frac{i}{2}\Omega(\varphi_1, \varphi_2) \tag{2.22}$$

is an inner product on $\mathcal{S}_{J_\mathcal{P}}$ [3]. In this context, the one-particle Hilbert space $\mathscr{H}_\mathcal{P}$ is given by the Cauchy completion of the Euclidean space $(S_{J_\mathcal{P}}, \langle\cdot|\cdot\rangle_{J_\mathcal{P}})$. It is straightforward to check that the Cauchy completions of $(\mathcal{P}, \langle\cdot|\cdot\rangle)$ and $(S_{J_\mathcal{P}}, \langle\cdot|\cdot\rangle_{J_\mathcal{P}})$ are isomorphic: Indeed, the $\mathbb{C}$-linear map $\kappa : S_{J_\mathcal{P}} \to \mathcal{P}$ such that $\kappa(\varphi) = \Phi$, $\varphi \in \mathcal{S}_{J_\mathcal{P}}$, $\Phi \in \mathcal{P}$, defines a unitary transformation of $\mathcal{S}_{J_\mathcal{P}}$ onto $\mathcal{P}$, i.e., $\langle\varphi_1|\varphi_2\rangle_{J_\mathcal{P}} = \langle\kappa(\varphi_1)|\kappa(\varphi_2)\rangle = \langle\Phi_1|\Phi_2\rangle$, $\forall\,\varphi_1, \varphi_2 \in \mathcal{S}_{J_\mathcal{P}}$. Finally, we will obtain a relation that is relevant for the algebraic formulation of the quantum theory. By the Schwartz inequality, for all $\varphi_1, \varphi_2 \in \mathcal{S}_{J_\mathcal{P}}$ we have $\|\varphi_1\|^2_{J_\mathcal{P}}\|\varphi_2\|^2_{J_\mathcal{P}} \geq |\langle\varphi_1|\varphi_2\rangle_{J_\mathcal{P}}|^2 \geq |\mathrm{Im}[\langle\varphi_1|\varphi_2\rangle_{J_\mathcal{P}}]|^2$, where $\|\cdot\|_{J_\mathcal{P}}$ denotes the norm associated with the inner product (2.22), so that $\mu_{J_\mathcal{P}}$ satisfies

$$\mu_{J_\mathcal{P}}(\varphi_1, \varphi_1)\,\mu_{J_\mathcal{P}}(\varphi_2, \varphi_2) \geq \frac{1}{4}\big(\Omega(\varphi_1, \varphi_2)\big)^2 . \tag{2.23}$$

2.2.1 Complex structures

In practice, the definition of the complex structure $J_\mathcal{P}$ is complete once a choice of complex functions $(y_\ell)_{\ell\in\mathbb{N}_0}$ satisfying (2.9) and (2.11) is given. In that case, we can construct an orthonormal basis $(\varphi_\ell = y_\ell Y_{\ell 0})_{\ell\in\mathbb{N}_0}$ for the one-particle Hilbert space $\mathscr{H}_\mathcal{P}$ and define $J_\mathcal{P}$ by imposing that the complex structure be diagonalized in $\mathcal{S}_\mathbb{C}$,

$$J_\mathcal{P}\varphi_\ell = i\varphi_\ell\,, \quad J_\mathcal{P}\bar{\varphi}_\ell = -i\bar{\varphi}_\ell\,. \tag{2.24}$$

Different choices for $(y_\ell)_{\ell\in\mathbb{N}_0}$ give rise in general to different complex structures. With the aim of characterizing the freedom in the election, consider the family $(y_{0\ell})_{\ell\in\mathbb{N}_0}$ defined by (2.12) satisfying the normalization condition (2.11). Denote by J_0 the corresponding complex structure. For any other normalized election of a family of linearly independent functions $(y_\ell = u_\ell + iv_\ell)_{\ell\in\mathbb{N}_0}$ we can write (in terms of the $u_{0\ell}$ and $v_{0\ell}$)

$$y_\ell(t) = u_\ell(t) + iv_\ell(t) = \alpha_\ell u_{0\ell}(t) + \beta_\ell v_{0\ell}(t) + i\big(\gamma_\ell u_{0\ell}(t) + \delta_\ell v_{0\ell}(t)\big)\,. \tag{2.25}$$

The normalization that we are choosing (2.11) yields the following condition for the real coefficients α_ℓ, β_ℓ, γ_ℓ, and δ_ℓ,

$$\alpha_\ell\delta_\ell - \beta_\ell\gamma_\ell = 1\,, \quad \forall\,\ell\in\mathbb{N}_0\,, \tag{2.26}$$

i.e.,

$$\left[\begin{array}{cc} \alpha_\ell & \beta_\ell \\ \gamma_\ell & \delta_\ell \end{array}\right] \in SL(2;\mathbb{R})\,, \quad \forall\,\ell\in\mathbb{N}_0\,.$$

It is well-known that $SL(2,\mathbb{R})$ is bijective (as a set) to $\mathbb{S}^1\times\mathbb{R}^2$, in the sense that any element of $SL(2,\mathbb{R})$ can be uniquely decomposed as the product of a rotation and an upper triangular matrix with unit determinant,

$$SL(2,\mathbb{R}) \ni \left[\begin{array}{cc} \alpha_\ell & \beta_\ell \\ \gamma_\ell & \delta_\ell \end{array}\right] = \left[\begin{array}{cc} \cos\theta_\ell & -\sin\theta_\ell \\ \sin\theta_\ell & \cos\theta_\ell \end{array}\right]\cdot\left[\begin{array}{cc} \rho_\ell & \nu_\ell \\ 0 & \rho_\ell^{-1} \end{array}\right] \tag{2.27}$$

for a unique choice of $\rho_\ell > 0$, $\nu_\ell \in \mathbb{R}$, $\theta_\ell \in [0, 2\pi)$. Different choices of the triplet $(\rho_\ell, \nu_\ell, \theta_\ell)$ correspond, in principle, to different complex structures on $\mathcal{S}$, defined through (2.24) with

$$\begin{aligned} y_\ell(t) &= \rho_\ell\cos\theta_\ell u_{0\ell}(t) + (\nu_\ell\cos\theta_\ell - \rho_\ell^{-1}\sin\theta_\ell)v_{0\ell}(t) \\ &+ i\Big(\rho_\ell\sin\theta_\ell u_{0\ell}(t) + (\nu_\ell\sin\theta_\ell + \rho_\ell^{-1}\cos\theta_\ell)v_{0\ell}(t)\Big)\,. \end{aligned}$$

However, this is not always the case. For instance, if we obtain y_ℓ from $y_{0\ell}$ by the rotation appearing in the decomposition (2.27),

$$y_\ell = u_\ell + iv_\ell = \cos\theta_\ell u_{0\ell} - \sin\theta_\ell v_{0\ell} + i(\sin\theta_\ell u_{0\ell} + \cos\theta_\ell v_{0\ell}) = e^{i\theta_\ell}y_{0\ell}\,,$$

the set $(\varphi_\ell = y_\ell Y_{\ell 0})_{\ell\in\mathbb{N}_0}$ defines a complex structure J through $J\varphi_\ell := i\varphi_\ell$ and $J\bar{\varphi}_\ell := -i\bar{\varphi}_\ell$. Now, it is straightforward to see that $J\varphi_\ell = i\varphi_\ell \Leftrightarrow Je^{i\theta_\ell}\varphi_{0\ell} = ie^{i\theta_\ell}\varphi_{0\ell}$, and $\mathbb{C}$-linearity implies $J\varphi_{0\ell} = i\varphi_{0\ell}$, i.e., $J = J_0$. Therefore, two different choices of the form $(\rho_\ell, \nu_\ell, \theta_\ell)$ and $(\rho_\ell, \nu_\ell, \tilde{\theta}_\ell)$, with $\theta_\ell \neq \tilde{\theta}_\ell$, give rise to the same complex structure. Then, in the following we will omit the angular part of $(\rho_\ell, \nu_\ell, \theta_\ell)$ by choosing $\theta_\ell = 0$ in (2.27). The complex structures defined trough (ρ_ℓ, ν_ℓ) and, hence, the corresponding Lagrangian subspaces $\mathcal{P}$, will generally yield irreducible *unitarily nonequivalent* Fock representations. This a well known property of any QFT in a generic curved spacetime, and can be considered as a serious drawback to the formulation of the theory. Obviously, this is not the case for a system of finite number of degrees of freedom, where the Stone-von Neumann's theorem can be applied [4]: For any Lagrangian subspace

$\mathcal{P}$ one obtains a quantum theory unitarily equivalent to the standard tensor product construction. Also, for the case of a massless scalar field evolving in a fixed *stationary* spacetime, there exists a preferred choice of Lagrangian subspace by virtue of the time translation symmetry [2]. In our case, in absence of this symmetry (or any extra constraint obtained after deparameterization, that would generate residual symmetries useful to select a preferred representation of the canonical commutation relations, as in the 3-torus case), no natural, preferred election of $\mathcal{P}$ is available. In other words, due to the time-dependence of the Hamiltonian, the solutions of $\mathcal{S}$ do not oscillate harmonically and, thus, it is not possible to uniquely define subspaces of positive and negative frequency solutions.

$SO(3)$-invariant complex structures

Our purpose now is to characterize those complex structures on the real solution space $\mathcal{S}^{KG}$ of the field equation $\mathring{g}^{ab}\mathring{\nabla}_a\mathring{\nabla}_b\varphi = 0$, invariant under the symmetries of $\mathbb{S}^2$ –the spatial manifold in our $(1+2)$-dimensional description– *without imposing* the symmetry condition $\mathcal{L}_\sigma\varphi = 0$. As we will show, once this is done it is straightforward to restrict them to the solution space $\mathcal{S}$. In particular, we will prove that all complex structures $J_\mathcal{P}$ as defined in previous sections are $SO(3)$-invariant; similarly, any $SO(3)$-invariant complex structure has an associated Lagrangian subspace $\mathcal{P}$ characterized by definite pairs (ρ_ℓ, ν_ℓ). With this aim in mind, let us consider the complexified solution space $\mathcal{S}^{KG}_\mathbb{C} = \mathcal{P}^{KG}_0 \oplus \bar{\mathcal{P}}^{KG}_0$ where

$$\begin{aligned}\mathcal{P}^{KG}_1 &:= \mathcal{P}^{KG}_0 = \mathrm{Span}\{y_{0\ell}Y_{\ell m}\,|\,\ell\in\mathbb{N}_0,\, m\in\{-\ell,\ldots,\ell\}\}\,,\\ \mathcal{P}^{KG}_2 &:= \bar{\mathcal{P}}^{KG}_0 = \mathrm{Span}\{\bar{y}_{0\ell}Y_{\ell m}\,|\,\ell\in\mathbb{N}_0,\, m\in\{-\ell,\ldots,\ell\}\}\,.\end{aligned}$$

Here, $Y_{\ell m}$ are the usual spherical harmonics on $\mathbb{S}^2$. There are two antilinear maps connecting the spaces $\mathcal{P}^{KG}_1$ and $\mathcal{P}^{KG}_2$ that we denote (in a slight notational abuse) with the same symbol $^- : \mathcal{P}^{KG}_1 \to \mathcal{P}^{KG}_2 : \psi_1 \mapsto \bar{\psi}_1$ and $^- : \mathcal{P}_2 \to \mathcal{P}^{KG}_1 : \psi_2 \mapsto \bar{\psi}_2$. Each one of these maps is the inverse of the other and their composition is the identity for every element of $\mathcal{P}^{KG}_1$ or $\mathcal{P}^{KG}_2$ (i.e., $\bar{\bar{\psi}} = \psi$). With their help, we can write the conjugation $^- : \mathcal{S}_\mathbb{C} \to \mathcal{S}_\mathbb{C}$ according to

$$\Psi = \begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix} \mapsto \bar{\Psi} := \begin{bmatrix}\bar{\psi}_2\\ \bar{\psi}_1\end{bmatrix},$$

with $\psi_1 \in \mathcal{P}^{KG}_1$ and $\psi_2 \in \mathcal{P}^{KG}_2$. The elements in the original *real* solution space $\mathcal{S}^{KG}$ can be easily characterized by using the previous conjugation as those of the form

$$\Phi = \begin{bmatrix}\varphi\\ \bar{\varphi}\end{bmatrix}$$

or, alternatively, as the real linear subspace of $\mathcal{S}^{KG}_\mathbb{C}$ given by $\mathcal{S}^{KG} = \{\Phi \in \mathcal{S}^{KG}_\mathbb{C}\,|\,\Phi = \bar{\Phi}\}$. The elements $\varphi_a \in \mathcal{P}^{KG}_a$, $a = 1, 2$, are complex functions $\varphi_a(t, s)$ defined on $(0, \pi) \times \mathbb{S}^2$.

There is a natural representation D_a of $SO(3)$ in $\mathcal{P}_a^{KG}$ defined by $(D_a(g)\varphi)(t,s) = \varphi(t, g^{-1}\cdot s)$, where $g^{-1}\cdot s$ denotes the action of the rotation $g^{-1} \in SO(3)$ on the point $s \in \mathbb{S}^2$. Then, the natural representation of $SO(3)$ in $\mathcal{S}_{\mathbb{C}}^{KG} = \mathcal{P}_1^{KG} \oplus \mathcal{P}_2^{KG}$ can be written in matrix form as

$$D(g) = \begin{bmatrix} D_1(g) & 0 \\ 0 & D_2(g) \end{bmatrix}, \quad g \in SO(3)\,,$$

in terms of the representations $(D_a, \mathcal{P}_a^{KG})$. Consider now a $\mathbb{C}$-linear map $J : \mathcal{S}_{\mathbb{C}}^{KG} \to \mathcal{S}_{\mathbb{C}}^{KG}$, in matrix notation

$$J = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix},$$

where the maps $J_{ab} : \mathcal{P}_b^{KG} \to \mathcal{P}_a^{KG}$ are $\mathbb{C}$-linear for $a, b \in \{1, 2\}$. The invariance of J under the action of the $SO(3)$ group implies

$$D(g)J = JD(g) \Leftrightarrow \begin{bmatrix} J_{11}D_1(g) & J_{12}D_2(g) \\ J_{21}D_1(g) & J_{22}D_2(g) \end{bmatrix} = \begin{bmatrix} D_1(g)J_{11} & D_1(g)J_{12} \\ D_2(g)J_{21} & D_2(g)J_{22} \end{bmatrix}, \ \forall\, g \in SO(3)\,.$$

We require that the restriction of J to $\mathcal{S}^{KG}$ is $\mathbb{R}$-linear, i.e., $J\Phi = \overline{J\Phi}$ for every $\Phi \in \mathcal{S}^{KG}$, which implies $J_{11}\varphi = \overline{J_{22}\bar{\varphi}}$ and $J_{21}\varphi = \overline{J_{12}\bar{\varphi}}$, this is,

$$J_{22} = \bar{J}_{11}\,, \quad J_{12} = \bar{J}_{21}\,, \tag{2.28}$$

where we have used the notation $\bar{A}\varphi := \overline{A\bar{\varphi}}$ to denote the $\mathbb{C}$-linear map $\bar{A} : P_b^{KG} \to P_a^{KG}$ $(a \neq b)$ obtained from the $\mathbb{C}$-linear map $A : P_a^{KG} \to P_b^{KG}$. Finally, we impose that J be a complex structure, $J^2 = -\mathrm{Id}_{\mathcal{S}_{\mathbb{C}}}$. This requires

$$J_{11}^2 + \bar{J}_{21}J_{21} = -\mathrm{Id}_1\,, \quad J_{21}J_{11} + \bar{J}_{11}J_{21} = 0\,. \tag{2.29}$$

It is convenient now to expand the vector spaces $\mathcal{P}_a^{KG}$ as

$$\mathcal{P}_a^{KG} = \bigoplus_{\ell=0}^{\infty} \mathcal{P}_a^{\ell}\,, \quad a = 1, 2\,,$$

with

$$\begin{aligned} \mathcal{P}_1^{\ell} &:= \mathrm{Span}\{y_{0\ell}\} \otimes \mathrm{Span}\{Y_{\ell m} \,|\, m \in \{-\ell, \dots, \ell\}\}\,, \\ \mathcal{P}_2^{\ell} &:= \mathrm{Span}\{\bar{y}_{0\ell}\} \otimes \mathrm{Span}\{Y_{\ell m} \,|\, m \in \{-\ell, \dots, \ell\}\}\,. \end{aligned}$$

This is useful because the operators $D_a(g)$ can be written as $D_a = \bigoplus_{\ell=0}^{\infty} D_a^{\ell}$, where each pair $(\mathcal{P}_a^{\ell}, D_a^{\ell})$ is an irreducible representation. Denoting as Π_a^{ℓ} the projectors on the linear spaces $\mathcal{P}_a^{\ell}$, we define

$$J_{ab}^{\ell_1\ell_2} := \Pi_a^{\ell_1} J_{ab} \Pi_b^{\ell_2} : \mathcal{P}_b^{\ell_2} \to \mathcal{P}_a^{\ell_1}\,.$$

In order to proceed with the characterization of the complex structures, we establish the following lemma.

Lemma 2.2.1 (Schur). *Let $D_1(g)$ and $D_2(g)$ be two finite dimensional, irreducible representations of the group G in the complex finite-dimensional linear spaces V_1 and V_2. Let us suppose that a linear operator $L : V_1 \to V_2$* commutes *with these representations, i.e., $D_2(g)L = LD_1(g)$, $\forall\, g \in G$. Then, either L is zero or it is invertible. In the latter case, both representations are equivalent and L is uniquely determined modulo a multiplicative constant.*

This lemma directly implies that $J^{\ell_1\ell_2}_{ab} = 0$, whenever $\ell_1 \neq \ell_2$, and $J^{\ell\ell}_{aa} = \jmath^{\ell}_{aa} I^{\ell}_{aa}$, where $\jmath^{\ell}_{aa} \in \mathbb{C}$ and I^{ℓ}_{aa} denotes the identity on $\mathcal{P}^{\ell}_{a}$, with $\jmath^{\ell}_{22} = \bar{\jmath}^{\ell}_{11}$ as a consequence of (2.28). Also,

$$J^{\ell\ell}_{12}(\bar{y}_{0\ell} \otimes v) = \jmath^{\ell}_{12} y_{0\ell} \otimes v, \quad J^{\ell\ell}_{21}(y_{0\ell} \otimes v) = \jmath^{\ell}_{21} \bar{y}_{0\ell} \otimes v, \quad \jmath^{\ell}_{12}, \jmath^{\ell}_{21} \in \mathbb{C}\,,$$

with $\jmath^{\ell}_{12} = \bar{\jmath}^{\ell}_{21}$ again as a consequence of (2.28). In conclusion, the general form of the mapping J is given by

$$J = \bigoplus_{\ell=0}^{\infty} \left[\begin{array}{cc} \jmath^{\ell}_{11} I^{\ell}_{11} & \jmath^{\ell}_{12} I^{\ell}_{12} \\ \bar{\jmath}^{\ell}_{12} I^{\ell}_{21} & \bar{\jmath}^{\ell}_{11} I^{\ell}_{22} \end{array} \right],$$

where I^{ℓ}_{aa} denotes the identity operator in $\mathcal{P}^{\ell}_{a}$ and the linear operators $I^{\ell}_{ab} : \mathcal{P}^{\ell}_{b} \to \mathcal{P}^{\ell}_{a}$ act according to $I^{\ell}_{12}(\bar{y}_{0\ell} \otimes v) = y_{0\ell} \otimes v$ and $I^{\ell}_{21}(y_{0\ell} \otimes v) = \bar{y}_{0\ell} \otimes v$. Conditions (2.29) defining J as a complex structure finally yield the following restrictions on $\jmath^{\ell}_{11}$ and $\jmath^{\ell}_{12}$,

$$|\jmath^{\ell}_{11}|^{\,2} - |\jmath^{\ell}_{12}|^{\,2} = 1, \quad \jmath^{\ell}_{11} \in i\mathbb{R} \setminus \{0\}\,, \quad \jmath^{\ell}_{12} \in \mathbb{C}\,. \tag{2.30}$$

The previous considerations apply to solutions of the Klein-Gordon equation without imposing the additional axial symmetry. This can be trivially taken into account at this point by realizing that it suffices to restrict ourselves to the one-dimensional subspaces (for each value of ℓ) spanned by the spherical harmonics $Y_{\ell 0}$. Note that on each subspace $\mathcal{P}^{\ell}_{1} \oplus \mathcal{P}^{\ell}_{2}$ the complex structure is completely fixed by a pair of complex parameters $(\jmath^{\ell}_{11}, \jmath^{\ell}_{12})$ subject to the conditions (2.30); the remaining freedom is then parameterized by two real numbers. This is what we found before by explicitly considering the solution space and the choice of the families of functions u_ℓ and v_ℓ.[5] According to (2.30), it suffices to take $\jmath^{\ell}_{11} = i$ and $\jmath^{\ell}_{12} = 0$, $\forall\, \ell \in \mathbb{N}_0$, to conclude that all complex structures $J_{\mathcal{P}}$ naturally defined by these families of functions are, in fact, $SO(3)$ invariant. Similarly, in accordance with the previous arguments it is also clear that any $SO(3)$-invariant complex structure, characterized by pairs $(\jmath^{\ell}_{11}, \jmath^{\ell}_{12})$ verifying (2.30), has an associated Lagrangian subspace $\mathcal{P}$ defined by a set $(y_\ell = \rho_\ell u_{0\ell} + (\nu_\ell + i\rho_\ell^{-1}) v_{0\ell})_{\ell\in\mathbb{N}_0}$. The formulas that relate the parameters ρ_ℓ and ν_ℓ to the definition of the invariant complex structure discussed in this section are calculated as follows. Once a fiducial basis $\varphi_{0\ell} = y_{0\ell} Y_{\ell 0}$ is chosen (2.12), any other complex structure defined by a different basis –satisfying

[5] Here, the choice $\jmath^{\ell}_{11} \in i\mathbb{R}_+$ is equivalent to the normalization for the Wronskian of u_ℓ and v_ℓ introduced in equation (2.11) and guarantees that the sesquilinear form (2.18) restricted to the subspace corresponding to the i eigenvalue of J (that we have denotes as $\mathcal{P}$ in previous sections) defines an inner product. Changing the sign in the Wronskian corresponds to taking $\jmath^{\ell}_{11} \in i\mathbb{R}_-$.

the normalization condition (2.11)– can be written in terms of $\varphi_{0\ell}$, by using (2.25) and (2.27), as

$$J\begin{bmatrix}\varphi_{0\ell}\\ \bar{\varphi}_{0\ell}\end{bmatrix}=\begin{bmatrix}\jmath^{\ell}_{11}I^{\ell}_{11} & \jmath^{\ell}_{12}I^{\ell}_{12}\\ \bar{\jmath}^{\ell}_{12}I^{\ell}_{21} & \bar{\jmath}^{\ell}_{11}I^{\ell}_{22}\end{bmatrix}\cdot\begin{bmatrix}\varphi_{0\ell}\\ \bar{\varphi}_{0\ell}\end{bmatrix},\tag{2.31}$$

where

$$\jmath^{\ell}_{11} = \frac{i}{2}(\alpha_\ell^2+\beta_\ell^2+\gamma_\ell^2+\delta_\ell^2)=\frac{i}{2}(\nu_\ell^2+\rho_\ell^{-2}+\rho_\ell^2)\,,\tag{2.32}$$

$$\jmath^{\ell}_{12} = -(\alpha_\ell\beta_\ell+\gamma_\ell\delta_\ell)+\frac{i}{2}(\beta_\ell^2+\delta_\ell^2-\alpha_\ell^2-\gamma_\ell^2)=-\rho_\ell\nu_\ell+\frac{i}{2}(\nu_\ell^2+\rho_\ell^{-2}-\rho_\ell^2)\,.\tag{2.33}$$

Note that, as expected, the complex structures defined by (2.32) and (2.33) do not depend on the parameters $\theta_\ell\in[0,2\pi)$ appearing in (2.27) but only on the pairs $(\rho_\ell,\nu_\ell)\in(0,+\infty)\times\mathbb{R}$.

2.2.2 Canonical commutation relations

The canonical field operators associated with a given time $t\in(0,\pi)$ are defined as operator-valued distributions on $\mathbb{S}^2$,

$$\hat{Q}(t,s) = \sum_{\ell=0}^{\infty}\left(y_\ell(t)\hat{a}_\ell+\bar{y}_\ell(t)\hat{a}_\ell^\dagger\right)Y_{\ell 0}(s)\,,\tag{2.34}$$

$$\hat{P}(t,s) = \sin t\sum_{\ell=0}^{\infty}\left(\dot{y}_\ell(t)\hat{a}_\ell+\dot{\bar{y}}_\ell(t)\hat{a}_\ell^\dagger\right)Y_{\ell 0}(s)\,.\tag{2.35}$$

In practice, these expressions can be obtained by formally promoting the Fourier coefficients in (2.8) to the creation and annihilation operators –$\hat{a}_\ell^\dagger$ and $\hat{a}_\ell$, respectively– associated with the basic vectors $\varphi_\ell\in\mathscr{H}_{\mathcal{P}}$. The infinite sums appearing in (2.34) and (2.35) do not converge, and the theory actually does not admit observables corresponding to the values of the field and its momentum at a given spacetime point (t,s). Rather, they must be interpreted in a distributional sense. Only the spacetime average of these expressions weighted by smooth functions on the 2-sphere are mathematically well-defined. Nevertheless, the above expressions can be used to perform formal calculations provided that only linear operations of them be involved. Given any pair of smooth axially-symmetric real-valued functions on the 2-sphere, $g_1,g_2\in C^\infty(\mathbb{S}^2;\mathbb{R})$ with $\mathcal{L}_\sigma g_k=0$, $k=1,2$, the above distributions define canonical field operators $(\hat{Q}_t[g_1],\hat{P}_t[g_2])$ just by multiplying the formal expressions (2.34) and (2.35) by g_1 and g_2, respectively, and integrating then over the round 2-sphere $\mathbb{S}^2$. In this way, we obtain

$$\hat{Q}_t[g_1]=\sum_{\ell=0}^{\infty}g_\ell^{(1)}\left(y_\ell(t)\hat{a}_\ell+\bar{y}_\ell(t)\hat{a}_\ell^\dagger\right)\,,\quad \hat{P}_t[g_2]=\sin t\sum_{\ell=0}^{\infty}g_\ell^{(2)}\left(\dot{y}_\ell(t)\hat{a}_\ell+\dot{\bar{y}}_\ell(t)\hat{a}_\ell^\dagger\right)\,,\tag{2.36}$$

where $g_k = \sum_{\ell=0}^{\infty} g_\ell^{(k)} Y_{\ell 0}$, $g_\ell^{(k)} \in \mathbb{R}$, $k = 1, 2$. It is straightforward to check that, by construction, the states with a finite number of particles define a common, invariant, dense domain of analytic vectors for these configuration and momentum operators, so that their essential self-adjointness is guaranteed and, hence, the existence of unique self-adjoint extensions for these operators (see Nelson's analytic vector theorem in [5]). Consider first the $\hat{Q}_t[g_1]$ operator. If $\psi^{(n)} \in \mathscr{P}_+^{(n)}(\mathscr{H}_{\mathcal{P}}^{\otimes n})$, then $\psi^{(n)} \in \mathscr{D}_{\hat{Q}_t[g_1]^m}$, for all m, and $\hat{Q}_t[g_1]\psi^{(n)} \in \mathscr{P}_+^{(n-1)}(\mathscr{H}_{\mathcal{P}}^{\otimes(n-1)}) \oplus \mathscr{P}_+^{(n+1)}(\mathscr{H}_{\mathcal{P}}^{\otimes(n+1)})$. Denote $\hat{a}_t(g_1) := \sqrt{2}\sum_{\ell=0}^{\infty} g_\ell^{(1)} y_\ell(t) \hat{a}_\ell$, so that $\hat{Q}_t[g_1] = \big(\hat{a}_t(g_1) + \hat{a}_t^\dagger(g_1)\big)/\sqrt{2}$. Relations (E.1) of *appendix E* imply $\|\hat{Q}_t[g_1]^m \psi^{(n)}\| \leq 2^{m/2}(n+m)^{1/2}(n+m-1)^{1/2} \cdots (n+1)^{1/2} \|g_1\|^m \|\psi^{(n)}\|$, where we have denoted $\|g_1\|^2 := \sum_{\ell=0}^{\infty} |g_\ell^{(1)} y_\ell(t)|^2$ which converges given the square-summability of $(g_\ell^{(1)})_{\ell \in \mathbb{N}_0}$ (recall that g is smooth) and the asymptotic behavior of $y_\ell(t) = O(\ell^{-1/2})$ (see next section). Therefore,

$$\sum_{m=0}^{\infty} \frac{|z|^m}{m!} \|\hat{Q}_t[g_1]^m \psi^{(n)}\| \leq \sum_{m=0}^{\infty} \frac{(\sqrt{2}|z|)^m}{m!} \left(\frac{(n+m)!}{n!}\right)^{1/2} \|g_1\|^m \|\psi^{(n)}\| < +\infty \,,$$

for all $z \in \mathbb{C}$. It directly follows that each vector $\psi = (\psi^{(n)})_{n \geq 0}$ in the dense domain of finite number of particles is analytic for $\hat{Q}_t[g_1]$. We can proceed in the same way to prove a similar result for the momentum operator $\hat{P}_t[g_2]$. In the next section, we will elucidate if the functional dependence in t of $\hat{Q}(t,s)$ and $\hat{P}(t,s)$ can be obtained by the action of a unitary operator in the Fock space $\mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$.

2.3 Unitarity of the quantum time evolution

We discuss in this section the unitarity of the quantum evolution for the models under consideration. A particularly convenient approach to this issue is given by the algebraic formulation of QFT, since the notion of unitary implementability of linear symplectic transformations on Hilbert spaces can be analyzed in a natural way within this framework. As explained in *appendix C*, the basic ingredients in the algebraic approach are (i) a unital C^*-algebra $\mathfrak{A}$, with observables[6] defining the subset of $*$-invariant elements, and (ii) positive normalized linear functionals (states) $\varpi : \mathfrak{A} \to \mathbb{C}$ with $\varpi(\mathbf{1}) = 1$ and $\varpi(A^*A) \geq 0$ for all $A \in \mathfrak{A}$. The value of a state ϖ on an observable $A \in \mathfrak{A}$, $A = A^*$, is interpreted as the expectation value of that observable in the physical state of the system represented by ϖ, $\langle A \rangle_\varpi = \varpi(A)$.

The construction of the appropriate C^*-algebra for free (linear) fields is straightforward. Consider the covariant phase space $\Gamma = (\mathcal{S}, \Omega)$ of smooth real classical solutions

[6]Some relevant physical observables, such as the stress-energy tensor of the quantum field, will not be represented as elements of $\mathfrak{A}$. In this sense, the $\mathfrak{A}$ algebra will encompass a *minimal* collection of physical observables sufficiently large to enable the theory to be formulated.

to the equation of motion given by (2.3) and (2.4); Γ has the structure of an infinite-dimensional symplectic vector space. As a consequence of the linearity of $\mathcal{S}$, the set of elementary classical observables $\mathcal{O}_c$ can be identified with the $\mathbb{R}$-vector space generated by linear functionals on Γ. Every vector $\varphi \in \Gamma$ has an associated functional $F_\varphi : \Gamma \to \mathbb{R}$ such that, for all $\psi \in \Gamma$,

$$F_\varphi(\psi) := \Omega(\varphi, \psi) = \sin t \int_{\mathbb{S}^2} |\gamma|^{1/2} \iota_t^* \Big(\psi \dot{\varphi} - \varphi \dot{\psi} \Big) .$$

Therefore, $\mathcal{O}_c = \mathrm{Span}\big\{\mathbb{I}, F_\varphi\big\}_{\varphi\in\Gamma}$. As expected [6], this set satisfies the condition that any regular function on Γ can be obtained as a (suitable limit of) sum of products of elements in $\mathcal{O}_c$, and also that it is closed under Poisson brackets, $\{F_\varphi(\cdot), F_\psi(\cdot)\} = F_\varphi(\psi)\mathbb{I}$. The abstract quantum algebra of observables is then given by the usual Weyl C^*-algebra $\mathscr{W}(\Gamma)$ on Γ generated by the elements $W(\varphi) = \exp(iF_\varphi(\cdot))$, $\varphi \in \Gamma$, satisfying for all $\varphi_1, \varphi_2 \in \Gamma$ the following relations

$$W(\varphi_1)^* = W(-\varphi_1) , \quad W(\varphi_1)W(\varphi_2) = \exp\left(-\frac{i}{2}\Omega(\varphi_1, \varphi_2)\right) W(\varphi_1 + \varphi_2) ,$$

which contain the information about the canonical commutation relations. The GNS construction (see *Theorem C.2.1* in *appendix C*) establishes that, given any state ϖ_0 on the algebra $\mathscr{W}(\Gamma)$, there exist a Hilbert space $\mathfrak{H}_{\varpi_0}$, a representation $\pi_{\varpi_0} : \mathscr{W}(\Gamma) \to \mathscr{B}(\mathfrak{H}_{\varpi_0})$ from the Weyl algebra to the collection of bounded linear operators on $\mathfrak{H}_{\varpi_0}$, and a cyclic vector $\Psi_{\varpi_0} \in \mathfrak{H}_{\varpi_0}$ such that $\varpi_0(A) = \langle \Psi_{\varpi_0} \,|\, \pi_{\varpi_0}(A)\Psi_{\varpi_0}\rangle_{\mathfrak{H}_{\varpi_0}}$, $\forall\, A \in \mathscr{W}(\Gamma)$. Moreover, the triplet $(\mathfrak{H}_{\varpi_0}, \pi_{\varpi_0}, \Psi_{\varpi_0})$ with these properties is unique up to unitary equivalence. The construction of the Fock spaces $\mathscr{F}_+(\mathscr{H}_\mathcal{P})$ depending on the Lagrangian subspaces $\mathcal{P}$ discussed in previous sections proves equivalent to the GNS construction for the (faithful) state $\varpi_0 : \mathscr{W}(\Gamma) \to \mathbb{C}$ defined as

$$\varpi_0(W(\varphi)) := \exp\left(-\frac{1}{2}\mu_{J_\mathcal{P}}(\varphi, \varphi)\right) , \tag{2.37}$$

with $\mu_{J_\mathcal{P}}$ given by equation (2.21) and the vacuum $\Psi_{\varpi_0} = |0\rangle_\mathcal{P}$ serving as the cyclic vector. Indeed, the value of the state ϖ_0 acting on the Weyl generators $W(\varphi)$ is interpreted as the expectation value of the associated operator $\pi_{\varpi_0}(W(\varphi))$ on the vacuum state $|0\rangle_\mathcal{P}$, i.e., $\varpi_0(W(\varphi)) = \langle \Psi_{\varpi_0} \,|\, \pi_{\varpi_0}(W(\varphi))\Psi_{\varpi_0}\rangle$. We have $\pi_{\varpi_0}(W(\varphi)) = \exp(i\hat{\Omega}(\varphi, \cdot))$, where the fundamental observables are defined as $\hat{\Omega}(\varphi, \cdot) = i\big(A(\kappa(\varphi)) - C(\kappa(\varphi))\big)$. Here, C and A are the creation and annihilation operators associated with $\kappa(\varphi)$, with $\kappa : \mathcal{S}_\mathbb{C} \to \mathcal{P}$ being the $\mathbb{C}$-linear projector defined by the splitting $\mathcal{S}_\mathbb{C} = \mathcal{P} \oplus \bar{\mathcal{P}}$. By using the Baker-Campbell-Hausdorff (BCH) relation, and taking into account that $[A(\kappa(\varphi)), C(\kappa(\varphi))] = \langle \varphi|\varphi\rangle_{J_\mathcal{P}} = \mu_{J_\mathcal{P}}(\varphi, \varphi)$, we finally get

$$\begin{aligned} \langle \Psi_{\varpi_0} \,|\, \pi_{\varpi_0}(W(\varphi))\Psi_{\varpi_0}\rangle &= \langle \Psi_{\varpi_0} \,|\, \exp(C(\kappa(\varphi))) \exp(-A(\kappa(\varphi)))\Psi_{\varpi_0}\rangle \exp\Big(-\frac{1}{2}\mu_{J_\mathcal{P}}(\varphi, \varphi)\Big) \\ &= \langle \Psi_{\varpi_0} \,|\, \Psi_{\varpi_0}\rangle \exp\Big(-\frac{1}{2}\mu_{J_\mathcal{P}}(\varphi, \varphi)\Big) . \end{aligned}$$

Since the vacuum state is normalized, we have $\langle \Psi_{\varpi_0} | \Psi_{\varpi_0} \rangle = 1$ and recover the expression (2.37). The state ϖ_0 is uniquely extended to $\mathscr{W}(\Gamma)$ by linearity and continuity. It clearly satisfies the positivity condition $\varpi_0(A^*A) \geq 0$, $A \in \mathscr{W}(\Gamma)$, for the basic elements $W(\varphi)$, although it does not automatically verify this condition for arbitrary complex linear combinations of these elements. A necessary and sufficient condition for positivity is in fact given by relation (2.23).

Every linear symplectic transformation $\mathcal{T} \in \mathrm{SP}(\Gamma)$, $\mathcal{T}^*\Omega(\varphi_1, \varphi_2) = \Omega(\mathcal{T}\varphi_1, \mathcal{T}\varphi_2) = \Omega(\varphi_1, \varphi_2)$, defines a (unique) $*$-automorphism $\alpha_{\mathcal{T}} \in \mathrm{Aut}(\mathscr{W}(\Gamma))$ such that $\alpha_{\mathcal{T}} \cdot W(\varphi) := W(\mathcal{T}\varphi)$. Given any point $\varphi = \sum_{\ell=0}^{\infty} (a_\ell y_\ell + \overline{a_\ell y_\ell}) Y_{\ell 0} \in \Gamma$, the action of $\mathcal{T}$ can be written in the form

$$\mathcal{T}\varphi = \sum_{\ell=0}^{\infty} \Big(\mathfrak{a}_\ell(a, \bar{a}) y_\ell + \overline{\mathfrak{a}_\ell(a, \bar{a}) y_\ell} \Big) Y_{\ell_1 0} \,,$$

with the complex coefficients

$$\mathfrak{a}_\ell(a, \bar{a}) = \sum_{\ell'=0}^{\infty} \Big(\alpha(\ell, \ell') a_{\ell'} + \beta(\ell, \ell') \bar{a}_{\ell'} \Big) \,, \quad \ell \in \mathbb{N}_0 \,.$$

Given a concrete Hilbert space representation $(\mathfrak{H}, \pi, \Psi)$ of the Weyl algebra $\mathscr{W}(\Gamma)$, for instance the Fock-like one, a (continuous) linear symplectic transformation $\mathcal{T} \in \mathrm{SP}(\Gamma)$ is said to be *unitarily implementable* on the Hilbert space $\mathfrak{H}$ if π and $\pi \circ \alpha_{\mathcal{T}}$ (or, equivalently, $\pi \circ \alpha_{\mathcal{T}}^{-1}$) are unitarily equivalent representations, i.e., there exists a unitary operator $\hat{U}_{\mathcal{T}} : \mathfrak{H} \to \mathfrak{H}$ such that $\hat{U}_{\mathcal{T}}^{-1}\, \pi(W(\varphi))\, \hat{U}_{\mathcal{T}} = \pi(\alpha_{\mathcal{T}} \cdot W(\varphi)) = \pi(W(\mathcal{T}\varphi))$, for all $W(\varphi) \in \mathscr{W}(\Gamma)$. Concretely, for the Fock representation space $\mathfrak{H} = \mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$, one has

$$\hat{U}_{\mathcal{T}}^{-1}\, \hat{a}_\ell\, \hat{U}_{\mathcal{T}} = \sum_{\ell'=0}^{\infty} \Big(\alpha(\ell, \ell') \hat{a}_{\ell'} + \beta(\ell, \ell') \hat{a}_{\ell'}^{\dagger} \Big) \,, \quad \ell \in \mathbb{N}_0 \,. \tag{2.38}$$

It is well known [7] that not every linear symplectic transformation $\mathcal{T}$ defined on the infinite dimensional symplectic linear space Γ can be unitarily implemented in the Fock space $\mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$. This is so because π_{ϖ_0} and its transform $\pi_{\varpi_0} \circ \alpha_{\mathcal{T}}$, whose action on basic observables is given by

$$\langle \Psi_{\varpi_0} \,|\, \pi_{\varpi_0} \circ \alpha_{\mathcal{T}}(W(\varphi)) \Psi_{\varpi_0} \rangle = \exp\left(-\frac{1}{4} \Omega\big((\mathcal{T}^{-1} \circ J_{\mathcal{P}} \circ \mathcal{T}) \varphi, \varphi \big) \right),$$

do not necessarily yield unitarily equivalent Fock space representations. This will be the case if and only if $J_{\mathcal{P}} - \mathcal{T}^{-1} \circ J_{\mathcal{P}} \circ \mathcal{T}$ is a Hilbert-Schmidt operator on the one-particle Hilbert space $\mathscr{H}_{\mathcal{P}}$ [2, 7]. This immediately translates into the condition

$$\sum_{\ell=0}^{\infty} \sum_{\ell'=0}^{\infty} |\beta(\ell, \ell')|^2 < +\infty \,.$$

In particular, we will focus on the symplectic transformations $\mathcal{T}_{(t_1,t_0)}$ defined in (2.16) representing the time evolution from $\iota_{t_0}(\mathbb{S}^2)$ to $\iota_{t_1}(\mathbb{S}^2)$. The corresponding condition for the unitary implementability of this transformation can be written from (2.16) and (2.17) as

$$\sum_{\ell=0}^{\infty} |\beta_\ell(t_1,t_0\,|\,y_\ell)|^2 < +\infty\,, \tag{2.39}$$

for all $t_0, t_1 \in (0,\pi)$, where

$$\beta_\ell(t_1,t_0\,|\,y_\ell) := i\big(\sin t_1 \bar{y}_\ell(t_0)\dot{\bar{y}}_\ell(t_1) - \sin t_0 \bar{y}_\ell(t_1)\dot{\bar{y}}_\ell(t_0)\big)\,.$$

Equivalently, we have to check if

$$\sum_{\ell=0}^{\infty} \mathrm{Re}^2[\beta_\ell(t_1,t_0\,|\,y_\ell)] < +\infty \quad \text{and} \quad \sum_{\ell=0}^{\infty} \mathrm{Im}^2[\beta_\ell(t_1,t_0\,|\,y_\ell)] < +\infty\,.$$

If these conditions are indeed verified, there will exist a unitary operator $\hat{U}(t_1,t_0)$: $\mathscr{F}_+(\mathscr{H}_\mathcal{P}) \to \mathscr{F}_+(\mathscr{H}_\mathcal{P})$, the so-called *unitary evolution operator*, such that

$$\hat{U}^{-1}(t_1,t_0)\hat{Q}(t_0,s)\hat{U}(t_1,t_0) = \hat{Q}(t_1,s)\,,\ \ \hat{U}^{-1}(t_1,t_0)\hat{P}(t_0,s)\hat{U}(t_1,t_0) = \hat{P}(t_1,s)\,,$$

with the field and momentum operators defined as in equations (2.34) and (2.35). At this point, we have to study the convergence of the previous series. Note, in particular, that their square summability depends only on its ultraviolet behavior (the zero mode corresponding to $\ell = 0$ plays no role in this context). Let us consider the real part of the β_ℓ coefficients. By using the expression for y_ℓ in terms of the ρ_ℓ and ν_ℓ coefficients, $y_\ell = \rho_\ell u_{0\ell} + (\nu_\ell + i\rho_\ell^{-1})v_{0\ell}$, it is possible to identify the dependence of $\mathrm{Re}[\beta_\ell(t_1,t_0\,|\,y_\ell)]$ on the choice of complex structures. This is given by

$$\mathrm{Re}[\beta_\ell(t_1,t_0\,|\,y_\ell)] \;=\; A_\ell(t_1,t_0) + 2\rho_\ell^{-1}\nu_\ell B_\ell(t_1,t_0)\,, \tag{2.40}$$

where

$$\begin{aligned}
A_\ell(t_1,t_0) &:= \sin t_1\big(u_{0\ell}(t_0)\dot{v}_{0\ell}(t_1) + v_{0\ell}(t_0)\dot{u}_{0\ell}(t_1)\big) - \sin t_0\big(u_{0\ell}(t_1)\dot{v}_{0\ell}(t_0) + \dot{u}_{0\ell}(t_0)v_{0\ell}(t_1)\big)\,,\\
B_\ell(t_1,t_0) &:= \sin t_1 v_{0\ell}(t_0)\dot{v}_{0\ell}(t_1) - \sin t_0 v_{0\ell}(t_1)\dot{v}_{0\ell}(t_0)\,.
\end{aligned}$$

The explicit form of A_ℓ and B_ℓ, derived in a straightforward way from (2.12), is

$$\begin{aligned}
A_\ell(t_1,t_0) &= \frac{\ell+1}{2}\Big(\mathscr{P}_{\ell+1}(\cos t_1)\mathscr{Q}_\ell(\cos t_0) - \mathscr{P}_{\ell+1}(\cos t_0)\mathscr{Q}_\ell(\cos t_1)\\
&\qquad +\mathscr{P}_\ell(\cos t_1)\big(\cos t_0 - \cos t_1)\mathscr{Q}_\ell(\cos t_0) - \mathscr{Q}_{\ell+1}(\cos t_0)\big)\\
&\qquad +\mathscr{P}_\ell(\cos t_0)\big((\cos t_0 - \cos t_1)\mathscr{Q}_\ell(\cos t_1) - \mathscr{Q}_{\ell+1}(\cos t_1)\big)\Big)\,,\\
B_\ell(t_1,t_0) &= -\frac{\ell+1}{2}\Big(\mathscr{Q}_\ell(\cos t_1)\mathscr{Q}_{\ell+1}(\cos t_0)\\
&\qquad -\big((\cos t_0 - \cos t_1)\mathscr{Q}_\ell(\cos t_1) + \mathscr{Q}_{\ell+1}(\cos t_1)\big)\mathscr{Q}_\ell(\cos t_0)\Big)\,.
\end{aligned}$$

By using the following asymptotic expansions for the first and second class Legendre functions ($\varepsilon < t < \pi - \varepsilon$, $\varepsilon > 0$) [8]

$$\begin{aligned}
\mathscr{P}_\ell(\cos t) &= \sqrt{\frac{2}{\pi\ell\sin t}}\cos\big((\ell+1/2)t-\pi/4\big)-\sqrt{\frac{1}{8\pi\ell^3\sin t}}\Big(\cos\big((\ell+1/2)t-\pi/4\big)\\
&- \frac{1}{2}\cot t\sin\big((\ell+1/2)-\pi/4\big)\Big)+O\big(\ell^{-5/2}\big)\,,\\
\mathscr{Q}_\ell(\cos t) &= \sqrt{\frac{\pi}{2\ell\sin t}}\cos\big((\ell+1/2)t+\pi/4\big)-\sqrt{\frac{\pi}{32\,\ell^3\sin t}}\Big(\cos\big((\ell+1/2)t+\pi/4\big)\\
&- \frac{1}{2}\cot t\sin\big((\ell+1/2)+\pi/4\big)\Big)+O\big(\ell^{-5/2}\big)\,,
\end{aligned} \tag{2.41}$$

we find that

$$\begin{aligned}
\mathrm{Re}[\beta_\ell(t_1,t_0\,|\,y_\ell)] \sim\ & -\frac{1}{2}\frac{\sin t_1-\sin t_0}{\sqrt{\sin t_0\sin t_1}}\sin[(\ell+1/2)(t_0+t_1)]\\
& -\frac{\pi\nu_\ell\rho_\ell^{-1}}{2\sqrt{\sin t_0\sin t_1}}\Big(\sin t_1\cos[(\ell+1/2)t_0+\pi/4]\sin[(\ell+1/2)t_1+\pi/4]\\
& -\sin t_0\cos[(\ell+1/2)t_1+\pi/4]\sin[(\ell+1/2)t_0+\pi/4]\Big)\,,
\end{aligned}$$

as $\ell \to +\infty$. The asymptotic behavior of $\mathrm{Re}[\beta_\ell(t_1,t_0\,|\,y_\ell)]$ leads us to conclude that, irrespective of the choice of (ρ_ℓ,ν_ℓ), it is not square summable and, hence, the quantum time evolution cannot be unitarily implemented for any choice of $SO(3)$-invariant complex structure.

2.3.1 Conformal field redefinitions

The negative conclusion concerning the impossibility of unitarily implementing the time evolution can be overcome much in the same way as in the three-torus 3-torus case, i.e., by introducing a redefinition of the fields in terms of which the model is formulated [9]. In our approach, this redefinition is appropriately interpreted from a geometrical point of view, being suggested by the functional form of the conformal factor $\sin t$ which appears in the auxiliary metric $\mathring{g}_{ab}$ (2.1). In the following, we will reintroduce the index i that labels the gravitational scalar ($i = 0$) and the matter scalars ($i \neq 0$) and consider the new fields

$$\xi_i := \sqrt{\sin t}\varphi_i\,. \tag{2.42}$$

The equations of motion are now

$$-\ddot{\xi}_i+\Delta_{\mathbb{S}^2}\xi_i=\frac{1}{4}(1+\csc^2 t)\xi_i\,,\quad \mathcal{L}_\sigma\xi_i=0\,. \tag{2.43}$$

These can be interpreted as the equations for scalar, axially symmetric fields with time-dependent mass term $\frac{1}{4}(1+\csc^2 t)$, evolving in $(0,\pi)\times\mathbb{S}^2$ with the *regular* –i.e. extensible to $\mathbb{R}\times\mathbb{S}^2$– fixed *static* background metric

$$\mathring{\eta}_{ab} = -(\mathrm{d}t)_a(\mathrm{d}t)_b + \gamma_{ab}\,. \tag{2.44}$$

Note that the singular behavior introduced by the conformal factor $\sin t$ in (2.1) is translated, in terms of the redefined fields, into the behavior of the time-dependent potential term, which is singular at $t=0$ and $t=\pi$. In spite of being singular at these instants of time, we expect to attain unitary dynamics if this potential is well behaved enough. In particular, it has the *correct* positive sign for all $t\in(0,\pi)$. Otherwise, the modes would satisfy harmonic oscillator equations with a negative time dependent square frequency; this would introduce a non-oscillatory behavior of the modes that, at the end of the day, may become again responsible for the failure of the unitarity condition. The field redefinition (2.42) can be incorporated in the model at the Lagrangian level by substituting $\phi_i=\xi_i/\sqrt{\sin t}$ in the action (2.2) to get the corresponding variational problem in terms of the new fields

$$\begin{aligned} s(\xi_i) \;=\; -\frac{1}{2}\sum_i\int_{[t_0,t_1]\times\mathbb{S}^2} |\mathring{\eta}|^{1/2}\mathring{\eta}^{ab}\Big((\mathrm{d}\xi_i)_a(\mathrm{d}\xi_i)_b - (\mathrm{d}\log\sin t)_a(\mathrm{d}\xi_i)_b\xi_i \\ +\frac{1}{4}(\mathrm{d}\log\sin t)_a(\mathrm{d}\log\sin t)_b\xi_i^2\Big)\,. \end{aligned} \tag{2.45}$$

Next, we will follow the method used in the preceding sections for the original φ fields. Some details will be omitted owing to their similarity with the previous derivations. The canonical phase space for the ξ-field equations is given again by $\Upsilon=(\mathbf{P},\omega)$, with $\mathbf{P}:=\{(Q,P)\in C^\infty(\mathbb{S}^2;\mathbb{R})\times C^\infty(\mathbb{S}^2;\mathbb{R})\,|\,\mathcal{L}_\sigma Q=0=\mathcal{L}_\sigma P\}$ and ω given by (2.5). We define the space $\mathcal{S}_\xi$ of smooth and symmetric real solutions to the Klein-Gordon equation (2.43) and expand $\xi\in\mathcal{S}_\xi$ as

$$\xi(t,s)=\sum_{\ell=0}^{\infty}\Big(b_\ell z_\ell(t)+\overline{b_\ell z_\ell(t)}\Big)Y_{\ell 0}(s)\,, \tag{2.46}$$

where $z_\ell(t)$ are complex functions satisfying the differential equations

$$\ddot{z}_\ell+\left(\frac{1}{4}(1+\csc^2 t)+\ell(\ell+1)\right)z_\ell=0\,. \tag{2.47}$$

The functions z_ℓ can be easily written in terms the functions y_ℓ appearing in (2.9) and satisfying (2.11),

$$z_\ell(t)=\sqrt{\sin t}\,y_\ell(t)\,,$$

the Wronskian being now normalized as

$$z_\ell\dot{\bar{z}}_\ell-\bar{z}_\ell\dot{z}_\ell=i\,. \tag{2.48}$$

This allows us to write the symplectic structure in $\mathcal{S}_\xi$, naturally derived from the variational principle (2.45), as

$$\Omega_\xi(\xi_1,\xi_2) \;=\; \int_{\mathbb{S}^2}|\gamma|^{1/2}\imath_t^*\Big(\xi_2\dot{\xi}_1-\xi_1\dot{\xi}_2\Big)=i\sum_{\ell=0}^{\infty}(\bar{b}_\ell^{(1)}b_\ell^{(2)}-\bar{b}_\ell^{(2)}b_\ell^{(1)})\,,\quad \xi_1,\xi_2\in\mathcal{S}_\xi\,.$$

Classical evolution

We now consider the classical functional time evolution operator $\mathcal{T}_{(t_1,t_0)}:\Gamma_\xi\rightarrow\Gamma_\xi$ in the covariant phase space $\Gamma_\xi=(\mathcal{S}_\xi,\Omega_\xi)$. As before, we will write it in the form

$$(\mathcal{T}_{(t_1,t_0)}\xi)(t,s):=\sum_{\ell=0}^{\infty}\Big(\mathfrak{b}_\ell(t_1,t_0)z_\ell(t)+\overline{\mathfrak{b}_\ell(t_1,t_0)z_\ell(t)}\Big)Y_{\ell0}(s)\,. \tag{2.49}$$

In this case, the map $\mathcal{T}_{(t_1,t_0)}=\mathfrak{I}_{t_0}\circ\mathfrak{I}_{t_1}^{-1}$ is constructed from

$$\mathfrak{I}_{t_1}^{-1}:\Gamma_\xi\rightarrow\Upsilon\,,\quad \xi\mapsto(Q,P)=\mathfrak{I}_{t_1}^{-1}(\xi)\,, \tag{2.50}$$

defined by

$$Q(s) \;:=\; \xi(t_1,s)=\sum_{\ell=0}^{\infty}\Big(b_\ell z_\ell(t_1)+\overline{b_\ell z_\ell(t_1)}\Big)Y_{\ell0}(s)\,, \tag{2.51}$$

$$\begin{aligned}P(s) \;&:=\; \dot{\xi}(t_1,s)-\frac{1}{2}\cot t_1\xi(t_1,s) \qquad (2.52)\\ &=\; \sum_{\ell=0}^{\infty}\Big(b_\ell\Big(\dot{z}_\ell(t_1)-\frac{1}{2}\cot t_1 z_\ell(t_1)\Big)+\overline{b_\ell\Big(\dot{z}_\ell(t_1)-\frac{1}{2}\cot t_1 z_\ell(t_1)\Big)}\Big)Y_{\ell0}(s)\,,\end{aligned}$$

and from

$$\mathfrak{I}_{t_0}:\Upsilon\rightarrow\Gamma_\xi\,,\quad (Q,P)\mapsto\xi=\mathfrak{I}_{t_0}(Q,P)\,, \tag{2.53}$$

defined, in terms of the Fourier coefficients b_ℓ of ξ (2.46), by

$$b_\ell(t_0)=-i\Big(\dot{\bar{z}}_\ell(t_0)-\frac{1}{2}\cot t_0\bar{z}_\ell(t_0)\Big)\int_{\mathbb{S}^2}|\gamma|^{1/2}Y_{\ell0}Q+i\bar{z}_\ell(t_0)\int_{\mathbb{S}^2}|\gamma|^{1/2}Y_{\ell0}P\,.$$

From these expressions, we finally obtain

$$\begin{aligned}\mathfrak{b}_\ell(t_1,t_0) \;&=\; i\Big(\bar{z}_\ell(t_0)\Big(\dot{z}_\ell(t_1)-\frac{1}{2}\cot t_1 z_\ell(t_1)\Big)-z_\ell(t_1)\Big(\dot{\bar{z}}_\ell(t_0)-\frac{1}{2}\cot t_0\bar{z}_\ell(t_0)\Big)\Big)\,b_\ell \qquad (2.54)\\ &+\; i\Big(\bar{z}_\ell(t_0)\Big(\dot{\bar{z}}_\ell(t_1)-\frac{1}{2}\cot t_1\bar{z}_\ell(t_1)\Big)-\bar{z}_\ell(t_1)\Big(\dot{\bar{z}}_\ell(t_0)-\frac{1}{2}\cot t_0\bar{z}_\ell(t_0)\Big)\Big)\,\bar{b}_\ell\,.\end{aligned}$$

Quantum evolution

The unitarity condition for the quantum evolution in the corresponding Fock space quantization becomes

$$\sum_{\ell=0}^{\infty} |\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)|^2 = \sum_{\ell=0}^{\infty}\Big(\mathrm{Re}^2[\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)] + \mathrm{Im}^2[\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)]\Big) < +\infty\,, \tag{2.55}$$

for all t_0,$t_1 \in (0,\pi)$, where

$$\beta_\ell^\xi(t_1,t_0\,|\,z_\ell) := i\bar z_\ell(t_0)\Big(\dot{\bar z}_\ell(t_1) - \frac{1}{2}\cot t_1 \bar z_\ell(t_1)\Big) - i\bar z_\ell(t_1)\Big(\dot{\bar z}_\ell(t_0) - \frac{1}{2}\cot t_0 \bar z_\ell(t_0)\Big)\,. \tag{2.56}$$

The general solution to equation (2.47) under the normalization condition (2.48) can be written again in terms of associated Legendre functions (2.12) in the form

$$\begin{aligned} z_\ell(t) &= \rho_\ell\sqrt{\sin t}\,u_{0\ell}(t) + (\nu_\ell + i\rho_\ell^{-1})\sqrt{\sin t}\,v_{0\ell}(t) \\ &= \rho_\ell\tilde u_{0\ell}(t) + (\nu_\ell + i\rho_\ell^{-1})\tilde v_{0\ell}(t)\,, \end{aligned}$$

where, as above, $SO(3)$-invariant complex structures differ from each other just in the pairs (ρ_ℓ,ν_ℓ), with $\rho_\ell > 0$ and $\nu_\ell \in \mathbb{R}$, and we have defined

$$\tilde u_{0\ell} := \sqrt{\sin t}\,u_{0\ell} \quad\text{and}\quad \tilde v_{0\ell} := \sqrt{\sin t}\,v_{0\ell}\,. \tag{2.57}$$

We have to discuss now the convergence condition expressed in (2.55). Let us first consider the real part

$$\mathrm{Re}[\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)] = \tilde A_\ell(t_1,t_0) + 2\nu_\ell\rho_\ell^{-1}\tilde B_\ell(t_1,t_0)$$

where

$$\begin{aligned} \tilde A_\ell(t_1,t_0) &:= \tilde u_{0\ell}(t_0)\dot{\tilde v}_{0\ell}(t_1) - \tilde u_{0\ell}(t_1)\dot{\tilde v}_{0\ell}(t_0) + \dot{\tilde u}_{0\ell}(t_1)\tilde v_{0\ell}(t_0) - \dot{\tilde u}_{0\ell}(t_0)\tilde v_{0\ell}(t_1) \\ &- \frac{1}{2}(\cot t_1 - \cot t_0)\left(\tilde u_{0\ell}(t_1)\tilde v_{0\ell}(t_0) + \tilde u_{0\ell}(t_0)\tilde v_{0\ell}(t_1)\right)\,, \\ \tilde B_\ell(t_1,t_0) &:= \tilde v_{0\ell}(t_0)\dot{\tilde v}_{0\ell}(t_1) - \tilde v_{0\ell}(t_1)\dot{\tilde v}_{0\ell}(t_0) - \frac{1}{2}(\cot t_1 - \cot t_0)\tilde v_{0\ell}(t_0)\tilde v_{0\ell}(t_1)\,. \end{aligned}$$

The asymptotic behaviors of $\tilde A_\ell$ and $\tilde B_\ell$ as $\ell \to +\infty$ can be obtained from (2.12) and (2.41),

$$\tilde A_\ell(t_1,t_0) \sim -\frac{1}{4\ell}(\cot t_1 - \cot t_0)\cos\big((\ell+1/2)(t_0+t_1)\big)\,, \tag{2.58}$$

$$\tilde B_\ell(t_1,t_0) \sim -\frac{\pi}{4}\sin\big((\ell+1/2)(t_1-t_0)\big)\,. \tag{2.59}$$

We then conclude that $\mathrm{Re}[\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)]$ is square summable if and only if

$$\big(\nu_\ell\rho_\ell^{-1}\big)_{\ell\in\mathbb{N}_0} \in \ell^2(\mathbb{R})\,. \tag{2.60}$$

For the imaginary part of the $\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)$ coefficients, we have

$$\mathrm{Im}[\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)] \;=\; \rho_\ell\nu_\ell\tilde{A}_\ell(t_1,t_0)+(\nu_\ell^2-\rho_\ell^{-2})\tilde{B}_\ell(t_1,t_0)+\rho_\ell^2\tilde{C}_\ell(t_1,t_0)\,,$$

where

$$\begin{aligned}\tilde{C}_\ell(t_1,t_0) \;&:=\; \tilde{u}_{0\ell}(t_0)\dot{\tilde{u}}_{0\ell}(t_1)-\tilde{u}_{0\ell}(t_1)\dot{\tilde{u}}_{0\ell}(t_0)-\frac{1}{2}(\cot t_1-\cot t_0)\tilde{u}_{0\ell}(t_0)\tilde{u}_{0\ell}(t_1)\\ &\sim\; -\frac{1}{\pi}\sin\big((\ell+1/2)(t_1-t_0)\big),\ \text{ when }\ \ell\to+\infty.\end{aligned} \tag{2.61}$$

The asymptotic behavior as $\ell\to+\infty$ of $\mathrm{Im}[\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)]$ can be obtained now from (2.58), (2.59), and (2.61). The imaginary part is then square summable if and only if

$$\big(\rho_\ell\nu_\ell/\ell\big)_{\ell\in\mathbb{N}_0}\in\ell^2(\mathbb{R})\ \text{ and }\ \big(\nu_\ell^2+4\rho_\ell^2/\pi^2-\rho_\ell^{-2}\big)_{\ell\in\mathbb{N}_0}\in\ell^2(\mathbb{R})\,. \tag{2.62}$$

Taking into account that conditions (2.60) and (2.62) must be satisfied jointly, we conclude that $\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)$ is square summable if and only if

$$\rho_\ell=\sqrt{\frac{\pi}{2}}+x_\ell>0\,,\ \ (x_\ell)_{\ell\in\mathbb{N}_0}\in\ell^2(\mathbb{R})\,,\ \text{ and }\ (\nu_\ell)_{\ell\in\mathbb{N}_0}\in\ell^2(\mathbb{R})\,. \tag{2.63}$$

We end this section by showing that the linear symplectic map $\mathcal{T}_{(t_1,t_0)}$ is continuous in the norm $||\cdot||=\sqrt{\langle\cdot|\cdot\rangle_{\mathcal{P}}}$ associated with the inner product (2.20) for all complex structures characterized by pairs (ρ_ℓ,ν_ℓ) verifying (2.63). That is, there exists some $K(t_1,t_0)>0$ such that

$$\|\kappa(\mathcal{T}_{(t_1,t_0)}\xi)\|\le K(t_1,t_0)\|\kappa(\xi)\|\,,$$

for all $\xi\in\mathcal{S}_\xi$, where $\kappa:\mathcal{S}_{\xi_\mathbb{C}}\to\mathcal{P}_\xi$ is the $\mathbb{C}$-linear projector defined by the splitting $\mathcal{S}_{\xi_\mathbb{C}}=\mathcal{P}_\xi\oplus\bar{\mathcal{P}}_\xi$. By using (2.49) and (2.54), it is straightforward to show that

$$\|\kappa(\mathcal{T}_{(t_1,t_0)}\xi)\|^2=\sum_{\ell=0}^{\infty}|\mathfrak{b}_\ell(t_1,t_0)|^2\le\sum_{\ell=0}^{\infty}\Big(|\alpha_\ell(t_1,t_0\,|\,z_\ell)|^2+|\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)|^2\Big)|b_\ell|^2\,, \tag{2.64}$$

where

$$\alpha_\ell^\xi(t_1,t_0\,|\,z_\ell)\;:=\;i\bar{z}_\ell(t_0)\Big(\dot{z}_\ell(t_1)-\frac{1}{2}\cot t_1 z_\ell(t_1)\Big)-iz_\ell(t_1)\Big(\dot{\bar{z}}_\ell(t_0)-\frac{1}{2}\cot t_0\bar{z}_\ell(t_0)\Big)\,,$$

and the $\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)$ coefficients are given by (2.56). We have shown above that the sequence $(|\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)|)_{\ell\in\mathbb{N}_0}$ is bounded (actually square summable) so in the case when the sequence $(|\alpha_\ell^\xi(t_1,t_0\,|\,z_\ell)|)_{\ell\in\mathbb{N}_0}$ be also bounded, the continuity of $\mathcal{T}_{(t_1,t_0)}$ follows directly from equation (2.64). It suffices to remember that $\alpha_\ell^\xi(t_1,t_0\,|\,z_\ell)$ and $\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)$ are Bogoliubov coefficients satisfying $|\alpha_\ell^\xi(t_1,t_0\,|\,z_\ell)|^2-|\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)|^2=1$ for all ℓ to conclude that $|\alpha_\ell^\xi(t_1,t_0\,|\,z_\ell)|\sim1$ as $\ell\to+\infty$. Therefore, it is clear that there exists a $K^2(t_1,t_0)>0$ such that $|\alpha_\ell^\xi(t_1,t_0\,|\,z_\ell)|^2+|\beta_\ell^\xi(t_1,t_0\,|\,z_\ell)|^2\le K^2(t_1,t_0)\,,\ \forall\,\ell\in\mathbb{N}_0\,$. Then, using (2.64), we get that $\|\kappa(\mathcal{T}_{(t_1,t_0)}\xi)\|^2\le K^2(t_1,t_0)\|\kappa(\xi)\|^2$ and, hence, $\mathcal{T}_{(t_1,t_0)}$ is continuous. In conclusion, by imposing suitable conditions (2.63) on the parameters ρ_ℓ and ν_ℓ, it is possible to find $SO(3)$-complex structures (equivalently, subspaces $\mathcal{P}$) such that the quantum dynamics can be unitarily implemented in $\mathcal{F}_+(\mathscr{H}_\mathcal{P})$.

2.4 Uniqueness of the Fock quantization

In the case of the $\mathbb{T}^3$ Gowdy models, the presence of an extra constraint remaining after deparameterization, and the corresponding $U(1)$ symmetry generated by it, gives the possibility of introducing a physically sensible criterion to select a preferred complex structure, namely, invariance under this symmetry [10]. This is not the case for the other compact topologies $\mathbb{S}^1 \times \mathbb{S}^2$ and $\mathbb{S}^3$ for which, as showed in *Chapter 1*, there are no extra constraints after deparameterization. In these cases, we will use the $SO(3)$ symmetry associated with the background metric to select a preferred class of complex structures. Once we require that the quantum dynamics is unitary, we will find that all of them are unitarily equivalent.[7]

To this end, let us recall some properties of the $SO(3)$-invariant complex structures considered in section 2.2.1. Any invariant complex structure J is related to the complex structure J_0 (defined for the ξ field by the set of functions $(z_{0\ell}(t) = \tilde{u}_{0\ell}(t) + i\tilde{v}_{0\ell})_{\ell\in\mathbb{N}_0}$ corresponding to $\rho_\ell = 1$ and $\nu_\ell = 0$) through a linear symplectic transformation T_J, so that $J = T_J \circ J_0 \circ T_J^{-1}$. Explicitly, making use of relation (2.31), a direct calculation shows

$$T_J = \bigoplus_{\ell=0}^{\infty} \left[\begin{array}{cc} (\tau_1^\ell)_J I_{11}^\ell & (\tau_2^\ell)_J I_{12}^\ell \\ (\bar{\tau}_2^\ell)_J I_{21}^\ell & (\bar{\tau}_1^\ell)_J I_{22}^\ell \end{array} \right], \tag{2.65}$$

with

$$\begin{aligned} (\tau_1^\ell)_J &:= \sqrt{(1 + |\jmath_{11}^\ell|)/2} \quad \text{(up to multiplicative phase)}, \\ (\tau_2^\ell)_J &:= \frac{i\jmath_{12}^\ell}{2(\tau_1^\ell)_J}. \end{aligned}$$

Note that J_0 does not lead to a unitary implementation of the dynamics. In this context, it is fixed just to compare different complex structures. Let us then consider any two $SO(3)$-invariant complex structures, J and J', for which the dynamics is unitary – they are thus characterized by pairs (ρ_ℓ, ν_ℓ) satisfying (2.63). They will define unitarily equivalent quantum theories if and only if the linear symplectic transformation $T_{J,J'} := T_J \circ T_{J'}^{-1}$ connecting them through $J = T_{J,J'} \circ J' \circ T_{J,J'}^{-1}$ is unitarily implementable. This is the case if and only if the sequence

$$\big((\tau_2^\ell)_J(\tau_1^\ell)_{J'} - (\tau_1^\ell)_J(\tau_2^\ell)_{J'}\big)_{\ell\in\mathbb{N}_0}$$

is square summable. Taking into account the relations (2.32) and (2.33), as well as the asymptotic behaviors (2.63), the previous condition is verified, so the quantum theories defined by J and J' are, indeed, unitarily equivalent. The simplicity of this result typifies the usefulness of the employed formalism.

[7]See also [11] for an independent proof of this result.

2.5 Self-adjointness and domain of quantum Hamiltonians

We analyze here an interesting feature of the quantum dynamics for these systems: The fact that, even though the evolution is unitarily implemented, the time-dependent quantum Hamiltonian, proved to be self-adjoint for each value of the time parameter, has the striking property that Fock space vectors corresponding to a finite number of particle-like excitations do not belong to its domain. We will then discuss the possibility of modifying the expression of the Hamiltonian at the classical level in order to avoid these problems regarding the domain of its quantum counterpart.

The classical Hamiltonian governing the dynamics on the canonical phase space $\Upsilon = (\mathbf{P}, \omega)$ in the ξ-description of the system is derived from the action (2.45). It is given by the time-dependent *indefinite*[8] quadratic form

$$H(Q,P;t) = \frac{1}{2}\int_{\mathbb{S}^2} |\gamma|^{1/2}\left(P^2 + \cot t\, PQ - Q\Delta_{\mathbb{S}^2}Q\right). \tag{2.66}$$

Note that, due to the nonautonomous nature of the classical Hamiltonian, the time evolution does not define a one-parameter symplectic group on Υ and we cannot apply Stone's theorem to justify the self-adjointness of the corresponding (one-parameter family of) operators in the quantum theory. Nevertheless, it is possible to show that the quantum Hamiltonian is self-adjoint for each value of the time parameter t by analyzing the unitary implementability on $\mathscr{F}_+(\mathscr{H}_\mathcal{P})$ of the one-parameter symplectic group generated by the *autonomous* Hamiltonian $H(\tau)$, once a value $t = \tau \in (0,\pi)$ has been fixed. Here, we will follow the efficient procedure employed in [12] for the Gowdy $\mathbb{T}^3$ model, subsequently generalized in [13] to discuss the self-adjointness of general quadratic operators in this context. We start by considering the auxiliary system $(\mathbf{P}, \omega, H(\tau))$, where the dynamics is governed by the classical autonomous Hamiltonian

$$H(\tau) = \frac{1}{2}\sum_{\ell=0}^{\infty}\left(K_\ell(\tau)b_\ell^2 + \bar{K}_\ell(\tau)\bar{b}_\ell^2 + 2G_\ell(\tau)\bar{b}_\ell b_\ell\right), \tag{2.67}$$

with

$$\begin{aligned}
K_\ell(\tau) &:= \left(\dot{z}_\ell(\tau) - \frac{1}{2}\cot\tau\, z_\ell(\tau)\right)^2 + \ell(\ell+1)z_\ell^2(\tau) + \cot\tau\left(\dot{z}_\ell(\tau) - \frac{1}{2}\cot\tau\, z_\ell(\tau)\right)z_\ell(\tau)\,,\\
G_\ell(\tau) &:= \left|\dot{z}_\ell(\tau) - \frac{1}{2}\cot\tau\, z_\ell(\tau)\right|^2 + \ell(\ell+1)|z_\ell(\tau)|^2\\
&+ \frac{1}{2}\cot\tau\left(\left(\dot{z}_\ell(\tau) - \frac{1}{2}\cot\tau\, z_\ell(\tau)\right)\bar{z}_\ell(\tau) + \left(\dot{\bar{z}}_\ell(\tau) - \frac{1}{2}\cot\tau\,\bar{z}_\ell(\tau)\right)z_\ell(\tau)\right).
\end{aligned} \tag{2.68}$$

[8]Note the appearance of a cross term involving Q and P.

The modes $b_\ell, \bar{b}_\ell$ are defined through the relations $Q_\ell := \int_{\mathbb{S}^2} |\gamma|^{1/2} Q Y_{\ell 0} = z_\ell(\tau) b_\ell + \bar{z}_\ell(\tau)\bar{b}_\ell$ and $P_\ell := \int_{\mathbb{S}^2} |\gamma|^{1/2} P Y_{\ell 0} = \big(\dot{z}_\ell(\tau) - (1/2)\cot\tau\, z_\ell(\tau)\big) b_\ell + \big(\dot{\bar{z}}_\ell(\tau) - (1/2)\cot\tau\, \bar{z}_\ell(\tau)\big)\bar{b}_\ell$. Their evolution in a fictitious time parameter $s \in \mathbb{R}$ is given by the linear equations[9]

$$\begin{aligned} \frac{\mathrm{d}b_\ell}{\mathrm{d}s} &= \{b_\ell, H(\tau)\} = -i\big(G_\ell(\tau) b_\ell + \bar{K}_\ell(\tau)\bar{b}_\ell\big)\,, \\ \frac{\mathrm{d}\bar{b}_\ell}{\mathrm{d}s} &= \{\bar{b}_\ell, H(\tau)\} = i\big(K_\ell(\tau) b_\ell + G_\ell(\tau)\bar{b}_\ell\big)\,. \end{aligned} \tag{2.69}$$

Using the normalization condition (2.48), we easily obtain the second-order differential equation

$$\frac{\mathrm{d}^2 b_\ell}{\mathrm{d}s^2} = -\Big(\ell(\ell+1) - \frac{1}{4}\cot^2\tau\Big) b_\ell\,, \tag{2.70}$$

whose solutions have a linear dependence on the initial conditions $b_\ell(s_0)$ and $\bar{b}_\ell(s_0)$,

$$b_\ell(s) = \alpha_\ell(s,s_0) b_\ell(s_0) + \beta_\ell(s,s_0)\bar{b}_\ell(s_0)\,,\ \ \bar{b}_\ell(s) = \overline{b_\ell(s)}\,. \tag{2.71}$$

This symplectic transformation is unitarily implementable on $\mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$ for each $s \in \mathbb{R}$, i.e., there exists a unitary operator $\hat{u}(s,s_0) : \mathscr{F}_+(\mathscr{H}_{\mathcal{P}}) \to \mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$ such that $\hat{u}^{-1}(s,s_0)\hat{b}_\ell \hat{u}(s,s_0) = \alpha_\ell(s,s_0)\hat{b}_\ell + \beta_\ell(s,s_0)\hat{b}_\ell^\dagger$ and $\hat{u}^{-1}(s,s_0)\hat{b}_\ell^\dagger \hat{u}(s,s_0) = \bar{\beta}_\ell(s,s_0)\hat{b}_\ell + \bar{\alpha}_\ell(s,s_0)\hat{b}_\ell^\dagger$, if and only if the Bogoliubov coefficients β_ℓ are square summable [7],

$$\sum_{\ell=0}^{\infty} |\beta_\ell(s,s_0)|^2 < +\infty\,. \tag{2.72}$$

Here, $\hat{b}_\ell^\dagger$ and $\hat{b}_\ell$ are the creation and annihilation operators associated with the modes $\xi_\ell = z_\ell Y_{\ell 0}$, respectively. Note that, for each value of $\tau \in (0,\pi)$, there exists $\ell_0 \in \mathbb{N}_0$ such that

$$\lambda_\ell^2 := \ell(\ell+1) - \frac{1}{4}\cot^2\tau > 0\,,\ \ \forall\, \ell > \ell_0\,.$$

In this case,

$$\begin{aligned} \alpha_\ell(s,s_0) &= \cos\big(\lambda_\ell(s-s_0)\big) - i\lambda_\ell^{-1} G_\ell(\tau)\sin\big(\lambda_\ell(s-s_0)\big)\,, \\ \beta_\ell(s,s_0) &= -i\lambda_\ell^{-1}\bar{K}_\ell(\tau)\sin\big(\lambda_\ell(s-s_0)\big)\,. \end{aligned}$$

It suffices to consider the modes corresponding to $\ell > \ell_0$, since the convergence of the series (2.72) depends, in practice, only on the high-frequency behavior of the β_ℓ coefficients. Taking into account the asymptotic expansions in ℓ

$$\begin{aligned} z_\ell(t) &= \frac{1}{\sqrt{2\ell}}\exp\big(-i[(\ell+1/2)t - \pi/4]\big) + O(\ell^{-3/2})\,, \\ \dot{z}_\ell(t) - \frac{1}{2}\cot t\, z_\ell(t) &= -i\sqrt{\frac{\ell}{2}}\exp\big(-i[(\ell+1/2)t - \pi/4]\big) + O(\ell^{-1/2})\,, \end{aligned} \tag{2.73}$$

[9]Here, $\{\cdot,\cdot\}$ denotes the Poisson bracket defined from (2.5), with $\{b_\ell, \bar{b}_{\ell'}\} = -i\delta(\ell,\ell')\mathbb{I}$.

we have $K_\ell(\tau) = O(1)$, so that $\sum_{\ell>\ell_0} \lambda_\ell^{-2}|K_\ell(\tau)|^2 \sin^2\big(\lambda_\ell(s-s_0)\big) < +\infty$, $\forall\, s \in \mathbb{R}$ and, hence, condition (2.72) is verified. Finally, the transformation (2.71) is implementable as a continuous, unitary, one-parameter group if it verifies the strong continuity condition in the auxiliary parameter s

$$\lim_{s\to s_0} \sum_{\ell=0}^{\infty} |b_\ell(s) - b_\ell(s_0)|^2 = 0\,, \quad s_0 \in \mathbb{R}\,. \tag{2.74}$$

Again, we can restrict ourselves to the modes $\ell > \ell_0$. It is straightforward to check that this condition holds for the solution (2.71) with square summable initial data b_ℓ and $\bar{b}_\ell$. Therefore, we have obtained a strongly continuous and unitary one-parameter group whose generator is self-adjoint according to Stone's theorem.

The quantum Hamiltonian of the models under consideration can be explicitly calculated as the strong limit

$$\mathrm{s}\!-\!\lim_{t_0\to t} \frac{\hat{U}(t,t_0) - \hat{\mathbb{I}}}{t-t_0} f = -i\hat{H}(t) f\,, \quad f \in \mathscr{D}_{\hat{H}(t)}\,, \tag{2.75}$$

where $\hat{U}(t,t_0)$ denotes the quantum evolution operator on $\mathscr{F}_+(\mathscr{H}_\mathcal{P})$, that can be univocally derived from the evolution of creation operators in the Heisenberg picture

$$\begin{aligned}
\hat{U}^{-1}(t,t_0)\,\hat{b}_\ell\,\hat{U}(t,t_0) &= \alpha_\ell^\xi(t,t_0\,|\,z_\ell)\hat{b}_\ell + \beta_\ell^\xi(t,t_0\,|\,z_\ell)\hat{b}_\ell^\dagger\,,\\
\hat{U}^{-1}(t,t_0)\,\hat{b}_\ell^\dagger\,\hat{U}(t,t_0) &= \bar{\beta}_\ell^\xi(t,t_0\,|\,z_\ell)\hat{b}_\ell + \bar{\alpha}_\ell^\xi(t,t_0\,|\,z_\ell)\hat{b}_\ell^\dagger\,,
\end{aligned}$$

and the evolution of the vacuum state $|0\rangle_\mathcal{P} := 1 \oplus 0 \oplus 0 \oplus \cdots \in \mathscr{F}_+(\mathscr{H}_\mathcal{P})$, that can be written in closed form as (see also [14 − 16])

$$\hat{U}(t,t_0)|0\rangle_\mathcal{P} = N(t,t_0)\exp\left(-\frac{1}{2}\sum_{\ell=0}^{\infty}\frac{\beta_\ell^\xi(t_0,t\,|\,z_\ell)}{\alpha_\ell^\xi(t_0,t\,|\,z_\ell)}\,\hat{b}_\ell^{\dagger 2}\right)|0\rangle_\mathcal{P}\,,$$

where $N(t,t_0)$ is fixed (up to an irrelevant multiplicative phase) by normalization

$$|N(t,t_0)| = \prod_{\ell\in\mathbb{N}_0} \frac{1}{\sqrt{|\alpha_\ell^\xi(t_0,t\,|\,z_\ell)|}}\,.$$

Note in particular that, as expected in a nonautonomous system, the vacuum state (and, hence, states with a finite number of particles) is not stable under time evolution. The previous result ensures the self-adjointness of the quantum Hamiltonian $\hat{H}(t)$ and the existence of a dense domain $\mathscr{D}_{\hat{H}(t)} \subset \mathscr{F}_+(\mathscr{H}_\mathcal{P})$, for each value of the time parameter $t \in (0,\pi)$. Unfortunately, the method employed here does not provide us with a characterization of such domains or the concrete expression of the quantum Hamiltonian. This can be done in a mathematically rigorous way by studying the differentiability (2.75) of $\hat{U}(t,t_0)$. Nevertheless, given the quadratic nature of the classical Hamiltonian, it is expected that this limit coincides with the operator directly promoted from the classical function up to normal ordering,

$$\hat{H}(t) \;=\; \frac{1}{2}\sum_{\ell=0}^{\infty}\Big(K_\ell(t)\,\hat{b}_\ell^2+\bar{K}_\ell(t)\,\hat{b}_\ell^{\dagger 2}+2G_\ell(t)\,\hat{b}_\ell^\dagger\hat{b}_\ell\Big)\,. \tag{2.76}$$

However, this operator does not have the Fock vacuum state $|0\rangle_{\mathcal{P}}$ in its domain due to the non-square summability of the K_ℓ sequence defined in (2.68). Indeed, the action of the quantum Hamiltonian on the vacuum $|0\rangle_{\mathcal{P}}$ is

$$\hat{H}(t)|0\rangle_{\mathcal{P}}=\frac{1}{\sqrt{2}}\sum_{\ell=0}^{\infty}\bar{K}_\ell(t)|2_\ell\rangle\,,$$

where $|2_\ell\rangle=2^{-1/2}\hat{b}_\ell^{\dagger 2}\,|0\rangle_{\mathcal{P}}$. The state $\hat{H}(t)|0\rangle_{\mathcal{P}}$ is normalizable if and only if $\sum_{\ell=0}^{\infty}|K_\ell(t)|^2 < +\infty$, a condition which is not verified since that $K_\ell(t)=O(1)$. As a consequence, the action of the operator is not defined either on the dense subspace of states with a finite number of particles. This difficulty can be overcome right from the start by realizing that the covariant phase space Γ_ξ defined by (2.45) can be equivalently derived from the simpler action

$$s_0(\xi) \;=\; -\frac{1}{2}\int_{[t_0,t_1]\times\mathbb{S}^2}|\mathring{\eta}|^{1/2}\mathring{\eta}^{ab}\Big((\mathrm{d}\xi)_a(\mathrm{d}\xi)_b+\frac{1}{4}(1+\csc^2 t)\,\xi^2\Big)\,. \tag{2.77}$$

This variational principle gives now a time-dependent, *positive definite*, diagonal Hamiltonian of the form

$$H_0(Q,P;t):=\frac{1}{2}\int_{\mathbb{S}^2}|\gamma|^{1/2}\left(P^2+Q\Big[\frac{1}{4}(1+\csc^2 t)-\Delta_{\mathbb{S}^2}\Big]Q\right)\,. \tag{2.78}$$

The Hamiltonians (2.66) and (2.78) obviously govern the same classical evolution. Note, however, that they are connected by a time-dependent symplectic transformation that, in principle, is not unitarily implementable. As a consequence, one possibly obtains nonequivalent quantum theories from them. The corresponding quantum Hamiltonian is given, after normal ordering, by

$$\hat{H}_0(t)=\frac{1}{2}\sum_{\ell=0}^{\infty}\Big(K_{0\ell}(t)\hat{b}_\ell^2+\bar{K}_{0\ell}(t)\hat{b}_\ell^{\dagger 2}+2G_{0\ell}(t)\hat{b}_\ell^\dagger\hat{b}_\ell\Big)\,, \tag{2.79}$$

where

$$\begin{aligned} K_{0\ell}(t) \;&:=\; \dot{z}_\ell^2(t)+\left(\frac{1}{4}\big(1+\csc^2 t\big)+\ell(\ell+1)\right)z_\ell^2(t)\,, \qquad (2.80)\\ G_{0\ell}(t) \;&:=\; \big|\dot{z}_\ell(t)\big|^2+\left(\frac{1}{4}\big(1+\csc^2 t\big)+\ell(\ell+1)\right)|z_\ell(t)|^2\,. \end{aligned}$$

There are no subtleties associated with the domain of this new quantum Hamiltonian in the sense that now the Fock space vacuum belongs to the its domain –in this case, $K_{0\ell}(t)$ defines a square summable sequence for each value of t. Moreover, the previous results concerning the unitary implementation of the time evolution and the uniqueness of the Fock representation are also valid in this case. Concretely, the biparametric family of complex structures for which the dynamics is unitary is characterized again by the pairs (2.63). In what follows, we will consider the dynamics of the system to be described by (2.78).

References

1 C. Crnković and E. Witten, in *300 Years of Gravitation*, edited by S. Hawking and W. Israel, Cambridge University Press, Cambridge (1987). C. Crnković, Class. Quantum. Grav. **5** (1988) 1557-1575. J. Lee and R. Wald, J. Math. Phys. **31**, 725 (1990). A. Ashtekar, L. Bombelli, and O. Reula, in *Mechanics, Analysis and Geometry : 200 Years After Lagrange*, edited by M. Francaviglia, North-Holland, New York (1991). G. Barnich, M. Henneaux, and C. Schomblond, Phys. Rev. D **44**, R939 (1991).

2 R. M. Wald, *Quantum field theory in curved spacetime and black hole thermodynamics*, The University of Chicago Press, USA (1994).

3 N. M. J. Woodhouse, *Geometric quantization*, Oxford University Press, USA; 2nd edition (1997).

4 E. Prugovečki. Quantum mechanics in Hilbert space. Academic Press, New York and London (1971).

5 M. Reed and B. Simon, *Methods of Modern Mathematical Physics*, Vol. I. Academic Press, New York, (1980).

6 A. Ashtekar, Commun. Math. Phys. **71**, 59-64 (1980).

7 D. Shale, Trans. Am. Math. Soc. **103**, 149 (1962).

8 G. N. Watson, “Asymptotic expansions of hypergeometric functions”, Trans. Cambridge Philos. Soc. **22** (1918) 277-308.

9 A. Corichi, J. Cortez, and G. A. Mena Marugán, Phys. Rev. D **73**, 041502 and 084020 (2006).

10 A. Corichi, J. Cortez, G. A. Mena Marugán, and J. M. Velhinho, Class. Quant. Grav. **23**, 6301 (2006).

11 J. Cortez, G. A. Mena Marugán, and J. M. Velhinho, Class. Quant. Grav. **25**, 105005 (2008).

12 C. G. Torre, Phys. Rev. D **66**, 084017 (2002).

13 J. F. Barbero G., D. G. Vergel, and E. J. S. Villaseñor, Phys. Rev. D **74**, 024003 (2006).

14 L. Parker, Phys. Rev. **183**, 5 (1969).

15 K. Pilch and N. P. Warner, Class. Quant. Grav. **4**, 1183 (1987).

16 C. G. Torre and M. Varadarajan, Phys. Rev. D **58**, 064007 (1998).

Chapter 3
Schrödinger Quantization

D. G. Vergel
Classical and Quantum Gravity 25, 175016 (2008)

J. F. Barbero G., D. G. Vergel, and E. J. S. Villaseñor
Physical Review D 74, 024003 (2006)

We will consider the Schrödinger representation for the linearly polarized Gowdy $\mathbb{S}^1 \times \mathbb{S}^2$ and $\mathbb{S}^3$ models coupled to massless scalar fields, where states act as functionals on the quantum configuration space $\overline{\mathscr{C}}$ for a fixed time t_0. Here, $\overline{\mathscr{C}}$ is an appropriate distributional extension of the classical configuration space $\mathscr{C}$, characterized in these cases by the space of tempered distributions on the 2-sphere. The Hilbert space then takes the form $\mathscr{H}_s(t_0) = L^2(\overline{\mathscr{C}}, \mathrm{d}\mu_{t_0})$. The identification of the Gaussian nature of the measure μ_{t_0}, the nonstandard representation of the momentum operator, and the relation between Schrödinger and Fock representations were exhaustively analyzed in [1] as a natural extension to the functional description of the Fock quantization of scalar fields in curved backgrounds [2]. In the QFT context, the Schrödinger representation has been historically pushed into the background in favor of the usual Fock quantization due to the difficulty in using it to address sensible questions regarding physical scattering processes. However, it is certainly the most natural representation in the context of canonical quantum gravity, in view of the splitting of spacetime into spatial sections of constant time. Furthermore, as was pointed out in [3] for the vacuum three-torus case, it provides a better understanding of the properties of the quantized field, since it is possible to determine the behavior of the typical field configurations through the study of the measure support.

3.1 Constructing the L^2 space

Let us denote by $\mathscr{S}$ the Schwartz space of smooth and symmetric test functions on the 2-sphere,

$$\mathscr{S} := \{f \in C^\infty(\mathbb{S}^2; \mathbb{R}) \mid \mathcal{L}_\sigma f = 0\},$$

endowed with the standard nuclear topology. Note that every element $f \in \mathscr{S}$ can be expanded as

$$f(s) = \sum_{\ell=0}^{\infty} f_\ell Y_{\ell 0}(s)\,, \quad s \in \mathbb{S}^2\,, \tag{3.1}$$

with $(f_\ell)_{\ell\in\mathbb{N}_0}$ being a sequence of rapidly decreasing real coefficients, such that $\lim_{\ell\to+\infty} \ell^n f_\ell = 0$, $\forall\, n \in \mathbb{N}_0$. As $\mathscr{S}$ is central to our future considerations, it is very useful to have as complete a characterization as possible. Concretely, we will revise the equivalent description of the topological structure of $\mathscr{S}$ in terms of the locally convex space of rapidly decreasing sequences in section 3.1.1.[1] The quantum configuration space used to define the Schrödinger representation is then the topological dual $\mathscr{S}'$ space of continuous linear functionals (tempered distributions) on $\mathscr{S}$. Note that this space includes the delta functions and their derivatives. Given a time of embedding t_0, the Schrödinger representation is introduced by defining a suitable Hilbert space $L^2(\mathscr{S}', \mathrm{d}\mu_{t_0})$, for a certain measure μ_{t_0}, in which the configuration observables act as *multiplication* operators. Here, the measure μ_{t_0} is implicitly assumed to be defined on the σ-algebra $\sigma(\mathrm{Cyl}(\mathscr{S}'))$ generated by the cylinder sets. As we will see later, given the Gaussian nature of the measure μ_{t_0}, the momentum operators will differ from the usual ones in terms of derivatives by a multiplicative term depending on the configuration variables,

$$\hat{P}_\ell(t_0)\Psi = -i\partial_{q_\ell}\Psi + \text{multiplicative term}\,.$$

We saw in *Chapter 2* that the phase space of the models under consideration can be alternatively described by solutions to the equation of motion in the covariant scheme or in terms of Cauchy data in the canonical formalism. In the present approach, it is especially convenient to construct the Weyl C^*-algebra of quantum observables from the canonical phase space scheme. The arguments used here will be, in any case, analogous to those employed in *section 2.3* within the covariant formalism. We start by constructing the set $\mathcal{O}_c$ of elementary classical observables of the theory. Again, the election is particularly simple given the linearity of the space $\mathbf{P} = \mathscr{S} \times \mathscr{S}$. In this case, $\mathcal{O}_c$ can be identified with the $\mathbb{R}$-vector space generated by linear functionals on $\mathbf{P}$. Every pair $\lambda := (-g, f) \in \mathbf{P}$, $f, g \in \mathscr{S}$, has an associated functional $L_\lambda : \mathbf{P} \to \mathbb{R}$ such that, for all $X = (Q, P) \in \mathbf{P}$,

$$L_\lambda(X) := \omega(\lambda, X) = \int_{\mathbb{S}^2} |\gamma|^{1/2}(fQ + gP)\,, \tag{3.2}$$

with the symplectic structure ω defined as in equation (2.5). In this way, $\mathcal{O}_c = \mathrm{Span}\{\mathbb{I}, L_\lambda\}_{\lambda\in\mathbf{P}}$. Again, this set satisfies the condition that any regular function on $\mathbf{P}$ can be obtained as a (suitable limit of) sum of products of elements in $\mathcal{O}_c$, and also that it is closed under Poisson brackets, $\{L_\lambda(\cdot), L_\nu(\cdot)\} = L_\nu(\lambda)\mathbb{I}$. Specifically, the configuration and momentum observables are objects of this type defined by the pairs

[1] For more details, the reader can consult [4]

$\lambda = (0, f)$ and $\lambda = (-g, 0)$, respectively

$$Q(f) := L_{(0,f)}(Q,P) = \int_{\mathbb{S}^2} |\gamma|^{1/2} f Q = \sum_{\ell=0}^{\infty} f_\ell Q_\ell \,, \tag{3.3}$$

$$P(g) := L_{(-g,0)}(Q,P) = \int_{\mathbb{S}^2} |\gamma|^{1/2} g P = \sum_{\ell=0}^{\infty} g_\ell P_\ell \,, \tag{3.4}$$

where the symmetric test functions have been expanded as explained at the beginning of this section –see the equation (3.1). Here, with the aim of simplifying the notation, we have used the same symbol to denote the canonical inclusion $\mathscr{S} \hookrightarrow \mathscr{S}'$ of $\mathscr{S}$ into $\mathscr{S}'$. In this way, $L_{(-g,f)}(Q,P) = Q(f) + P(g)$. Given the canonical phase space $\Upsilon = (\mathbf{P}, \omega)$, the corresponding Weyl C^*-algebra $\mathscr{W}(\Upsilon)$ is generated by the elements $W(\lambda) = \exp(iL_\lambda(\cdot))$, $\lambda \in \mathbf{P}$, satisfying the conditions

$$W(\lambda_1)^* = W(-\lambda_1) \,, \quad W(\lambda_1)W(\lambda_2) = \exp\big(-\frac{i}{2}\omega(\lambda_1,\lambda_2)\big) W(\lambda_1+\lambda_2) \,, \tag{3.5}$$

for all $\lambda_1, \lambda_2 \in \mathbf{P}$. Since the generators of this algebra and the one defined in *section 2.3* satisfy the same Weyl relations, there exists a unique $*$-isomorphism connecting them.

From now on, we will implicitly assume the use of a concrete $SO(3)$-invariant complex structure $J_{\mathcal{P}}$ satisfying the conditions (2.63), so that the dynamics is unitarily implemented on the Fock space $\mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$. Let $\mathfrak{I}_{t_0} : \mathbf{P} \to \mathcal{S}_\xi$, $t_0 \in (0, \pi)$, be the symplectomorphism introduced in *section 2.1* which defines for each pair of Cauchy data $(Q, P) \in \mathbf{P}$ the unique solution $\xi \in \mathcal{S}_\xi$ such that $\xi(t_0, s) = Q(s)$ and $\dot{\xi}(t_0, s) = P(s)$ under the evolution given by the Hamiltonian (2.78). This is,

$$\xi(t,s) = (\mathfrak{I}_{t_0}(Q,P))(t,s) = \sum_{\ell=0}^{\infty} \Big(b_\ell(t_0) z_\ell(t) + \overline{b_\ell(t_0) z_\ell(t)} \Big) Y_{\ell 0}(s) \in \mathcal{S}_\xi \,, \tag{3.6}$$

with

$$b_\ell(t_0) := i\bar{z}_\ell(t_0) P_\ell - i\dot{\bar{z}}_\ell(t_0) Q_\ell \,. \tag{3.7}$$

This map gives rise to a natural ω-compatible complex structure on the canonical phase space,

$$J_{t_0} := \mathfrak{I}_{t_0}^{-1} \circ J_{\mathcal{P}} \circ \mathfrak{I}_{t_0} : \mathbf{P} \to \mathbf{P} \,,$$

such that

$$(Q,P) \in \mathbf{P} \mapsto J_{t_0}(Q,P) = (A(t_0)Q + B(t_0)P, D(t_0)Q + C(t_0)P) \in \mathbf{P} \,, \tag{3.8}$$

where $A(t_0), B(t_0), C(t_0), D(t_0) : \mathscr{S} \to \mathscr{S}$ are linear operators satisfying, by virtue of the ω-compatibility, the relations [5]

$$\langle f, B(t_0) f' \rangle = \langle B(t_0) f, f' \rangle \,, \quad \langle g, D(t_0) g' \rangle = \langle D(t_0) g, g' \rangle \,, \quad \langle f, A(t_0) g \rangle = -\langle C(t_0) f, g \rangle \,,$$

for all $f, g, f', g' \in \mathscr{S}$. Here, we have denoted

$$\langle f, g \rangle := \int_{\mathbb{S}^2} |\gamma|^{1/2} f g \, .$$

Also, given the condition $J_{t_0}^2 = -\mathrm{Id}_{\mathbf{P}}$, we have

$$\begin{aligned} A^2(t_0) + B(t_0)D(t_0) &= -\mathbf{1} \, , \quad A(t_0)B(t_0) + B(t_0)C(t_0) = 0 \, , \\ C^2(t_0) + D(t_0)B(t_0) &= -\mathbf{1} \, , \quad D(t_0)A(t_0) + C(t_0)D(t_0) = 0 \, . \end{aligned}$$

Thereby, assuming $B(t_0)$ invertible, the $C(t_0)$ and $D(t_0)$ operators can be expressed in terms of the $A(t_0)$ and $B(t_0)$ operators through the relations

$$C(t_0) = -B^{-1}(t_0)A(t_0)B(t_0) \quad \text{and} \quad D(t_0) = -B^{-1}(t_0)(\mathbf{1} + A^2(t_0)) \, ,$$

respectively, in such a way that the complex structure J_{t_0} is fully characterized by them. Using the normalization condition (2.48) and equation (3.6) it is straightforward to obtain[2]

$$\begin{aligned} \big(A(t_0)Q\big)(s) &= \sum_{\ell=0}^{\infty} \big(\dot{\bar{z}}_\ell(t_0) z_\ell(t_0) + \dot{z}_\ell(t_0)\bar{z}_\ell(t_0)\big) Q_\ell Y_{\ell 0}(s) \, , \\ \big(B(t_0)P\big)(s) &= -2\sum_{\ell=0}^{\infty} |z_\ell(t_0)|^2 P_\ell Y_{\ell 0}(s) \, . \end{aligned} \tag{3.9}$$

It is worth noting that, given the rapidly decreasing nature of the sequences $(Q_\ell)_{\ell\in\mathbb{N}_0}$ and $(P_\ell)_{\ell\in\mathbb{N}_0}$, as well as the asymptotic behavior of the z_ℓ functions decaying like (2.73), the $A(t_0)$ and $B(t_0)$ operators are well defined on $\mathscr{S}$. In addition, $B(t_0)$ has an inverse operator $B^{-1}(t_0) : \mathscr{S} \to \mathscr{S}$ given by

$$\big(B^{-1}(t_0)P\big)(s) = -\frac{1}{2}\sum_{\ell=0}^{\infty} |z_\ell(t_0)|^{-2} P_\ell Y_{\ell 0}(s) \, . \tag{3.10}$$

Summarizing, a fixed complex structure $J_{\mathcal{P}} : \mathcal{S}_\xi \to \mathcal{S}_\xi$ on the covariant phase space determines a one-parameter family of complex structures $J_t : \mathbf{P} \to \mathbf{P}$, $t \in (0, \pi)$, on the canonical phase space. Once a time of embedding t_0 is fixed, the corresponding complex structure J_{t_0} is fully characterized by the pairs (3.9). The Schrödinger quantization associated with time t_0 consists then in a representation of the canonical commutation relations in terms of self-adjoint operators in a space of complex-valued functionals $\Psi : \mathscr{S}' \to \mathbb{C}$ belonging to a certain Hilbert space $\mathscr{H}_s(t_0) = L^2(\mathscr{S}', \mathrm{d}\mu_{t_0})$. The functionals

[2]Note that the zero mode $\ell = 0$ has been included into the spherical harmonic expansion of the test functions. The $B(t_0)$ operator is well defined even for this mode, ultimately as a consequence of equation (2.47) verified by the z_ℓ functions, where the squared frequency is positive definite $\forall\, t \in (0, \pi)$ when $\ell = 0$.

representing the pure states of the system are, thus, square integrable with respect to the measure μ_{t_0}. Due to the infinite dimensionality of the quantum configuration space $\overline{\mathscr{C}} = \mathscr{S}'$, it is not possible to define a Lebesgue-type translation invariant measure μ_{t_0} –such a measure does not exists– but rather a probability one, i.e., a measure satisfying $\int_{\mathscr{S}'} \mathrm{d}\mu_{t_0} = 1$. This representation is constructed in such a way that it is associated with the state $\varpi_{t_0} : \mathscr{W}(\Upsilon) \to \mathbb{C}$ on the Weyl algebra $\mathscr{W}(\Upsilon)$ whose action on the elementary observables is given by

$$\varpi_{t_0}(W(\lambda)) = \exp\left(-\frac{1}{4}\omega(J_{t_0}(\lambda), \lambda)\right), \quad \lambda \in \mathbf{P}\,. \tag{3.11}$$

We will check in section 3.3 that the Schrödinger representations corresponding to different values of the time parameter are unitarily equivalent owing to the unitary implementability of the dynamics. We require that the configuration observables are represented as *multiplication* operators, so that for $\lambda = (0, f) \in \mathbf{P}$,

$$\pi_s(t_0) \cdot W(\lambda)|_{\lambda=(0,f)} = \exp(i\hat{Q}_{t_0}[f])\,, \quad \left(\hat{Q}_{t_0}[f]\Psi\right)[\tilde{Q}] = \tilde{Q}(f)\Psi[\tilde{Q}]\,, \tag{3.12}$$

where $\tilde{Q} \in \mathscr{S}'$ denotes a generic distribution of $\mathscr{S}'$ and $\tilde{Q}(f)$ gives the usual pairing between $\mathscr{S}$ and $\mathscr{S}'$, $\Psi \in \mathscr{D}_{\hat{Q}_{t_0}[f]} \subset \mathscr{H}_s(t_0)$ (the self-adjointness of the configuration and momentum operators will be discussed in subsection 3.2), and $\pi_s(t_0) : \mathscr{W}(\Upsilon) \to \mathscr{B}(\mathscr{H}_s(t_0))$ is the map from the Weyl algebra to the collection of bounded linear operators on the Hilbert space $\mathscr{H}_s(t_0)$. The expectation value (3.11) evaluated at $\lambda = (0, f)$ yields

$$\varpi_{t_0}(W(\lambda))|_{\lambda=(0,f)} = \exp\left(\frac{1}{4}\langle f, B(t_0)f\rangle\right). \tag{3.13}$$

The left hand side of this equation corresponds to the vacuum expectation value of the $\pi_s(t_0) \cdot W(\varphi)$ operator, so it must coincide with the integral

$$\int_{\mathscr{S}'} \bar{\Psi}_0^{(t_0)}\big(\exp(i\hat{Q}_{t_0}[f])\Psi_0^{(t_0)}\big)\, \mathrm{d}\mu_{t_0}[\tilde{Q}] = \int_{\mathscr{S}'} e^{i\tilde{Q}(f)} \mathrm{d}\mu_{t_0}[\tilde{Q}]\,, \tag{3.14}$$

where $\Psi_0^{(t_0)} \in \mathscr{H}_s(t_0)$ is the normalized vacuum state. Comparing (3.13) and (3.14), we finally get

$$\int_{\mathscr{S}'} e^{i\tilde{Q}(f)}\, \mathrm{d}\mu_{t_0}[\tilde{Q}] = \exp\left(\frac{1}{4}\langle f, B(t_0)f\rangle\right). \tag{3.15}$$

In order to interpret this result, let us introduce the covariance operator $\check{\mathcal{C}}_{t_0} : \mathbf{P} \to \mathbb{R}$ defined as $\check{\mathcal{C}}_{t_0}(f, g) := \langle f, -B(t_0)g/2\rangle$, $f, g \in \mathscr{S}$. Since $|z_\ell(t_0)|^2$ is bounded and positive definite $\forall\, t \in (0, \pi)$ and $\forall\, \ell \in \mathbb{N}_0$, it follows that $\check{\mathcal{C}}_{t_0}$ is a nondegenerate, positive, definite, and continuous bilinear form on the topological vector space $\mathscr{S}$. Now, the Bochner-Minlos theorem, which plays a key role in the characterization of measures on functional spaces, states [6]:

Theorem 3.1.1 (Bochner-Minlos). *Let $\check{\mathcal{C}}$ be a positive continuous nondegenerate bilinear form on $\mathscr{S}\times\mathscr{S}$, written symbolically $\check{\mathcal{C}}(f,g)=\langle f,\mathcal{C}g\rangle$. Then, there exists a unique Gaussian integration measure $\mathrm{d}\mu_{\mathcal{C}}$ on $\mathscr{S}'$ with covariance $\mathcal{C}$ and mean zero. The corresponding generating function (or Fourier transform) is given explicitly as $\int_{\mathscr{S}'}\exp(i\phi(f))\mathrm{d}\mu_{\mathcal{C}}[\phi]=\exp(-\langle f,\mathcal{C}f\rangle/2)$.*

Thus, according to this result, we have that μ_{t_0} is the unique Gaussian integration measure (with covariance $\mathcal{C}(t_0):=-B(t_0)/2$) defined by the covariance operator $\check{\mathcal{C}}_{t_0}$. The generating function is given in this case by equation (3.15).

3.1.1 Properties of the measure

In order to easily visualize the nature of the measure μ_{t_0}, note that upon restriction on any number of coordinate directions in $\mathscr{S}'$, say $\tilde{Q}_\ell=\tilde{Q}(Y_{\ell 0})$, $\ell=0,1,\dots,n$, we obtain

$$\mathrm{d}\mu_{t_0}|_{(\tilde{Q}_\ell)_{\ell=0}^n}=\prod_{\ell=0}^{n}\frac{1}{\sqrt{2\pi}}\,|z_\ell(t_0)|^{-1}\exp\left(-\frac{1}{2}|z_\ell(t_0)|^{-2}\tilde{Q}_\ell^2\right)\mathrm{d}\tilde{Q}_\ell\,, \tag{3.16}$$

in terms of the Lebesgue measures $\mathrm{d}\tilde{Q}_\ell$ [6]. Now, we will prove that the support of the μ_{t_0}-measure is smaller than $\mathscr{S}'$. Concretely, it is given by the topological dual of the subspace of symmetric functions in the Sobolev space $H^\epsilon(\mathbb{S}^2)$ on the 2-sphere, for any $\epsilon>0$. With this aim, we will use some well-established consequences of the Bochner-Minlos theorem, closely relying on the analysis developed in [7]. We first point out that the space of test functions $\mathscr{S}$ is topologically isomorphic to $\varsigma=\bigcap_{r\in\mathbb{Q}}\varsigma_r$, where

$$\varsigma_r:=\left\{f=\{f_\ell\}_{\ell=0}^\infty\;|\;\|f\|_r^2:=\sum_{\ell=0}^{\infty}(\ell+1/2)^{2r}f_\ell^2<+\infty\right\},$$

endowed with the Fréchet topology induced by the norms $(\|\cdot\|_r)_{r\in\mathbb{Q}}$. As a corollary to the Bochner-Minlos theorem, one has that if the covariance $\check{\mathcal{C}}_{t_0}$ is continuous in the norm associated with some ς_r, then the associated Gaussian measure μ_{t_0} has support on any set of the form [7]

$$\left\{f\;|\;\sum_{\ell=0}^{\infty}(\ell+1/2)^{-2r-1-2\epsilon}f_\ell^2<+\infty\,,\;\epsilon>0\right\}\subset\bigcup_{r\in\mathbb{Q}}\varsigma_r=\varsigma'\,, \tag{3.17}$$

where ς' is the topological dual of ς.[3] In particular, given the asymptotic behavior of the z_ℓ functions (2.73), it is straightforward to check the continuity in the norm corresponding to $r=-1/2$, i.e.,

$$\langle f,\mathcal{C}(t_0)f\rangle\leq N(t_0)\sum_{\ell=0}^{\infty}(\ell+1/2)^{-1}f_\ell^2$$

[3]Here, $g\in\varsigma'$ is associated with the linear functional $L_g(f):=\sum_{\ell=0}^\infty f_\ell g_\ell$, $f\in\varsigma$.

for a certain constant $N(t_0) \in \mathbb{R}_+$. According to this, the measure μ_{t_0} is concentrated on the set (3.17) for $r = -1/2$, which can be identified with the topological dual $\mathfrak{h}'_\epsilon$ of the subspace of symmetric functions in the Sobolev space[4] $H^\epsilon(\mathbb{S}^2)$, for any $\epsilon > 0$,

$$\mathfrak{h}_\epsilon := \Big\{ f \in H^\epsilon(\mathbb{S}^2) \;\Big|\; \mathcal{L}_\sigma f = 0\,,\; \|f\|_\epsilon^2 := \sum_{\ell=0}^{\infty} (\ell + 1/2)^{2\epsilon} f_\ell^2 < +\infty \Big\}\,,\;\; \epsilon > 0\,,$$

where f_ℓ are the Fourier coefficients of the function f. We then conclude that the typical field configurations are not as singular as the delta functions or their derivatives. Note, however, that the subset $\mathfrak{b} \subset \mathfrak{h}'_\epsilon$ of symmetric $L^2(\mathbb{S}^2)$ functions has also measure zero. Indeed, consider the characteristic function $\chi_{\mathfrak{b}}$ of the measurable set $\mathfrak{b}$, defined by

$$\chi_{\mathfrak{b}}[\tilde{Q}] := \lim_{\alpha \to +0} \exp\left(-\alpha \sum_{\ell=0}^{\infty} \tilde{Q}_\ell^2 \right), \tag{3.18}$$

so that $\chi_{\mathfrak{b}}[\tilde{Q}] = 1$, for $\tilde{Q} \in \mathfrak{b}$, vanishing anywhere else. Making use of the restriction (3.16) and applying the Lebesgue monotone convergence theorem it is straightforward to obtain

$$\mu_{t_0}(\mathfrak{b}) = \int_{\mathscr{S}'} \chi_{\mathfrak{b}}[\tilde{Q}]\, \mathrm{d}\mu_{t_0}[\tilde{Q}] = \lim_{\alpha \to +0} \lim_{n \to +\infty} \prod_{\ell=0}^{n} \frac{1}{\sqrt{1 + 2\alpha |z_\ell(t_0)|^2}}\,. \tag{3.19}$$

The limit of the product vanishes as $n \to +\infty$ due to the nonconvergence of the series $\sum_{\ell=0}^{\infty} \log(1 + 2\alpha |z_\ell(t_0)|^2)$, and hence $\mu_{t_0}(\mathfrak{b}) = 0$. Since $\mathscr{S} \hookrightarrow \mathfrak{b}$, we have that, as usual for a field theory, the μ_{t_0}-measure is not supported on the classical configuration space $\mathscr{S}$. This is precisely the reason why a suitable distributional extension of $\mathscr{S}$ must be chosen as measure space in order to construct the L^2 space for the Schrödinger representation.

Finally, note that the Bochner-Minlos theorem (see *Theorem 3.1.1*) gives the support of the measure as a linear subspace of the original measure space. In order to find a finer (nonlinear) characterization of this support, one can apply the methods developed in [8] for countable products of Gaussian measures. According to that reference, given a sequence $\{\Delta_k\}$, $\Delta_k > 1$, $k = 1, 2, \ldots$, the μ_{t_0}-measure of the set

$$Z_{t_0}(\{\Delta_k\}) := \Big\{ \tilde{Q} \in \mathscr{S}' \mid \exists\, N \in \mathbb{N} \text{ s.t. } |\tilde{Q}_\ell| < |z_\ell(t_0)| \sqrt{2 \log \Delta_\ell}\,,\;\; \text{for } \ell \geq N \Big\}$$

is one (resp. zero) if $\sum_k 1/(\Delta_k \sqrt{\log \Delta_k})$ converges (resp. diverges). Concretely, this condition is satisfied for $\Delta_\ell^{(\alpha)} := (1 + \ell)^\alpha$, with $\alpha > 1$, whereas it is not verified for the same sequence with $\alpha = 1$. Thus, $\mu_{t_0}(Z_{t_0}(\{\Delta_\ell^{(\alpha)}\})) = 1$ for $\alpha > 1$, and the measure vanishes on the set corresponding to $\alpha = 1$.

[4] This is, $H^\epsilon(\mathbb{S}^2) = \big\{ f \in L^2(\mathbb{S}^2) \mid \|f\|_\epsilon^2 = \sum_\ell (\ell + 1/2)^{2\epsilon} \sum_{m=-\ell}^{\ell} f_{\ell m}^2 < +\infty \big\}$, where the spherical Fourier transform $f \mapsto f_{\ell m}$ is defined as $f_{\ell m} := \int_{\mathbb{S}^2} |\gamma|^{1/2} f(s) \overline{Y}_{\ell m}(s)$.

3.2 Canonical commutation relations

Next, we will obtain the representation of the basic momentum observables following the discussion developed in [1], adapted here to our definitions and conventions. We will realize that both the representation of the momentum operator and the choice of the μ_{t_0} measure are interrelated, in the sense that the information on the complex structure $J_{\mathcal{P}}$ used to construct the Fock representation is encoded in both of them. We start by computing the expectation value

$$\begin{aligned}\varpi_{t_0}(W(\lambda))|_{\lambda=(-g,f)} &= \left\langle \Psi_0^{(t_0)} \right| \exp\Big(i\big(\hat{Q}_{t_0}[f]+\hat{P}_{t_0}[g]\big)\Big)\, \Psi_0^{(t_0)} \big\rangle_{\mathscr{H}_s(t_0)} \\ &= \exp\left(\frac{i}{2}\langle f,g\rangle\right) \left\langle \Psi_0^{(t_0)} \right| \exp\Big(i\hat{Q}_{t_0}[f]\Big) \exp\Big(i\hat{P}_{t_0}[g]\Big)\, \Psi_0^{(t_0)} \big\rangle_{\mathscr{H}_s(t_0)} ,\end{aligned}$$

where we have used the BCH relation to separate operators. We take the general expression

$$\Big(\hat{P}_{t_0}[g]\Psi\Big)[\tilde{Q}] = -i(D_{\tilde{Q}}\Psi)[g] - i\tilde{Q}\,(M(t_0)g)\,\Psi[\tilde{Q}]\,,$$

consisting of the expected directional derivative of the functional $\Psi\in\mathscr{D}_{\hat{P}_{t_0}[g]}\subset\mathscr{H}_s(t_0)$ in the direction defined by $\tilde{Q}\in\mathscr{S}'$ (this will acquire a definite sense in terms of the modes $\tilde{Q}_\ell$) plus an extra linear multiplicative term. Now, we must determine the expression of the new operator $M(t_0):\mathscr{S}\to\mathscr{S}$. Taking into account that for Gaussian measures the vacuum state is a constant functional, and using again the BCH formula, it is straightforward to obtain

$$\begin{aligned}\varpi_{t_0}(W(\lambda))|_{\lambda=(-g,f)} &= \exp\left(\frac{i}{2}\langle f,g\rangle - \frac{1}{2}\langle g, M(t_0)g\rangle\right)\int_{\mathscr{S}'} e^{i\tilde{Q}(f-iM(t_0)g)}\mathrm{d}\mu_{t_0}[\tilde{Q}] \\ &= \exp\left(\frac{i}{2}\langle f,g\rangle - \frac{1}{2}\langle g, M(t_0)g\rangle\right)\exp\Big(\frac{1}{4}\big(\langle f,B(t_0)f\rangle \\ &\quad -\langle M(t_0)g, B(t_0)M(t_0)g\rangle - 2i\langle f, B(t_0)M(t_0)g\rangle\big)\Big)\,,\end{aligned}$$

where we have used the generating function definition (3.15) and also the relation $\langle M(t_0)g, B(t_0)f\rangle = \langle f, B(t_0)M(t_0)g\rangle$. The left hand side of the above equation can be easily calculated by using the expressions (3.8) and (3.11), as well as the relation $\langle f, A(t_0)g\rangle = -\langle g, C(t_0)f\rangle$,

$$\varpi_{t_0}(W(\lambda))|_{\lambda=(-g,f)} = \exp\left(\frac{1}{4}\big(\langle f,B(t_0)f\rangle - \langle g, D(t_0)g\rangle - 2\langle f, A(t_0)g\rangle\big)\right).$$

A simple comparison between the two expressions obtained for $\varpi_{t_0}(W(\lambda))$, $\lambda=(-g,f)\in\mathbf{P}$, leads us to conclude that, for all $f,g\in\mathscr{S}$,

$$\begin{aligned}\langle f, A(t_0)g\rangle &= -i\langle f,g\rangle + i\langle M(t_0)g, B(t_0)f\rangle\,, &(3.20)\\ \langle g, D(t_0)g\rangle &= -2\langle g, M(t_0)g\rangle + \langle M(t_0)g, B(t_0)M(t_0)g\rangle\,. &(3.21)\end{aligned}$$

From (3.20) we finally obtain

$$M(t_0) = B^{-1}(t_0)\big(\mathbf{1} - iA(t_0)\big)\,,$$

whereas (3.21) simply becomes a consistency relation. Therefore, the representation of the momentum observable is given by

$$\begin{aligned}&\pi_s(t_0)\cdot W(\lambda)|_{\lambda=(-g,0)} = \exp(i\hat{P}_{t_0}[g])\,,\\ &\left(\hat{P}_{t_0}[g]\Psi\right)[\tilde{Q}] = -i(D_{\tilde{Q}}\Psi)[g] - i\tilde{Q}\left(B^{-1}(t_0)(\mathbf{1} - iA(t_0))g\right)\Psi[\tilde{Q}]\,. \end{aligned}\tag{3.22}$$

Note that the unusual multiplicative term depends both on the measure μ_{t_0} –uniquely characterized by the operator $B(t_0)$– and the operator $A(t_0)$. It guarantees that the momentum operator is symmetric with respect to the inner product $\langle\cdot|\cdot\rangle_{\mathscr{H}_s(t_0)}$. Indeed, just by using the Gaussian integration by parts formula

$$\int_{\mathscr{S}'}(D_{\tilde{Q}}\Psi)[f]\,\mathrm{d}\mu_{t_0}[\tilde{Q}] = \int_{\mathscr{S}'}\tilde{Q}(\mathcal{C}^{-1}(t_0)f)\Psi[\tilde{Q}]\,\mathrm{d}\mu_{t_0}[\tilde{Q}]\,,$$

that can be easily deduced from (3.16), we obtain

$$\begin{aligned}\big\langle\Phi\,\big|\,\hat{P}_{t_0}[g]\Psi\big\rangle_{\mathscr{H}_s(t_0)} &= i\big\langle(D_{\tilde{Q}}\Phi)[g]\,\big|\,\Psi\big\rangle_{\mathscr{H}_s(t_0)} + i\big\langle\Phi\,\big|\,\tilde{Q}\big(B^{-1}(t_0)(\mathbf{1}+iA(t_0))g\big)\Psi\big\rangle_{\mathscr{H}_s(t_0)}\\ &= i\big\langle(D_{\tilde{Q}}\Phi)[g] + \tilde{Q}\big(B^{-1}(t_0)(\mathbf{1}-iA(t_0))g\big)\Phi\,\big|\,\Psi\big\rangle_{\mathscr{H}_s(t_0)}\\ &= \big\langle\hat{P}_{t_0}[g]\Phi\,\big|\,\Psi\big\rangle_{\mathscr{H}_s(t_0)}\,,\ \ \forall\,\Phi,\Psi\in\mathscr{D}_{\hat{P}_{t_0}[g]}\,.\end{aligned}$$

Let us now denote $\hat{Q}_\ell(t_0) := \hat{Q}_{t_0}[Y_{\ell 0}]$ and $\hat{P}_\ell(t_0) := \hat{P}_{t_0}[Y_{\ell 0}]$, where the $\hat{Q}_{t_0}[f]$ operator has been defined in (3.12). By considering the normalization condition (2.48) and equation (3.10), we get

$$\big(B^{-1}(t_0)(\mathbf{1} - iA(t_0))Y_{\ell 0}\big)(s) = i\frac{\dot{\bar{z}}_\ell(t_0)}{\bar{z}_\ell(t_0)}Y_{\ell 0}(s)\,,$$

and, hence, we finally obtain

$$\hat{Q}_\ell(t_0)\Psi = \tilde{Q}_\ell\Psi\,,\quad \hat{P}_\ell(t_0)\Psi = -i\frac{\partial\Psi}{\partial\tilde{Q}_\ell} + \frac{\dot{\bar{z}}_\ell(t_0)}{\bar{z}_\ell(t_0)}\tilde{Q}_\ell\Psi\,,\tag{3.23}$$

where Ψ is a functional of the components $\tilde{Q}_\ell$. The canonical commutation relations $[\hat{Q}_\ell(t_0),\hat{P}_{\ell'}(t_0)] = i\delta(\ell,\ell')\hat{\mathbb{I}}$ and $[\hat{Q}_\ell(t_0),\hat{Q}_{\ell'}(t_0)] = 0 = [\hat{P}_\ell(t_0),\hat{P}_{\ell'}(t_0)]$ are obviously satisfied on the appropriate domains.

It is possible to relate the Fock and Schrödinger representations through the action of the annihilation and creation operators on wave functionals [1]. Making use of equations (3.7) and (3.23), we get

$$\hat{b}_\ell(t_0) = \bar{z}_\ell(t_0)\frac{\partial}{\partial\tilde{Q}_\ell}\,,\quad \hat{b}_\ell^\dagger(t_0) = -z_\ell(t_0)\frac{\partial}{\partial\tilde{Q}_\ell} + \frac{1}{\bar{z}_\ell(t_0)}\tilde{Q}_\ell\,.\tag{3.24}$$

In particular, the vacuum state is given by the unit constant functional (up to multiplicative phase)

$$\Psi_0^{(t_0)}[\tilde{Q}] = 1\,, \;\; \forall\, \tilde{Q} \in \mathscr{S}'\,.$$

There exists a map $\hat{V}_{t_0} : \mathscr{F}_+(\mathscr{H}_{\mathcal{P}}) \to \mathscr{H}_s(t_0)$ that unitarily connects the creation and annihilation operators of both representations [6]. Given the annihilation and creation operators associated with the modes $z_\ell Y_{\ell 0}$, $\hat{b}_\ell$ and $\hat{b}_\ell^\dagger$ respectively, the expressions (3.24) correspond to $\hat{V}_{t_0}\, \hat{b}_\ell\, \hat{V}_{t_0}^{-1}$ and $\hat{V}_{t_0}\, \hat{b}_\ell^\dagger\, \hat{V}_{t_0}^{-1}$, respectively. These relations, and the action $\Psi_0^{(t_0)} = \hat{V}_{t_0}|0\rangle_{\mathcal{P}}$ on the Fock vacuum state $|0\rangle_{\mathcal{P}} \in \mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$, univocally characterize the unitary transformation $\hat{V}_{t_0}$. The general procedure that we have followed guarantees the self-adjointness of the configuration and momentum operators in the Schrödinger representation. Indeed, the self-adjoint operators $\hat{Q}_{t_0}[f]$ and $\hat{P}_{t_0}[g]$ with dense domain in the Fock space $\mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$ corresponding to the fixed value $t = t_0$ (see equation (2.36)) are unitarily related to (3.12) and (3.22) through the unitary transformation $\hat{V}_{t_0}$.

Finally, the probabilistic interpretation of the models is given by the usual Born correspondence rules [9]: Given $f \in \mathscr{S}$, the theoretical probability that a measurement carried out in the pure state Ψ at a certain time to determine the value of $\tilde{Q}(f)$ will yield a result contained in the Borel set $\Delta \in \mathrm{Bor}(\mathbb{R})$ for some $\tilde{Q} \in \mathscr{S}'$ is given by

$$\mathrm{P}_\Psi^{\hat{Q}_{t_0}[f]}(\Delta) = \|\Psi\|_{\mathscr{H}_s(t_0)}^{-2} \big\langle \Psi \,\big|\, E^{\hat{Q}_{t_0}[f]}(\Delta)\Psi \big\rangle_{\mathscr{H}_s(t_0)} = \|\Psi\|_{\mathscr{H}_s(t_0)}^{-2} \int_{V_{f,\Delta}} \big|\Psi[\tilde{Q}]\big|^2 \,\mathrm{d}\mu_{t_0}[\tilde{Q}]\,, \tag{3.25}$$

where $E^{\hat{Q}_{t_0}[f]}(\Delta)$ is the spectral measure univocally associated with $\hat{Q}_{t_0}[f]$, defined by $\big(E^{\hat{Q}_{t_0}[f]}(\Delta)\Psi\big)[\tilde{Q}] = \chi_{V_{f,\Delta}}[\tilde{Q}]\,\Psi[\tilde{Q}]$, with $\chi_{V_{f,\Delta}}$ being the characteristic function of the measurable set $V_{f,\Delta} := \{\tilde{Q} \in \mathscr{S}' \,|\, \tilde{Q}(f) \in \Delta\} \in \sigma(\mathrm{Cyl}(\mathscr{S}'))$. Here, $\|\cdot\|_{\mathscr{H}_s(t_0)}$ denotes the norm associated with the inner product $\langle\cdot|\cdot\rangle_{\mathscr{H}_s(t_0)}$. According to this, the measure μ_{t_0} admits the following physical interpretation: It defines the probability measure (3.25) for the vacuum state $\Psi_0^{(t_0)}$.

3.3 Unitary equivalence of Schrödinger representations

Let us consider the symplectomorphism (2.13) $\tau_{(t_1,t_0)} := \mathfrak{I}_{t_1}^{-1} \circ \mathfrak{I}_{t_0} : \mathbf{P} \to \mathbf{P}$, $t_1 > t_0$, which implements the classical time evolution from the embedding $\iota_{t_0}(\mathbb{S}^2)$ to $\iota_{t_1}(\mathbb{S}^2)$ on the canonical phase space. It induces a one-parameter family of states on the Weyl algebra: Starting from the initial state ϖ_{t_0} defined in equation (3.11), the dynamical evolution in the algebraic formulation of the theory is given by $\varpi_{t_1} = \varpi_{t_0} \circ \alpha_{(t_1,t_0)}^{-1}$ in the Schrödinger picture, with $\alpha_{(t_1,t_0)} : \mathscr{W}(\Upsilon) \to \mathscr{W}(\Upsilon)$ being the $*$-automorphism univocally associated with the symplectic transformation $\tau_{(t_1,t_0)}$ defined by $\alpha_{(t_1,t_0)} \cdot W(\lambda) :=$

$W(\tau_{(t_1,t_0)}(\lambda))$. The evolved state ϖ_{t_1} acts on the elementary observables as

$$\varpi_{t_1}(W(\lambda)) = \exp\big(-\omega(J_{t_1}(\lambda),\lambda)/4\big)\,,$$

where the complex structure

$$J_{t_1} := \tau_{(t_1,t_0)} \circ J_{t_0} \circ \tau^{-1}_{(t_1,t_0)} = \mathfrak{I}^{-1}_{t_1} \circ J_{\mathcal{P}} \circ \mathfrak{I}_{t_1} : \mathbf{P} \to \mathbf{P}$$

defines the Schrödinger representation[5] $\mathscr{H}_s(t_1)$ corresponding to the time value t_1. The condition of unitary equivalence of Schrödinger representations corresponding to different values $t_0 < t_1$ of the time parameter clearly amounts to demanding the unitary implementability of the symplectic transformation $\tau_{(t_1,t_0)}$ in the $\mathscr{H}_s(t_0)$ representation. In that case, $J_{t_1} - J_{t_0}$ is a Hilbert-Schmidt operator in the one-particle Hilbert space constructed from J_{t_0} (or equivalently J_{t_1}), and there exists a unitary transformation $\hat{V}_{(t_1,t_0)} : \mathscr{H}_s(t_0) \to \mathscr{H}_s(t_1)$ mapping the configuration and momentum operators from one representation into the other, in such a way that

$$\begin{aligned} \hat{V}_{(t_1,t_0)}\,\hat{b}_\ell(t_0)\,\hat{V}^{-1}_{(t_1,t_0)} &= \alpha_\ell(t_1,t_0\,|\,z_\ell)\hat{b}_\ell(t_1) + \beta_\ell(t_1,t_0\,|\,z_\ell)\hat{b}^\dagger_\ell(t_1)\,, \\ \hat{V}_{(t_1,t_0)}\,\hat{b}^\dagger_\ell(t_0)\,\hat{V}^{-1}_{(t_1,t_0)} &= \bar{\beta}_\ell(t_1,t_0\,|\,z_\ell)\hat{b}_\ell(t_1) + \bar{\alpha}_\ell(t_1,t_0\,|\,z_\ell)\hat{b}^\dagger_\ell(t_1)\,, \end{aligned} \tag{3.26}$$

where

$$\alpha_\ell(t_1,t_0\,|\,z_\ell) := i\Big(\bar{z}_\ell(t_0)\dot{z}_\ell(t_1) - z_\ell(t_1)\dot{\bar{z}}_\ell(t_0)\Big),\quad \beta_\ell(t_1,t_0\,|\,z_\ell) := i\Big(\bar{z}_\ell(t_0)\dot{\bar{z}}_\ell(t_1) - \bar{z}_\ell(t_1)\dot{\bar{z}}_\ell(t_0)\Big).$$

This is precisely ensured by the square summability of the β_ℓ coefficients appearing in the Bogoliubov transformation (3.26), exactly the same condition that guarantees the unitary implementation of the quantum time evolution in the Fock space $\mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$. We then conclude that the unitarity of the quantum dynamics in the Fock representation guarantees the equivalence of the Schrödinger representations corresponding to different times t_0, t_1. The map $\hat{V}_{(t_1,t_0)} = \hat{V}_{t_1}\,\hat{U}(t_1,t_0)\,\hat{V}^{-1}_{t_0}$ relating them is completely characterized by the relations (3.26) and the action on the vacuum state $\Psi_0^{(t_0)} \in \mathscr{H}_s(t_0)$, given by

$$\Big(\hat{V}_{(t_1,t_0)}\Psi_0^{(t_0)}\Big)[\tilde{Q}] = \prod_{\ell=0}^{\infty} \frac{|z_\ell(t_1)|^{1/2}}{|z_\ell(t_0)|^{1/2}} \exp\left(-\frac{1}{2}\frac{\beta_\ell(t_1,t_0\,|\,z_\ell)}{\bar{z}_\ell(t_0)\bar{z}_\ell(t_1)}\tilde{Q}_\ell^2\right) \in \mathscr{H}_s(t_1)\,, \tag{3.27}$$

where we have used the fact that $\hat{b}_\ell(t_0)\Psi_0^{(t_0)} = 0$, $\forall\,\ell \in \mathbb{N}_0$, and the expressions (2.48), (3.24), and (3.26) to obtain the differential equations verified by this state; namely,

$$\partial\hat{V}_{(t_1,t_0)}\Psi_0^{(t_0)}/\partial\tilde{Q}_\ell = -\big(\beta_\ell(t_1,t_0\,|\,z_\ell)/\bar{z}_\ell(t_0)\bar{z}_\ell(t_1)\big)\tilde{Q}_\ell\hat{V}_{(t_1,t_0)}\Psi_0^{(t_0)}\,,\ \ \ell \in \mathbb{N}_0\,.$$

Equation (3.27) must be interpreted as the limit in the $\mathscr{H}_s(t_1)$-norm of the Cauchy sequence of normalized vectors $f_n \in \mathscr{H}_s(t_1)$ obtained by extending the product (3.27) to a finite integer $n \in \mathbb{N}$.

[5]Here, we will make a notational abuse and simply denote the triplet $\big(\mathscr{H}_s(t), \pi_s(t), \Psi_0^{(t)}\big)$ as $\mathscr{H}_s(t)$.

The mutual absolute continuity of any two Gaussian measures associated with different times $t_0, t_1 \in (0,\pi)$ is also verified, i.e., they have the same zero measure sets. This property requires that the operator $\mathcal{C}(t_1) - \mathcal{C}(t_0)$ is Hilbert-Schmidt [8, 10, 11], which is satisfied in our case. Indeed, it is straightforward to check that the sequence

$$\big(|z_\ell(t_1)|^2 - |z_\ell(t_0)|^2\big)_{\ell\in\mathbb{N}_0}$$

is square summable. In fact, it is possible to show that the equivalence of measures is a necessary condition for the unitary equivalence between Schrödinger representations, and that any possible unitary equivalence between them is of the form $\Psi \mapsto \big(\mathrm{d}\mu_{t_1}/\mathrm{d}\mu_{t_0}\big)^{1/2}\exp(iF)\Psi$, with $\mathrm{d}\mu_{t_1}/\mathrm{d}\mu_{t_0}$ denoting the Radon-Nikodym derivative of μ_{t_1} with respect to μ_{t_0} and F being a real functional [12].

On the contrary, for the original scalar field $\varphi = \xi/\sqrt{\sin t}$, for which the time evolution is not unitary, we get the nonequivalence of the representations obtained for different times, and also the impossibility of such continuity. In this case, the mutual singularity of measures can be expected, as proved for the vacuum Gowdy $\mathbb{T}^3$ model in [3]. This typifies the advantage of using the re-scaled fields making the quantum dynamics unitary, for in this case it is possible to obtain a unique (up to unitary equivalence) Schrödinger representation for these models and, as a direct consequence, the mutual absolute continuity of the measures corresponding to different times. Neither of these properties can be attained for the original variables. In this last situation, even if the failure of the unitarity of time evolution and the mutual singularity of measures are not serious obstacles for a suitable probabilistic interpretation of the models [3, 13], we must face the lack of uniqueness of the representation.

Note that the map $\hat{V}_{t_0} : \mathscr{F}_+(\mathscr{H}_{\mathcal{P}}) \to \mathscr{H}_s(t_0)$ introduced in subsection 3.2 does not connect the configuration and momentum operators of the Fock representation, $\hat{Q}_\ell(t) = z_\ell(t)\hat{b}_\ell + \bar{z}_\ell(t)\hat{b}_\ell^\dagger$ and $\hat{P}_\ell(t) = \dot{z}_\ell(t)\hat{b}_\ell + \dot{\bar{z}}_\ell(t)\hat{b}_\ell^\dagger$, respectively, with those of the Schrödinger one (except for $t = t_0$). However, owing to the unitary implementability of the dynamics, there exists also a unitary transformation $\hat{W}_{t_0}(t) : \mathscr{F}_+(\mathscr{H}_{\mathcal{P}}) \to \mathscr{H}_s(t_0)$, such that

$$\begin{aligned}
\hat{W}_{t_0}(t)\,\hat{b}_\ell\,\hat{W}_{t_0}^{-1}(t) &= \alpha_\ell(t,t_0\,|\,z_\ell)\hat{b}_\ell(t_0) + \beta_\ell(t,t_0\,|\,z_\ell)\hat{b}_\ell^\dagger(t_0)\,,\\
\hat{W}_{t_0}(t)\,\hat{b}_\ell^\dagger\,\hat{W}_{t_0}^{-1}(t) &= \bar{\beta}_\ell(t,t_0\,|\,z_\ell)\hat{b}_\ell(t_0) + \bar{\alpha}_\ell(t,t_0\,|\,z_\ell)\hat{b}_\ell^\dagger(t_0)\,,
\end{aligned}$$

relating these operators. In terms of the unitary evolution operator on $\mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$, we have $\hat{W}_{t_0}(t) = \hat{V}_{t_0}\,\hat{U}^{-1}(t,t_0)$. Finally, given the quantum Hamiltonian (2.79) in the Fock representation, with dense domain $\mathscr{D}_{\hat{H}_0(t)} \subset \mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$ spanned by the states with a finite number of particles, the corresponding operator in the $\mathscr{H}_s(t_0)$ representation is given by $\hat{W}_{t_0}(t)\,\hat{H}_0(t)\,\hat{W}_{t_0}^{-1}(t)$,

$$\frac{1}{2}\sum_{\ell=0}^{\infty}\left(-\frac{\partial^2}{\partial\tilde{Q}_\ell^2} - 2i\frac{\dot{\bar{z}}_\ell(t_0)}{\bar{z}_\ell(t_0)}\tilde{Q}_\ell\frac{\partial}{\partial\tilde{Q}_\ell} + \left(\frac{\dot{\bar{z}}_\ell^2(t_0)}{\bar{z}_\ell^2(t_0)} + \frac{1}{4}\big(1+\csc^2 t\big) + \ell(\ell+1)\right)\big(\tilde{Q}_\ell^2 - |z_\ell(t_0)|^2\big)\right),$$

modulo an irrelevant real term proportional to the identity. Note, by contrast, that the complex independent term appearing in the previous expression is necessary to ensure that the operator is self-adjoint. This Hamiltonian is defined in the dense subspace $\hat{W}_{t_0}(t)\mathscr{D}_{\hat{H}_0(t)} = \{\hat{W}_{t_0}(t)f \mid f \in \mathscr{D}_{\hat{H}_0(t)}\} \subset \mathscr{H}_s(t_0)$ generated by the cyclic vector $\hat{W}_{t_0}(t)|0\rangle_{\mathcal{P}} \in \mathscr{H}_s(t_0)$.

3.4 Unitary evolution operator

In this final section we provide a general procedure to obtain the unitary evolution operator $\hat{U}_{t_0}(t,t') : \mathscr{H}_s(t_0) \to \mathscr{H}_s(t_0)$ written explicitly in closed form in terms of the field and momentum operators. The strategy that we follow is to generalize the results already known for a single harmonic oscillator with time-dependent frequency to a system consisting of an infinite number of uncoupled harmonic oscillators [14, 15]. The reader is referred to *appendix D* for a detailed study of these topics. Analogously to the one-dimensional case, when the dynamics is unitarily implementable we define the time evolution propagator through the relation

$$\big(\hat{U}_{t_0}(t,t')\Psi\big)[\tilde{Q}] = \int_{\mathscr{S}'} K_{t_0}\big(\tilde{Q},t;\tilde{Q}',t'\big)\Psi[\tilde{Q}']\,\mathrm{d}\mu_{t_0}[\tilde{Q}']\,.$$

where a straightforward calculation formally provides[6]

$$\begin{aligned} K_{t_0}\big(\tilde{Q},t;\tilde{Q}',t'\big) &= \prod_{\ell=0}^{\infty}\sqrt{2\pi}|z_\ell(t_0)|\exp\left(\frac{i}{2}\left(\frac{\dot{z}_\ell(t_0)}{z_\ell(t_0)}\tilde{Q}_\ell'^2 - \frac{\dot{\bar{z}}_\ell(t_0)}{\bar{z}_\ell(t_0)}\tilde{Q}_\ell^2\right)\right) \\ &\times\; K_\ell\big(\tilde{Q}_\ell,t;\tilde{Q}_\ell',t'\big)\exp\left(-i\int_{t'}^{t}\mathrm{d}\tau\,\vartheta_\ell(\tau)\right), \end{aligned}$$

with K_ℓ denoting the well-known Feynman propagator (D.20) associated with the one-dimensional oscillator of squared frequency $\kappa_\ell(t) := \ell(\ell+1) + (1+\csc^2 t)/4$, written in terms of the $c_\ell(t,t')$ and $s_\ell(t,t')$ solutions to the equation of motion (2.47) (see equation (D.2) in *appendix D*). These functions are the unique solutions to (2.47) such that $c_\ell(t',t') = 1$, $\partial_t c_\ell(t',t') = 0$, $s_\ell(t',t') = 0$, and $\partial_t s_\ell(t',t') = 1$. They are given in terms of the associated Legendre functions by expressiones (D.51) in *appendix D*, substituting $\omega = \sqrt{\ell(\ell+1)}$. Finally, the term ϑ_ℓ comes from taking normal order in the quantum Hamiltonian; explicitly,

$$\vartheta_\ell(t) = -\frac{1}{2}\big(|\dot{z}_\ell(t_0)|^2 + \kappa_\ell(t)|z_\ell(t_0)|^2\big) \sim -\frac{\ell}{2} \quad \text{as} \quad \ell \to +\infty\,.$$

At first sight, the application of the techniques employed in *appendix D* for the single oscillator should allow us to factorize the evolution operator in the form

$$\hat{U}_{t_0}(t,t') = \hat{T}^{-1}_{t_0,\boldsymbol{\rho}}(t)\,\hat{R}_{t_0,\boldsymbol{\rho}}(t,t')\,\hat{T}_{t_0,\boldsymbol{\rho}}(t')\,, \tag{3.28}$$

[6] The reader may wish to compare this expression with equations (D.22) and (D.23) in *appendix D*.

where, given an *arbitrary* sequence $\boldsymbol{\rho}(t) = (\rho_\ell(t))_{\ell\in\mathbb{N}_0}$ of solutions to the auxiliary Ermakov-Pinney equations [16, 17]

$$\ddot{\rho}_\ell + \kappa_\ell(t)\rho_\ell = 1/\rho_\ell^3\,,$$

the $\hat{T}_{\boldsymbol{\rho}}(t)$ and $\hat{R}_{\boldsymbol{\rho}}(t,t')$ operators are univocally characterized up to phases by their action on annihilation and creation operators,

$$\begin{aligned}
\hat{T}^{-1}_{t_0,\boldsymbol{\rho}}(t)\,\hat{b}_\ell(t_0)\,\hat{T}_{t_0,\boldsymbol{\rho}}(t) &= i\left(\dot{z}_\ell(t_0)\bar{z}_\ell(t_0)\rho_\ell(t) - \frac{z_\ell(t_0)\dot{\bar{z}}_\ell(t_0)}{\rho_\ell(t)} - |z_\ell(t_0)|^2\dot{\rho}_\ell(t)\right)\hat{b}_\ell(t_0)\\
&+ i\left(\bar{z}_\ell(t_0)\dot{\bar{z}}_\ell(t_0)\Big(\rho_\ell(t) - \frac{1}{\rho_\ell(t)}\Big) - \bar{z}_\ell^2(t_0)\dot{\rho}_\ell(t)\right)\hat{b}^\dagger_\ell(t_0)\,,\\
\hat{R}^{-1}_{t_0,\boldsymbol{\rho}}(t,t')\,\hat{b}_\ell(t_0)\,\hat{R}_{t_0,\boldsymbol{\rho}}(t,t') &= \Big(\cos\gamma_\ell(t,t') - i(|z_\ell(t_0)|^2 + |\dot{z}_\ell(t_0)|^2)\sin\gamma_\ell(t,t')\Big)\hat{b}_\ell(t_0)\\
&- i(\bar{z}_\ell^2(t_0) + \dot{\bar{z}}_\ell^2(t_0))\sin\gamma_\ell(t,t')\hat{b}^\dagger_\ell(t_0)\,,
\end{aligned}$$

and similarly for $\hat{b}^\dagger_\ell(t_0)$. Here, we have denoted

$$\gamma_\ell(t,t') := \int_{t'}^{t}\frac{\mathrm{d}\tau}{\rho_\ell^2(\tau)}\,.$$

Nevertheless, even in the case of $\hat{U}_{t_0}(t,t')$ being well-defined as unitary operator, the factorization (3.28) is ill-defined. Indeed, the necessary and sufficient condition for $\hat{T}_{t_0,\boldsymbol{\rho}}(t)$ to be unitary for each value of t is given by

$$\sum_{\ell=0}^{\infty}\left|z_\ell(t_0)\dot{z}_\ell(t_0)\big(\rho_\ell(t) - 1/\rho_\ell(t)\big) - z_\ell^2(t_0)\dot{\rho}_\ell(t)\right|^2 < +\infty\,,\quad \forall\, t\in(0,\pi)\,. \tag{3.29}$$

Similarly, it is straightforward to show that $\hat{R}_{t_0,\boldsymbol{\rho}}(t,t_0)$ is unitarily implementable if and only if

$$\sum_{\ell=0}^{\infty}\left|(z_\ell^2(t_0) + \dot{z}_\ell^2(t_0))\sin\gamma_\ell(t,t')\right|^2 < +\infty\,,\quad \forall\, t,t_0\in(0,\pi)\,. \tag{3.30}$$

The asymptotic expansions (2.73) lead us to conclude that conditions (3.29) and (3.30) are not verified and, hence, neither $\hat{T}_{t_0,\boldsymbol{\rho}}(t)$ nor $\hat{R}_{t_0,\boldsymbol{\rho}}(t,t')$ are unitary for those systems. In the case of $\hat{R}_{t_0,\boldsymbol{\rho}}(t,t')$, this conclusion follows readily, irrespective of $\boldsymbol{\rho}(t)$. For $\hat{T}_{t_0,\boldsymbol{\rho}}(t)$, a necessary condition for (3.29) to be satisfied is given by

$$\sum_{\ell=0}^{\infty}|\rho_\ell(t) - 1/\rho_\ell(t)|^2 < +\infty \;\Leftrightarrow\; \lim_{\ell\to+\infty}\rho_\ell(t) = 1\,,\quad \forall\, t\in(0,\pi)\,,$$

where we have taken into account the fact that the real sequence $\boldsymbol{\rho}(t)$ is positive and bounded for all t. According to equation (D.12) in *appendix D*, this implies $s_\ell(t,t_0)\sim$

$\sin C(t,t_0)$ as $\ell \to +\infty$, where $C(t,t_0)$ is a *nonzero* function whose form we do not need to specify. This is in conflict with the asymptotic behavior of $s_\ell(t,t_0)$ for the systems under study, given by $s_\ell(t,t_0) \sim 0$ as $\ell \to +\infty$ for all $t,t_0 \in (0,\pi)$. In the context of the search of semiclassical states for the Gowdy models, the nonunitarity of the $\hat{T}_{t_0,\boldsymbol{\rho}}(t)$ operator makes it difficult to apply the techniques developed in *subsection D.3* of *appendix D* for a single time-dependent harmonic oscillator. This point will be discussed in depth in the conclusions of the thesis, where we will take advantage of the unitary implementability of the dynamics in order to define a family of coherent states for these systems. Obviously, this does not prevent us from defining other well-defined factorizations for $\hat{U}_{t_0}(t,t')$ different from (3.28). A particularly convenient choice is given by

$$\hat{U}_{t_0}(t,t') = \hat{\mathcal{D}}_{t_0,\boldsymbol{\rho}}(t,t')\,\hat{\mathcal{R}}_{t_0,\boldsymbol{\rho}}(t,t')\,\hat{\mathcal{S}}_{t_0,\boldsymbol{\rho}}(t,t')\,,$$

with

$$\begin{aligned}
\hat{\mathcal{D}}_{t_0,\boldsymbol{\rho}}(t,t') &:= \hat{D}^{-1}_{t_0,\boldsymbol{\rho}}(t)\,\hat{D}_{t_0\boldsymbol{\rho}}(t')\,,\\
\hat{\mathcal{S}}_{t_0,\boldsymbol{\rho}}(t,t') &:= \hat{D}^{-1}_{t_0,\boldsymbol{\rho}}(t')\,\hat{S}^{-1}_{t_0,\boldsymbol{\rho}}(t)\,\hat{T}_{t_0,\boldsymbol{\rho}}(t')\,,\\
\hat{\mathcal{R}}_{t_0,\boldsymbol{\rho}}(t,t') &:= \hat{T}^{-1}_{t_0,\boldsymbol{\rho}}(t')\,\hat{R}_{t_0,\boldsymbol{\rho}}(t,t')\,\hat{T}_{t_0,\boldsymbol{\rho}}(t')\,,
\end{aligned}$$

where $\hat{D}_{t_0,\boldsymbol{\rho}}(t)$ and $\hat{S}_{t_0,\boldsymbol{\rho}}(t)$ are displacement and squeeze operators of the type defined in *subsection D.2.2* of *appendix D*, in such a way that

$$\begin{aligned}
\hat{\mathcal{D}}^{-1}_{t_0,\boldsymbol{\rho}}(t,t')\,\hat{b}_\ell(t_0)\,\hat{\mathcal{D}}_{t_0,\boldsymbol{\rho}}(t,t') &= \left(1 + i|z_\ell(t_0)|^2\left(\frac{\dot{\rho}_\ell(t)}{\rho_\ell(t)} - \frac{\dot{\rho}_\ell(t')}{\rho_\ell(t')}\right)\right)\hat{b}_\ell(t_0)\\
&+ i\bar{z}_\ell^2(t_0)\left(\frac{\dot{\rho}_\ell(t)}{\rho_\ell(t)} - \frac{\dot{\rho}_\ell(t')}{\rho_\ell(t')}\right)\hat{b}^\dagger_\ell(t_0)\,,\\
\hat{\mathcal{S}}^{-1}_{t_0,\boldsymbol{\rho}}(t,t')\,\hat{b}_\ell(t_0)\,\hat{\mathcal{S}}_{t_0,\boldsymbol{\rho}}(t,t') &= i\Bigg(\dot{z}_\ell(t_0)\bar{z}_\ell(t_0)\frac{\rho_\ell(t')}{\rho_\ell(t)} - z_\ell(t_0)\dot{\bar{z}}_\ell(t_0)\frac{\rho_\ell(t)}{\rho_\ell(t')}\\
&+ |z_\ell(t_0)|^2\frac{\dot{\rho}_\ell(t')}{\rho_\ell(t')}\left(\frac{\rho_\ell(t)}{\rho_\ell(t')} - \frac{\rho_\ell(t')}{\rho_\ell(t)}\right)\Bigg)\hat{b}_\ell(t_0)\\
&+ i\bar{z}_\ell(t_0)\left(\bar{z}_\ell(t_0)\frac{\dot{\rho}_\ell(t')}{\rho_\ell(t')} - \dot{\bar{z}}_\ell(t_0)\right)\left(\frac{\rho_\ell(t)}{\rho_\ell(t')} - \frac{\rho_\ell(t')}{\rho_\ell(t)}\right)\hat{b}^\dagger_\ell(t_0)\,,
\end{aligned}$$

$$\begin{aligned}\hat{\mathcal{R}}^{-1}_{t_0\boldsymbol{\rho}}(t,t')\,\hat{b}_\ell(t_0)\,\hat{\mathcal{R}}_{t_0,\boldsymbol{\rho}}(t,t') &= \Bigg(\cos\gamma_\ell(t,t') + i\Bigg(\big(z_\ell(t_0)\dot{\bar{z}}_\ell(t_0) + \dot{z}_\ell(t_0)\bar{z}_\ell(t_0)\big)\dot{\rho}_\ell(t')\rho_\ell(t') \\ &- |z_\ell(t_0)|^2\left(\dot{\rho}_\ell^2(t') + \frac{1}{\rho_\ell^2(t')}\right) - |\dot{z}_\ell(t_0)|^2\rho_\ell^2(t')\Bigg) \\ &\times \sin\gamma_\ell(t,t')\Bigg)\,\hat{b}_\ell(t_0) + i\Bigg(2\bar{z}_\ell(t_0)\dot{\bar{z}}_\ell(t_0)\dot{\rho}_\ell(t')\rho_\ell(t') \\ &- \dot{\bar{z}}_\ell^2(t_0)\rho_\ell^2(t') - \bar{z}_\ell^2(t_0)\left(\dot{\rho}_\ell^2(t') + \frac{1}{\rho_\ell^2(t')}\right)\Bigg)\sin\gamma_\ell(t,t')\,\hat{b}_\ell^\dagger(t_0)\,,\end{aligned}$$

and similarly for $\hat{b}_\ell^\dagger(t_0)$. Here, the solutions ρ_ℓ to the Ermakov-Pinney equations are conveniently selected as

$$\rho_\ell(t) = \sqrt{\frac{\sin t}{2}\left(\pi\mathscr{P}_\ell^2(\cos t) + \frac{4}{\pi}\mathscr{Q}_\ell^2(\cos t)\right)}\,,\quad \ell\in\mathbb{N}_0\,, \tag{3.31}$$

with the asymptotic expansions

$$\rho_\ell(t) = 1/\sqrt{|\ell|} + O\big(|\ell|^{-3/2}\big)\,,\quad \dot{\rho}_\ell(t) = C(t)/|\ell|^{5/2} + O\big(|\ell|^{-7/2}\big)\,,$$

as $\ell\to+\infty$. Here, $C(t)$ is a function of time whose form we do not need to specify. Recall that the unitary evolution operator does not depend on the concrete choice of $\boldsymbol{\rho}$. The election (3.31) is motivated by the fact that the usual ρ_ℓ solutions to the Ermakov-Pinney equations for Minkowskian free scalar fields evolving in a spacetime $\mathbb{R}\times\mathbb{T}^3$ with closed spatial sections are, precisely, $\rho_\ell(t) = 1/\sqrt{|\ell|}$, $\ell\in\mathbb{Z}\setminus\{0\}$. In this way, the functions z_ℓ and $\dot{z}_\ell$ (2.73), as well as ρ_ℓ, approach those corresponding to the free Minkowskian system at high frequencies, for which the evolution is well defined and unitary. It is straightforward to check the unitary implementability of the above transformations in the Hilbert space $\mathscr{H}_s(t_0)$.

References

1 A. Corichi, J. Cortez, and H. Quevedo, Phys. Rev. D **66**, 085025 (2002); Class. Quant. Grav. **20**, L83 (2003); Annals Phys. **313**, 446478 (2004).

2 R. M. Wald, *Quantum Field Theory in Curved Spacetime and Black Hole Thermodynamics*, The University of Chicago Press, USA (1994).

3 C. G. Torre, Class. Quant. Grav. **24**, 1 (2007).

4 D. A. Dubin and M. A. Hennings, *Quantum Mechanics, Algebras and Distributions*, Longman Scientific & Technical (1990).

5 A. Ashtekar and A. Magnon, Proc. Roy. Soc. Lond. A**346**, 375 (1975).

6 J. Glimm and A. Jaffe, *Quantum Physics. A Functional Integral Point of View* (Second Edition), Springer (1984).

7 B. Simon, *Functional Integration and Quantum Physics*, Academic Press, New York, (1974).

8 J. M. Mourão, T. Thiemann, and J. M. Velhinho, J. Math. Phys. **40**, 2337 (1999).

9 E. Prugovečki, *Quantum Mechanics in Hilbert Space* (Second Edition), Academic Press, New York, (1981).

10 B. Simon, *The* $P(\phi)_2$ *Euclidean (Quantum) Field Theory*, Princeton University Press, Princeton, NJ, (1974).

11 Y. Yamasaki, *Measures on Infinite Dimensional Spaces*, World Scientific, Singapure, (1985).

12 A. Corichi, J. Cortez, G. A. Mena Marugán, and J. M. Velhinho, Phys. Rev. D **76**, 124031 (2007).

13 C. G. Torre, Phys. Rev. D **66**, 084017 (2002).

14 H. R. Lewis Jr. and W. B. Riesenfeld, J. Math. Phys. **10**, 1458 (1969).

15 M. Fernández Guasti and H. Moya-Cessa, J. Phys. A **36**, 2069 (2003).

16 V. P. Ermakov, Univ. Izv. Kiev. **20**, 1 (1880); see Appl. Anal. Discrete Math. **2**, 123-145 (2008) for an English translation of Ermakov's original paper.

17 E. Pinney, Proc. Am. Math. Soc. **1**, 681 (1950).

Conclusions

Throughout this thesis, we have studied the linearly polarized $\mathbb{S}^1 \times \mathbb{S}^2$ and $\mathbb{S}^3$ Gowdy models coupled to massless scalar fields in a rigorous and self-contained way, paying special attention to the mathematical aspects of their classical formulations and exact quantizations. Concretely, we have carefully applied modern (symplectic) differential-geometric techniques to the description of these dynamical systems. The presence of both initial and final singularities, as well as the inhomogeneity and anisotropy of space, justify the great interest in these models. Firstly, in *Chapter 1*, we have analyzed their Hamiltonian formalism as a necessary first step towards their quantization by gauge fixing and deparameterization.[7] After performing a Geroch symmetry reduction and an appropriate conformal transformation, these models can be interpreted as (1+2)-dimensional gravity systems coupled to a set of massless scalar fields with axial symmetry. As analyzed in this chapter, the description of these models requires a careful discussion of the regularity conditions that the metric must satisfy on the symmetry axis. These conditions give rise to the so-called *polar constraints*, which are shown to be first class and necessary to guarantee the differentiability of the other constraints present in the models.

An important issue to analyze on this type of cosmological models is the so-called *problem of time* in general relativity. Since there are not preferred foliations of the space-time, one has to consider all of them jointly with the aim of satisfying the principle of general covariance. As a consequence, the well-known Hamiltonian constraint is directly obtained within the canonical ADM formalism of the theory. In the case of a closed universe, the time evolution is purely gauge and the Hamiltonian of the system is restricted to vanish on the physical phase space. Thus, in order to recover the dynamics, one has to apply some *ad hoc* procedure such as deparameterization, based on a partial gauge fixation of the system. Obviously, different deparameterizations give rise in general to nonequivalent quantum theories. In our case, by imposing gauge fixing conditions similar to those employed in the literature for the familiar 3-torus case, and after a suitable series of canonical transformations suggested by very simple gauge transformations verified by some natural variables, one arrives at a reduced phase-space description where the dynamics of the systems is governed by nonautonomous quadratic Hamiltonians

[7] In addition, our study would allow us to follow other roads to quantization such as the viewpoint pioneered by M. Varadarajan in [1].

depending on a time parameter $t \in (0, \pi)$. The function $\sin t$ in their denominators explicitly shows that both initial and final singularities are present in these models. This is in contrast with the 3-torus case, where only an initial (or final) singularity appears. The usefulness of the deparameterization employed in this text consists in encoding the local degrees of freedom of the systems in massless scalar fields evolving in the *same* fixed background spacetime, conformal to the Einstein metric on $(0, \pi) \times \mathbb{S}^2$, so that one can apply standard techniques of QFT in order to exactly quantize the models. In this context, the time singularities of the metric are described by the time-conformal factor, given again by the function $\sin t$, so that the metric becomes singular whenever it cancels.

An interesting feature of both the 3-handle and the 3-sphere models is the fact that after deparameterization there are no constraints left, so that they can be completely described by the time-dependent Hamiltonian. This is again in contrast with the situation for the 3-torus topology where, in addition to the dynamics generated by the nonautonomous Hamiltonian, there is an extra $U(1)$ symmetry generated by a residual global constraint that must be appropriately taken into account.

In *Chapter 2*, we have studied the Fock quantization of the models. Concretely, we have focused our attention on the problem of unitarily implementing the quantum time evolution. It is expedient to tackle this roblem within the algebraic formalism of QFT. As a first result, we have proved the impossibility to get unitary dynamics when the systems are written in terms of their original variables, irrespectively of the $SO(3)$-invariant complex structures adapted to the round $\mathbb{S}^2$ background used to construct the symmetric Fock spaces. This result generalizes the conclusion reached in [2] for the 3-torus case to the topologies under consideration in this thesis. The lack of unitary dynamics could certainly lead us to conclude that the models quantized in this way are not physically acceptable. However, one may adopt the point of view proposed in [3] and [4] according to which these nonunitary Heisenberg formulations, though pathological in other respects, remain physically viable thanks to the fact that some relevant quantum observables can be described as self-adjoint operators and, hence, their probability interpretations are safe. Indeed, this is the case for the field and momentum operators, and also for the quantum Hamiltonian which is self-adjoint for each value of the time parameter.[8] Nevertheless, it is possible to overcome the failure of dynamics to be unitarily implemented by performing a suitable time-dependent redefinition of the fields at the Lagrangian level involving *precisely* the conformal factor $\sin t$ mentioned above. Furthermore, by demanding the unitarity of the dynamics and invariance under the $SO(3)$ symmetry associated with the background metric, the existence of a unique (up to unitary equivalence) Fock representation can be easily proved for these systems.

It is important to point out that this method, successfully applied to the Gowdy

[8]Recall that the dynamics does not generate a one-parameter symplectic group on the phase space for these models. Due to this fact, Stone's theorem does not apply and the existence of a self-adjoint Hamiltonian is not in conflict with the absence of unitary time evolution.

models in order to obtain unitary dynamics, is not of general validity and cannot be generalized to other highly symmetric spacetime backgrounds. Consider, for instance, the case of a massless scalar field evolving in a fixed de Sitter background. As shown in reference [5], it is impossible to find a time-dependent conformal redefinition of the field leading to a unitary implementation of the dynamics on any Fock space built from an $SO(4)$-symmetric complex structure. The ultimate reason that the method employed in the Gowdy models does not work in this case is the fact that the time-dependent potential terms appearing in the equations of motion after the field redefinitions are not as well behaved as the ones that show up in the treatment of the Gowdy models. A common situation in this case is that the field ends up verifying a Klein-Gordon equation with a *tachyonic* time-dependent mass term.

Finally, *Chapter 3* has been devoted to the construction of the Schrödinger representation for the 3-handle and 3-sphere Gowdy models, completing in this way the quantization of these systems previously performed within the Fock scheme. Here, the Hilbert space takes the form of a L^2 probability space of tempered distributions on the 2-sphere, endowed with a time-dependent Gaussian measure, whose support is analyzed by applying the Bochner-Minlos theorem. In particular, we have shown that the interrelation between measure theory and representation of quantum operators involves the appearance of unusual linear multiplicative terms in the momentum operators.

It is important in this context to highlight the advantage of using the re-scaled fields that make the quantum dynamics unitary. In this case, the Schrödinger representations corresponding to different values of the time parameter are unitarily equivalent. This guarantees at the same time the mutual absolute continuity of the corresponding measures.

As far as the support of the measure or the unitary implementability of the dynamics are concerned, the discussions and results obtained for these models are analogous to those found for the vacuum 3-torus model in [6] and [7]. It could be argued that this similarity is somehow expected owing to the fact that the critical features of these systems are determined by their ultraviolet behaviors, and these should not be sensitive to the topology of the spacetimes. This argument can be found, for instance, in [8] concerning the simplest generalization of Minkowski space quantum field theory to the $\mathbb{R} \times \mathbb{T}^3$ spacetime with closed spatial sections. This compactification can modify the long-wavelength behavior of the system, but not the ultraviolet one, so that both spacetimes suffer from the same ultraviolet divergence properties. Such statement is clearly intuitive, but it is not obvious to what extent it is also true for quantum field theories in non-locally isometric spacetimes, like those corresponding to the Gowdy models. In this respect, the similarity of the results is probably due to the similar structure of the differential equations verified by the mode functions.

The final issue discussed in this chapter is the construction of the unitary evolution operator, written explicitly in closed form in terms of the field and momentum operators. Although the resulting operator has been calculated in the restricted context of the Schrödinger quantization, it is clear that this study remains valid for other faithful representations of the Weyl algebra, offering the possibility to explore different choices for the quantization of the systems such as the polymer one [9].

We will conclude by commenting some open problems and questions that will be tackled elsewhere. To this end, let us first probe the existence of semiclassical states for the models under consideration. As shown in *appendix D*, the explicit expression of the quantum unitary evolution for the single harmonic oscillator as a product of unitary operators turns out to be very useful to construct semiclassical states for some relevant one-dimensional dynamical systems (including Gowdy-type oscillators). However, there are obstructions that arise when dealing with systems of infinite oscillators –particularly, the nonunitarity of the $T_{\boldsymbol{\rho}}(t)$ operator (see *section 3.4* in *Chapter 3*)–, making the application of the techniques developed in *appendix D* particularly difficult. In order to avoid these difficulties, we will probe an alternative procedure to construct semiclassical states that takes advantage of the unitary implementability of the quantum time evolution. We start by constructing the analogs of the minimal wave packets of the one-dimensional harmonic oscillator (see for example [10]). In what follows, we will assume the use of a complex structure $J_{\mathcal{P}}$ such that the dynamics is unitarily implementable on the associated symmetric Fock space $\mathscr{F}_+(\mathscr{H}_{\mathcal{P}})$ (see *Chapter 2*). Given a square summable sequence $\mathbf{C} := (C_\ell)_{\ell\in\mathbb{N}_0} \in \ell^2(\mathbb{C})$ belonging to the one-particle Hilbert space, consider the state

$$|\mathbf{C}\rangle = \mathrm{e}^{-\|\mathbf{C}\|^2/2}\exp\left(\sum_{\ell=0}^{\infty} C_\ell \hat{b}_\ell^\dagger\right)|0\rangle_{\mathcal{P}}\,,$$

where $|0\rangle_{\mathcal{P}}$ is the vacuum state, corresponding in this context to $\mathbf{C}=\mathbf{0}$, and $\|\mathbf{C}\|^2 = \sum_{\ell=0}^{\infty}|C_\ell|^2$. Vectors defined in this way appear as coherent superpositions of states with arbitrary number of particles. Let $\hat{U}(t,t_0)$ be the unitary evolution operator in the Fock representation, with $t_0\in(0,\pi)$ being a fixed initial value of the time parameter. We can now introduce the annihilation and creation operators in the Heisenberg picture corresponding to evolution *backwards* in time,

$$\begin{aligned}
\hat{\mathfrak{b}}_\ell(t_0,t) &:= \hat{U}(t,t_0)\,\hat{b}_\ell\,\hat{U}^{-1}(t,t_0) = \bar{\alpha}_\ell(t,t_0|z_\ell)\hat{b}_\ell - \beta_\ell(t,t_0|z_\ell)\hat{b}_\ell^\dagger\,,\\
\hat{\mathfrak{b}}_\ell^\dagger(t_0,t) &:= \hat{U}(t,t_0)\,\hat{b}_\ell^\dagger\,\hat{U}^{-1}(t,t_0) = -\bar{\beta}_\ell(t,t_0|z_\ell)\hat{b}_\ell + \alpha_\ell(t,t_0|z_\ell)\hat{b}_\ell^\dagger\,,
\end{aligned}$$

satisfying the Heisenberg algebra for all $t,t_0\in(0,\pi)$. Here, α_ℓ and β_ℓ are the Bogoliubov coefficients appearing in equation (3.26) of *Chapter 3*. We then evolve the $|\mathbf{C}\rangle$ states in the Schrödinger picture to obtain

$$\begin{aligned}
|\mathbf{C};t,t_0\rangle := \hat{U}(t,t_0)|\mathbf{C}\rangle &= e^{-\|\mathbf{C}\|^2/2}\hat{U}(t,t_0)\exp\left(\sum_{\ell=0}^{\infty} C_\ell\hat{b}_\ell^\dagger\right)|0\rangle_{\mathcal{P}}\\
&= e^{-\|\mathbf{C}\|^2/2}\exp\left(\sum_{\ell=0}^{\infty} C_\ell\hat{\mathfrak{b}}_\ell^\dagger(t_0,t)\right)|0;t,t_0\rangle_{\mathcal{P}}\,,
\end{aligned}$$

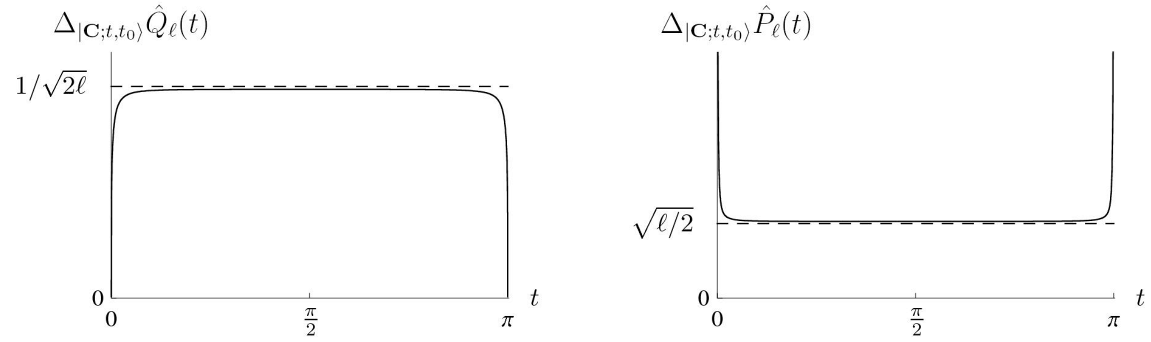

Figure 3.1: Asymptotic behavior of the variances of the field and momentum operators $\hat{Q}_\ell(t)$ and $\hat{P}_\ell(t)$ in the states $|\mathbf{C};t,t_0\rangle$, $t,t_0\in(0,\pi)$, at high frequencies. These graphics can be considered as the limit of *figure D.2* in *appendix D* when $\ell\to+\infty$.

with $\hat{\mathfrak{b}}_\ell(t_0,t)|\mathbf{C};t,t_0\rangle=C_\ell|\mathbf{C};t,t_0\rangle$, $\forall\,\ell\in\mathbb{N}_0$, and $|0;t,t_0\rangle_{\mathcal{P}}:=\hat{U}(t,t_0)|0\rangle_{\mathcal{P}}$. By definition, the one-parameter family of states obtained in this way verifies the Schrödinger equation with initial condition $|\mathbf{C};t_0,t_0\rangle=|\mathbf{C}\rangle$, and is closed under time evolution as well, $\hat{U}(t_2,t_1)|\mathbf{C};t_1,t_0\rangle=|\mathbf{C};t_2,t_0\rangle$. We can now calculate the uncertainties for the field and momentum operators in the $|\mathbf{C};t,t_0\rangle$ states. We easily obtain (see *figure 3.1*)

$$\begin{aligned}\Delta_{|\mathbf{C};t,t_0\rangle}\hat{Q}_\ell(t) &= \big|z_\ell(t)\alpha_\ell(t,t_0\,|\,z_\ell)+\bar{z}_\ell(t)\bar{\beta}_\ell(t,t_0\,|\,z_\ell)\big|\sim\frac{1}{\sqrt{2\ell}}\quad\text{when}\quad\ell\to+\infty\,,\\ \Delta_{|\mathbf{C};t,t_0\rangle}\hat{P}_\ell(t) &= \big|\dot{z}_\ell(t)\alpha_\ell(t,t_0\,|\,z_\ell)+\dot{\bar{z}}_\ell(t)\bar{\beta}_\ell(t,t_0\,|\,z_\ell)\big|\sim\sqrt{\frac{\ell}{2}}\quad\text{when}\quad\ell\to+\infty\,,\end{aligned}$$

where, for fixed values of t_0, these asymptotic behaviors converge uniformly in t for time intervals away from the classical singularities at $t=0$ and $t=\pi$. We then conclude that the $|\mathbf{C};t,t_0\rangle$ vectors are states of minimum uncertainty far enough from the singularities. They can be used to probe the existence of large quantum gravity effects in several ways. For instance, one may construct suitable regularized operators to represent the (3- or 4-dimensional) metric of these models by using arguments similar to those employed in the linearly polarized Einstein-Rosen waves [11, 12] and the Schmidt model [13] (see the *Table 1* in the *Introduction* to this thesis). Calculating the expectation values of these operators in the coherent states, one may deduce the additional conditions (if any) that the sequences $\mathbf{C}\in\ell^2(\mathbb{C})$ should satisfy in order to admit an approximate classical behavior. In this respect, it would be important to analyze if the metric quantum fluctuation are relevant for all states.

In addition, one may proceed as in [14] for the 3-torus case by appropriately promoting the quadratic invariant ${}^{(4)}R_{abcd}{}^{(4)}R^{abcd}$ into a quantum mechanical operator. According to that reference, one should be able to unambiguously fix the operator order by requiring that the expectation values of this quantity in the coherent states exactly reproduce the classical results far from the singularities. In analogy with the results of [14], even if the expectation values in other states (such as linear combinations of coherent states) give nonclassical results, it is expected that the classical singularities persist in all cases. This physical consideration is supported by the purely quantum behavior of the uncertainties of the field and momentum operators in the coherent states at the classical spacetime singularities.

As a natural extension of the work developed in this thesis, it would be interesting to couple gravity to different types of matter, for instance to electromagnetic fields [15], and find out if it is still possible to exactly solve the resulting systems. In this case, the dynamics is expected to be entirely described by the transverse part of the gravitational field and the components of the electromagnetic vector potential coupled in a nonlinear way. This nonlinearity should cause an evolution significantly different from that of the models in vacuum or coupled to scalar fields. It may be useful in this context to follow a classification of solutions similar to the one given in [16] for the 3-torus case. A fact that will play a relevant role here is the possibility of describing again these reduced models in the different Gowdy spatial topologies as field theories in certain conformally stationary curved backgrounds.

Another important issue to study at the classical level is the explicit characterization of all observables of these models. The objective here would be to obtain all functions on the phase space which have (weakly) vanishing Poisson brackets with the Hamiltonian, momentum, and polar constraints, following the general procedure outlined in [17] for the vacuum 3-torus case.

In addition, in order to complete the quantization of the $\mathbb{S}^1 \times \mathbb{S}^2$ and $\mathbb{S}^3$ Gowdy models, one could perform a discussion similar to the one developed in [18] for the vacuum 3-torus topology in order to prove that the redefinition of the fields involving the conformal factor $\sin t$ is, in fact, the only reasonable one (up to multiplicative constants) providing unitary dynamics under the $SO(3)$-invariance condition.

Finally, one can go beyond the Gowdy cosmologies and cover more general dynamical systems by considering generic nonautonomous quadratic Hamiltonians. These can be analyzed from the perspective of some recent works on this subject [19] in which Lie systems in quantum mechanics are studied from a geometrical point of view, developing methods to obtain the time evolution operators associated with time-dependent Schrödinger equations of Lie-type. These techniques may be successfully applied to infinite-dimensional quadratic Hamiltonian systems by following a functional description similar to the one performed in *Chapter 3*. In particular, the different resulting factorizations for the time evolution operators may be especially useful to define alternative families of semiclassical states for these systems.

The study of the Gowdy models has made a notable contribution to the current development of advanced theoretical cosmology. In particular, we want to remark the usefulness of the $\mathbb{S}^1 \times \mathbb{S}^2$ and $\mathbb{S}^3$ Gowdy models as testing grounds for quantum gravity theories such as loop quantum gravity. Even if the classical Hamiltonian formulation is more complicated for these topologies than for the 3-torus case, one finally obtains nonautonomous quadratic Hamiltonian systems without extra constraints. This fact provides a notable simplification of the quantization process given the unnecessary distinction between kinematical and physical Hilbert spaces, which is precisely one of the difficulties encountered in the treatment of the 3-torus model. In conclusion, we expect that the reader has convinced himself of the importance of the Gowdy models and other symmetry reductions as useful systems to gain valuable insights into the mathematical aspects of general relativity and the current formulation of quantum field theory in curved spacetimes, as well as to probe the behavior of gravity in its quantum regime.

References

1 M. Varadarajan, Phys. Rev. D **75**, 044018 (2007).

2 A. Corichi, J. Cortez, and G. A. Mena Marugán, Phys. Rev. D **73**, 084020 (2006).

3 C. G. Torre, Phys. Rev. D **66**, 084017 (2002).

4 T. Jacobson, in *Conceptual Problems of Quantum Gravity*, edited by A. Ashtekar and J. Stachel, Birkhäuser, Boston (1991).

5 D. G. Vergel and E. J. S. Villaseñor, Class. Quant. Grav. **25**, 145008 (2008).

6 C. G. Torre, Class. Quant. Grav. **24**, 1 (2007).

7 A. Corichi, J. Cortez, G. A. Mena Marugán, and J. M. Velhinho, Phys. Rev. D **76**, 124031 (2007).

8 N. D. Birrell and P. C. W. Davies, *Quantum Fields in Curved Space*, Cambridge University Press, (1982).

9 A. Ashtekar and J. Lewandowski, Class. Quant. Grav. **18**, L117-28 (2001). A Ashtekar, J. Lewandowski, and H. Sahlmann, Class. Quant. Grav. **20**, L11-1 (2003).

10 C. Itzykson and J.-B. Zuber, *Quantum Field Theory*, Dover Publications (2005).

11 A. Ashtekar, Phys. Rev. Lett. **77**, 4864-4867 (1996).

12 M. E. Angulo and G. A. Mena Marugán, Int. J. Mod.Phys. D **9**, 669-686 (2000).

13 C. Beetle, Adv. Theor. Math. Phys. **2**, 471-495 (1998).

14 V. Husain, Class. Quant. Grav. **4**, 1587 (1987).

15 M. Carmeli, Ch. Charach, and S. Malin, Phys. Rep. **76**, 79-156 (1981).

16 Ch. Charach, Phys. Rev. D **19**, 3516-3523 (1979).

17 C. G. Torre, Class. Quant. Grav. **23**, 1543-1556 (2006).

18 J. Cortez, G. A. Mena Marugán, and J. M. Velhinho, Phys. Rev. D **75**, 084027 (2007).

19 J. F. Cariñena, J. Grabowski, and G. Marmo, Rept. Math. Phys. **60**, 237-258 (2007). J. F. Cariñena, J. de Lucas, and M. F. Rañada, J. Phys. A: Math. Theor. **41**, 304029 (2008). J. F. Cariñena, J. de Lucas, and A. Ramos, accepted for publication in the Int. J. Theor. Phys., preprint at arXiv:0811.4386.

Appendix A

Symmetry Reduction in General Relativity

In this appendix, the method of symmetry reduction developed by Geroch in [1] is generalized for a nonvacuum 4-dimensional spacetime with a spacelike hypersurface orthogonal Killing vector field.[1] Concretely, we couple gravity to a massless scalar field. At the end of this study, we introduce a conformal transformation that provides a notable simplification of the equations of motion. Specifically, they become equivalent to the 3-dimensional Einstein-Klein-Gordon equations corresponding to two uncoupled symmetric massless scalar fields, one of them related to the logarithm of the norm of the Killing vector field and the other being simply proportional to the original field. The reader will find *Chapter 10* and *Appendices C* and *D* of reference [2] particularly useful in this context.

A.1 Geroch reduction technique

Let $\left({}^{(4)}\mathcal{M}, {}^{(4)}g_{ab}\right)$ be a spacetime with an everywhere spacelike and hypersurface orthogonal Killing vector field ξ^a. Let M denote the collection of all integral curves of ξ^a, called the *space of orbits* of ξ^a –an element of M is, therefore, a curve in ${}^{(4)}\mathcal{M}$ everywhere tangential to ξ^a. We will assume in the following that M is a smooth manifold and can be identified with one of the 3-dimensional hypersurfaces embedded in ${}^{(4)}\mathcal{M}$ which is everywhere orthogonal to the ξ^a trajectories, so that each orbit intersects M in exactly one point. The metric that ${}^{(4)}g_{ab}$ induces on M is

$${}^{(3)}g_{ab} = {}^{(4)}g_{ab} - \lambda^{-1}\xi_a\xi_b \,,$$

where $\xi_a := {}^{(4)}g_{ab}\xi^b$, $\lambda := {}^{(4)}g_{ab}\xi^a\xi^b > 0$.

Let ${}^{(3)}R_{ab}$, ${}^{(3)}\nabla_a$ and ${}^{(3)}\Box := {}^{(3)}g^{ab(3)}\nabla_a{}^{(3)}\nabla_b$ be, respectively, the Ricci tensor, the

[1]In reference [1], the reader will find a more extensive analysis of the vacuum case than the one performed here, allowing the Killing vector field to be either spacelike or timelike, and not necessarily hypersurface orthogonal.

Levi-Civita connection and the d'Alembert operator associated with ${}^{(3)}g_{ab}$. Given a tensor field on the manifold M, say $T^{a_1\cdots a_m}{}_{b_1\cdots b_n}$, the metric connection ${}^{(3)}\nabla_a$ acts according to the formula [2]

$$ {}^{(3)}\nabla_e T^{a_1\cdots a_m}{}_{b_1\cdots b_n} = {}^{(3)}g^{a_1}{}_{a'_1}\cdots{}^{(3)}g^{a_m}{}_{a'_m}\,{}^{(3)}g_{b_1}{}^{b'_1}\cdots{}^{(3)}g_{b_n}{}^{b'_n}\,{}^{(3)}g_e{}^f\,{}^{(4)}\nabla_f T^{a'_1\cdots a'_m}{}_{b'_1\cdots b'_n}\,, $$

where ${}^{(4)}\nabla_a$ is the Levi-Civita connection associated with the original 4-dimensional metric ${}^{(4)}g_{ab}$. Note that the indices of any tensor field on M can be raised or lowered with either the metric ${}^{(3)}g_{ab}$ or ${}^{(4)}g_{ab}$.

We proceed now to calculate the Riemann tensor on M. Let k^a be an arbitrary vector field defined on M. Then,

$$ \begin{aligned} {}^{(3)}\nabla_a{}^{(3)}\nabla_b k_c &= {}^{(3)}g_a{}^{p\,(3)}g_b{}^{q\,(3)}g_c{}^{r\,(4)}\nabla_p\left({}^{(3)}g_q{}^{s\,(3)}g_r{}^{t\,(4)}\nabla_s k_t\right) \\ &= {}^{(3)}g_a{}^{p\,(3)}g_b{}^{s\,(3)}g_c{}^{t\,(4)}\nabla_p{}^{(4)}\nabla_s k_t \\ &- \lambda^{-1\,(3)}g_a{}^{p\,(3)}g_b{}^{q\,(3)}g_c{}^{r}\left({}^{(4)}\nabla_p\xi_q\right)\xi^{s\,(4)}\nabla_s k_r \\ &- \lambda^{-1\,(3)}g_a{}^{p\,(3)}g_b{}^{q\,(3)}g_c{}^{r}\left({}^{(4)}\nabla_p\xi_r\right)\xi^{t\,(4)}\nabla_q k_t\,, \end{aligned} \tag{A.1} $$

where $k_a := {}^{(3)}g_{ab}k^b$. Next, we antisymmetrize over indices a and b and eliminate the derivatives of k_c on the right hand side of (A.1) by using the vanishing of the Lie derivative $\mathcal{L}_\xi k_r = 0$ for the second term, and the orthogonality condition $\xi^t k_t = 0$ for the third one. In this way, we get

$$ \begin{aligned} {}^{(3)}\nabla_{[a}{}^{(3)}\nabla_{b]}k_c &= {}^{(3)}g_a{}^{p\,(3)}g_b{}^{q\,(3)}g_c{}^{r\,(4)}\nabla_{[p}{}^{(4)}\nabla_{q]}k_r \\ &+ \lambda^{-1\,(3)}g_a{}^{p\,(3)}g_b{}^{q\,(3)}g_c{}^{r}\left({}^{(4)}\nabla_p\xi_q\right)\left({}^{(4)}\nabla_r\xi_s\right)k^s \\ &+ \lambda^{-1\,(3)}g_{[a}{}^{p\,(3)}g_{b]}{}^{q\,(3)}g_c{}^{r}\left({}^{(4)}\nabla_p\xi_r\right)\left({}^{(4)}\nabla_q\xi_t\right)k^t\,. \end{aligned} $$

Since k_c is arbitrary, the Riemann tensor ${}^{(3)}R_{abcd}$ of the manifold M is related to ${}^{(4)}R_{abcd}$ of ${}^{(4)}\mathcal{M}$ by the analogue of the first Gauss-Codazzi relation[2]

$$ \begin{aligned} {}^{(3)}R_{abcd} &= {}^{(3)}g_{[a}{}^{p\,(3)}g_{b]}{}^{q\,(3)}g_{[c}{}^{r\,(3)}g_{d]}{}^{s}\Big({}^{(4)}R_{pqrs} + 2\lambda^{-1}\left({}^{(4)}\nabla_p\xi_q\right)\left({}^{(4)}\nabla_r\xi_s\right) \\ &\quad +2\lambda^{-1}\left({}^{(4)}\nabla_p\xi_r\right)\left({}^{(4)}\nabla_q\xi_s\right)\Big)\,. \end{aligned} \tag{A.2} $$

By virtue of the hypersurface orthogonality of ξ^a, we have[3]

$$ {}^{(4)}\nabla_a\xi_b = \lambda^{-1}\xi_{[b}{}^{(3)}\nabla_{a]}\lambda\,. \tag{A.3} $$

[2]Here, we take the convention $2{}^{(n)}\nabla_{[a}{}^{(n)}\nabla_{b]}k_c =: {}^{(n)}R_{abc}{}^d k_d$, ${}^{(n)}R_{ab} := {}^{(n)}R_{acb}{}^c$ $(n = 3, 4)$. With the aim of obtaining the equation (A.2), we make use of the identities ${}^{(4)}R_{abcd} = -{}^{(4)}R_{bacd} = -{}^{(4)}R_{abdc}$, as well as of the Killing equation ${}^{(4)}\nabla_{(a}\xi_{b)} = 0$.

[3]Take the expression ${}^{(4)}\nabla_a\xi_b = \delta_a{}^{[p}\delta_b{}^{q]}\left({}^{(4)}\nabla_p\xi_q\right) = -\frac{1}{4\lambda}{}^{(4)}\epsilon^{e_1e_2pq\,(4)}\epsilon_{e_1e_2ab}\xi_r\xi^r\left({}^{(4)}\nabla_p\xi_q\right)$, with ${}^{(4)}\epsilon$ being the volume form naturally associated with ${}^{(4)}g_{ab}$ satisfying ${}^{(4)}\nabla_a{}^{(4)}\epsilon_{bcde} = 0$ and ${}^{(4)}\epsilon_{abcd}{}^{(4)}\epsilon^{abcd} = 4!$, and make use of the relations ${}^{(4)}\epsilon^{[e_1e_2pq}\xi^{r]} = 0$ and ${}^{(4)}\epsilon_{abcd}\xi^{b\,(4)}\nabla^c\xi^d = 0$, the last one being a direct consequence of the hypersurface orthogonality of ξ^a.

We also require the formula for the second derivative of the Killing vector field ξ^a,

$$ {}^{(4)}\nabla_a {}^{(4)}\nabla_b \xi_c = {}^{(4)}R_{cba}{}^d \xi_d \,. \tag{A.4} $$

Making use of equations (A.3) and (A.4), we obtain

$$ {}^{(3)}\Box\lambda = \frac{1}{2}\lambda^{-1}{}^{(3)}g^{ab}\left({}^{(3)}\nabla_a\lambda\right)\left({}^{(3)}\nabla_b\lambda\right) - 2\,{}^{(4)}R_{ab}\xi^a\xi^b \,. $$

Contracting (A.2) once, using (A.3) and (A.4), and taking again the hypersurface orthogonality of ξ^a into account, we get

$$ {}^{(3)}R_{ab} = \frac{1}{2}\lambda^{-1}{}^{(3)}\nabla_a {}^{(3)}\nabla_b\lambda - \frac{1}{4}\lambda^{-2}\left({}^{(3)}\nabla_a\lambda\right)\left({}^{(3)}\nabla_b\lambda\right) + {}^{(3)}g_a{}^{c}\,{}^{(3)}g_b{}^{d}\,{}^{(4)}R_{cd} \,. $$

We can then enunciate the following theorem.

Theorem A.1.1. *Consider a system consisting in 4-dimensional gravity minimally coupled to a massless scalar field ϕ, so that*

$$ {}^{(4)}R_{ab} = 8\pi G_N \left({}^{(4)}\nabla_a\phi\right){}^{(4)}\nabla_b\phi \,, \quad {}^{(4)}\Box\phi := {}^{(4)}g^{ab}\,{}^{(4)}\nabla_a {}^{(4)}\nabla_b\phi = 0 \,, \tag{A.5} $$

where G_N denotes the Newton constant. The symmetry of the system implies $\mathcal{L}_\xi\phi = 0$. In terms of 3-dimensional quantities, the basic equations of motion are given by

$$ \begin{aligned} {}^{(3)}R_{ab} &= \frac{1}{2}\lambda^{-1}{}^{(3)}\nabla_a {}^{(3)}\nabla_b\lambda - \frac{1}{4}\lambda^{-2}\left({}^{(3)}\nabla_a\lambda\right)\left({}^{(3)}\nabla_b\lambda\right) \\ &\quad + 8\pi G_N\left({}^{(3)}\nabla_a\phi\right){}^{(3)}\nabla_b\phi \,, && \text{(A.6)} \\ {}^{(3)}\Box\phi &= -\frac{1}{2}\lambda^{-1}{}^{(3)}g^{ab}\left({}^{(3)}\nabla_a\phi\right){}^{(3)}\nabla_a\lambda \,, && \text{(A.7)} \\ {}^{(3)}\Box\lambda &= \frac{1}{2}\lambda^{-1}{}^{(3)}g^{ab}\left({}^{(3)}\nabla_a\lambda\right)\left({}^{(3)}\nabla_b\lambda\right) . && \text{(A.8)} \end{aligned} $$

Proof. Indeed, we may rewrite the last relation in (A.5) in the form

$$ \begin{aligned} {}^{(4)}\Box\phi &= {}^{(3)}\Box\phi + \lambda^{-1}\xi^a\xi^b\,{}^{(4)}\nabla_a {}^{(4)}\nabla_b\phi \\ &= {}^{(3)}\Box\phi - \lambda^{-1}\xi^a({}^{(4)}\nabla_a\xi^b){}^{(4)}\nabla_b\phi \\ &= {}^{(3)}\Box\phi + \frac{1}{2}\lambda^{-1}{}^{(3)}g^{ab}\left({}^{(3)}\nabla_a\phi\right){}^{(3)}\nabla_a\lambda \,, \end{aligned} $$

where we have used the relations ${}^{(4)}\nabla_a\left(\xi^b\,{}^{(4)}\nabla_b\phi\right) = 0$ and (A.3), the first of them being a consequence of the vanishing of the Lie derivative $\mathcal{L}_\xi\phi = 0$. □

A.2 Conformal transformation

Since ξ^a is an everywhere spacelike vector field, its norm $\lambda = {}^{(4)}g_{ab}\xi^a\xi^b$ is a strictly positive function on ${}^{(4)}\mathcal{M}$ and, hence, the metric

$$g_{ab} := \lambda^{(3)}g_{ab}$$

arises from ${}^{(3)}g_{ab}$ via a well-defined conformal transformation. Denote by R_{ab}, ∇_a and $\Box$ the Riemann tensor, the Levi-Civita connection and the d'Alembert operator associated with the new 3-metric g_{ab}, respectively. Recall, in particular, that the action of the derivative operators ${}^{(3)}\nabla_a$ and ∇_a coincide over scalars. For any scalar function f, we have [2]

$$\nabla_a\nabla_b f = {}^{(3)}\nabla_a{}^{(3)}\nabla_b f - C^c{}_{ab}{}^{(3)}\nabla_c f\,, \tag{A.9}$$

where

$$C^c{}_{ab} := \delta^c{}_{(a}{}^{(3)}\nabla_{b)}\log\lambda - \frac{1}{2}{}^{(3)}g_{ab}{}^{(3)}g^{cd\,(3)}\nabla_d\log\lambda\,. \tag{A.10}$$

Similarly, we have the relation between the Ricci tensors

$$\begin{aligned} {}^{(3)}R_{ab} &= R_{ab} + \frac{1}{2}\nabla_a\nabla_b\log\lambda + \frac{1}{2}g_{ab}g^{cd}\nabla_c\nabla_d\log\lambda \\ &+ \frac{1}{4}\left(\nabla_a\log\lambda\right)\left(\nabla_b\log\lambda\right) - \frac{1}{4}g_{ab}g^{cd}\left(\nabla_c\log\lambda\right)\left(\nabla_d\log\lambda\right). \end{aligned} \tag{A.11}$$

Then, it is straightforward to prove the following theorem.

Theorem A.2.1. *The 4-dimensional system considered in the* Theorem A.1.1 *can be thought of as 3-dimensional general relativity coupled to two uncoupled symmetric massless scalar fields* $\phi_1 := \log\lambda$ *and* $\phi_2 := \sqrt{16\pi G_N}\phi$. *This reduced model satisfies the Einstein-Klein-Gordon equations*

$$R_{ab} = \frac{1}{2}\left(\nabla_a\log\lambda\right)\left(\nabla_b\log\lambda\right) + 8\pi G_N\left(\nabla_a\phi\right)\nabla_b\phi\,, \tag{A.12}$$

$$\Box\phi = 0\,, \quad \Box\log\lambda = 0\,. \tag{A.13}$$

Proof. Substituting $f = \phi$ and $f = \log\lambda$ in (A.9), and using (A.7) and (A.8), it is straightforward to obtain the equations (A.13). Finally, writing ${}^{(3)}\nabla_a{}^{(3)}\nabla_b\lambda$ in terms of quantities associated with the 3-metric g_{ab} as in (A.9) and (A.10), and making use of equations (A.6), (A.11), and (A.13), we finally obtain (A.12). □

References

1 R. Geroch, J. Math. Phys. **12**, 918-924 (1971); **13**, 394-404 (1972).

2 R. M. Wald, *General Relativity*, The University of Chicago Press, Chicago and London (1984).

Appendix B
Symplectic Geometry Applied to Analytical Mechanics

The purpose of this appendix is to introduce the basics of symplectic geometry, profusely applied throughout the thesis, and show their usefulness for the description of Lagrangian and Hamiltonian classical systems –assumed in what follows to have a finite number of degrees of freedom with the aim of simplifying their analysis. The interested reader will find extensive studies on this subject in references [1] and [2].

B.1 Symplectic manifolds

Let V be a real m-dimensional vector space ($m < +\infty$) and $\omega \in \Lambda^2 V$ a 2-form on V. Consider the linear mapping $\chi_\omega : V \to V^*$ (with V^* the dual space of V) defined as

$$\chi_\omega(u) := i_u\omega\,, \quad (i_u\omega)(v) = \omega(u,v)\,, \quad u, v \in V\,, \tag{B.1}$$

with $i_u\omega$ being the inner product of the vector u by ω. Let $\mathrm{Im}\chi_\omega$ and $\ker\chi_\omega := \{u \in V \,|\, i_u\omega = 0\}$ be the image and the kernel of χ_ω, respectively. We define the *rank of* ω, denoted $\mathrm{rank}\,\omega$, as the dimension of $\mathrm{Im}\chi_\omega$. This is an even number smaller or equal to $\dim V$. The dimension of the kernel $\ker\chi_\omega$ is called the *corank of* ω, being denoted $\mathrm{corank}\omega$. If $\mathrm{corank}\,\omega = 0$, then $\dim V = \mathrm{rank}\,\omega$, and ω is said to be *nondegenerate, regular* or *of maximal rank*.

We will say that every nondegenerate 2-form ω on a real m-dimensional vector space V defines a *symplectic structure* on it. The form ω is called *symplectic* in this case, and the pair (V,ω) a *symplectic vector space*. The dimension of V is then an even number, i.e., $m = 2n$ for some integer n. It is possible to show that, given a real vector space V of even dimension $2n$ and a 2-form ω on V, ω is nondegenerate iff the linear mapping (B.1) is an isomorphism, or equivalently, iff $\omega^n := \omega \wedge \ldots \wedge \omega$ (n times) defines a volume form on V.

Let M^m be a smooth (C^∞) m-dimensional manifold, and ω a 2-form on M^m. The rank (corank) of ω at a point $x \in M^m$ is defined as the rank (corank) of the form

$\omega(x) \in \Lambda^2(T_x M^m)$. We will say that ω is nondegenerate or of maximal rank if for every point $x \in M^m$, $\omega(x)$ is nondegenerate; in this case, the 2-form ω defines an *almost symplectic form* on M^m. Then, M^m has even dimension $m = 2n$ and the pair (M^{2n}, ω) is called an *almost symplectic manifold.* Note that since ω^n is a volume form on M^{2n} every almost symplectic manifold is orientable. Furthermore, the linear mapping $\chi_\omega : \mathfrak{X}(M^{2n}) \to \Lambda^1(M^{2n})$ defined by

$$\chi_\omega(X) = i_X \omega\,, \;\; X \in \mathfrak{X}(M^{2n})\,, \tag{B.2}$$

is an isomorphism. An almost symplectic form ω on a manifold M^{2n} is said to be *symplectic* if it is closed, i.e., $\mathrm{d}\omega = 0$. In this case, the pair (M^{2n}, ω) is called a *symplectic manifold.*[1]

Let (M^{2n}, ω) and $(\tilde{M}^{2n}, \tilde{\omega})$ be two symplectic manifolds of same dimension. A *symplectic transformation* is a mapping $\phi \in C^\infty(M^{2n}; \tilde{M}^{2n})$ such that $\phi^* \tilde{\omega} = \omega$, i.e.,

$$\tilde{\omega}(\mathrm{d}\phi(x) X_1, \mathrm{d}\phi(x) X_2) = \omega(X_1, X_2)\,,$$

for all $x \in M^{2n}$, $X_1, X_2 \in T_x M^{2n}$. The map ϕ is a local diffeomorphism; if it is also a global diffeomorphism, then it is called a *symplectomorphism.* In particular, when $M^{2n} = \tilde{M}^{2n}$, a symplectic transformation ϕ preserves the symplectic form, $\phi^* \omega = \omega$, and is called a (global) *canonical transformation.*

Let (M^{2n}, ω) be a symplectic manifold. A vector field X on M^{2n} is called a *symplectic vector field* or *infinitesimal canonical transformation* if its flow consists of symplectic transformations. In this case, the following statements are equivalent: (i) X is a symplectic vector field; (ii) $\mathcal{L}_X \omega = 0$; (iii) $i_X \omega = \mathrm{d}f$ (locally) for some function f, i.e., $\mathrm{d}(i_X \omega) = 0$. The equivalence between (i) and (ii) is straightforward to show, given the definition of the Lie derivative and the fact that the flow of X, φ_t, is a symplectic transformation: $\mathcal{L}_X \omega := \mathrm{d}/\mathrm{d}t|_{t=0}(\varphi_t^* \omega) = \lim_{t\to 0}(\varphi_t^* \omega - \omega)/t = 0$. The equivalence of (ii) and (iii) follows from the H. Cartan formula, $\mathcal{L}_X = i_X \mathrm{d} + \mathrm{d} i_X$, so that $\mathcal{L}_X \omega = \mathrm{d} i_X \omega$, and the Poincaré lemma. We can now prove the so-called *Liouville theorem*:

[1]For systems with infinite degrees of freedom, one must be careful with functional analysis [3]. Consider a Banach space $\mathcal{E}$ and let $\omega : \mathcal{E} \times \mathcal{E} \to \mathbb{R}$ be a continuous linear mapping on it. Define the (also continuous and linear) mapping $\chi_\omega : \mathcal{E} \to \mathcal{E}^*$, where $\mathcal{E}^*$ denotes the topological dual of $\mathcal{E}$, such that $\mathcal{E} \ni e \mapsto \chi_\omega(e) \,:\, \chi_\omega(e) \cdot f = \omega(e, f)$, $f \in \mathcal{E}$; ω is said to be *weakly nondegenerate* if χ_ω is an injection, i.e., $\omega(e, f) = 0$, $\forall\, f \in \mathcal{E} \Rightarrow e = 0$; ω is called *strongly nondegenerate* if χ_ω is an isomorphism. Note that, if $\mathcal{E}$ is a finite-dimensional space, the distinction between weak and strong nondegeneracy is unnecessary. This is not the case for infinite-dimensional spaces. Let $\mathcal{P}$ be a manifold modeled on a Banach space $\mathcal{E}$; a 2-form ω on $\mathcal{P}$ is called *symplectic* if: (i) ω is exact, i.e., $\mathrm{d}\omega = 0$; (ii) for each point $x \in \mathcal{P}$, $\omega_x : T_x\mathcal{P} \times T_x\mathcal{P} \to \mathbb{R}$ is a strongly nondegenerate map. If ω_x is weakly nondegenerate, it is said to be *weakly symplectic.* Although in this appendix we have restricted ourselves to the study of finite-dimensional systems, the main results presented here can be properly generalized for weakly symplectic manifolds.

Theorem B.1.1 (Liouville). *The flow φ_t of an infinitesimal canonical transformation preserves the volume form ω^n, $\forall\, t \in I \subseteq \mathbb{R}$.*

Proof. Indeed, since $\varphi_t^*\omega = \omega$ by definition, we have $\varphi_t^*\omega^n = \varphi_t^*(\omega \wedge \ldots \wedge \omega) = (\varphi_t^*\omega) \wedge \ldots \wedge (\varphi_t^*\omega) = (\varphi_t^*\omega)^n = \omega^n$. □

Finally, we enunciate the *Darboux theorem*, as a consequence of which any two symplectic manifolds of the same dimension are locally symplectomorphic:

Theorem B.1.2 (Darboux). *An almost symplectic manifold (M^{2n}, ω) is symplectic (i.e., $\mathrm{d}\omega = 0$) iff for each point $x \in M^{2n}$ there exists a coordinate neighborhood U with local coordinates $(x^1, \ldots, x^{2n})$ such that the symplectic form can be written*

$$\omega = \sum_{i=1}^{n} \mathrm{d}x^i \wedge \mathrm{d}x^{n+i}$$

in U. These coordinates are called symplectic *or* canonical coordinates *on M^{2n}, and will be denoted from now on as $x^i = q^i$, $x^{n+i} = p_i$, $1 \leq i \leq n$.*

B.2 Hamiltonian systems

B.2.1 Autonomous Hamiltonian systems

Let (M^{2n}, ω) be a symplectic manifold. Denote by $\mathcal{F}(M^{2n})$ the ring of smooth functions $C^\infty(M^{2n}; \mathbb{R})$, endowed with the structure of an infinite-dimensional $\mathbb{R}$-vector space with respect to the basic vector operations of sum and products by real scalars. Given a function $H \in \mathcal{F}(M^{2n})$, its exterior derivative $\mathrm{d}H$ is a 1-form on M^{2n} and, hence, there is by virtue of the isomorphism (B.2) a unique vector field $X_H := \chi_\omega^{-1}(\mathrm{d}H) \in \mathfrak{X}(M^{2n})$ such that

$$i_{X_H}\omega = \mathrm{d}H \tag{B.3}$$

called the *Hamiltonian vector field associated with the Hamiltonian function H*. The triplet (M^{2n}, ω, H) is said to characterize an *autonomous Hamiltonian system*. In view of equation (B.3), it is clear that every Hamiltonian vector field on (M^{2n}, ω) defines an infinitesimal canonical transformation.[2] This is the more general geometric framework for the description of time-independent classical Hamiltonian systems; in this context, M^{2n} is identified with the *phase space* of the system and each point $x \in M^{2n}$ represents a possible (pure) state. Once a point x_0 of this space is fixed as an initial state, the dynamical trajectory of the system is simply given by the (unique) integral curve of the

[2] In general, however, an infinitesimal canonical transformation X on M^{2n} does not define a Hamiltonian vector field, since an equation of the form (B.3) is not necessarily satisfied globally. Nevertheless, there will be a neighborhood U for each point $x \in M^{2n}$ and a function H in U such that $X = X_H$ in U. Owing to this fact, any infinitesimal canonical transformation is said to be *locally Hamiltonian*.

Hamiltonian vector field X_H crossing that point.

Take canonical coordinates (q^i, p_i) in (M^{2n}, ω) and consider the isomorphism $\chi_\omega : X \in \mathfrak{X}(M^{2n}) \mapsto \chi_\omega(X) = i_X\omega \in \Lambda^1 M^{2n}$. It is straightforward to check that $\chi_\omega(\partial/\partial q^i) = \mathrm{d}p_i$, $\chi_\omega(\partial/\partial p_i) = -\mathrm{d}q^i$, so that $\chi_\omega^{-1}(\mathrm{d}q^i) = -\partial/\partial p_i$, $\chi_\omega^{-1}(\mathrm{d}p_i) = \partial/\partial q^i$. From the previous equations, we deduce that given a vector field X on M^{2n} with local expression $X = X^i\partial/\partial q^i + \tilde{X}^i\partial/\partial p_i$ (in the following formulae we will implicitly assume summation over i), then $\chi_\omega(X) = -\tilde{X}^i\mathrm{d}q^i + X^i\mathrm{d}p_i$. Similarly, given a 1-form α on M^{2n} locally given by $\alpha = \alpha_i\mathrm{d}q^i + \tilde{\alpha}_i\mathrm{d}p_i$, then $\chi_\omega^{-1}(\alpha) = \tilde{\alpha}_i\partial/\partial q^i - \alpha_i\partial/\partial p_i$. Since $\mathrm{d}H = (\partial H/\partial q^i)\mathrm{d}q^i + (\partial H/\partial p_i)\mathrm{d}p_i$, we obtain

$$X_H = \chi_\omega^{-1}(\mathrm{d}H) = \sum_{i=1}^{n}\left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i}\frac{\partial}{\partial p_i}\right). \tag{B.4}$$

The time evolution (in the Heisenberg picture) of any observable $f \in \mathcal{F}(M^{2n})$ is then given by $\dot{f} := \mathcal{L}_{X_H} f$. Note, in particular, that for an autonomous Hamiltonian system the Hamiltonian H is a *first integral*, i.e., it remains constant along every curve solution of the system (indeed, $\mathcal{L}_{X_H} H = 0$).

Let $\sigma : I = (-\epsilon, \epsilon) \to M^{2n}$, $\epsilon > 0$, be an integral curve of X_H, i.e., $X_H|_{\sigma(t)} = \dot{\sigma}(t)$, $t \in I$; in local coordinates, $\sigma(t) = (q^i(t), p_i(t))$, $\dot{\sigma}(t) = (\mathrm{d}q^i/\mathrm{d}t)\partial/\partial q^i + (\mathrm{d}p_i/\mathrm{d}t)\partial/\partial p_i$ (sum over i). Making use of (B.4), we finally get the so-called (canonical) *Hamilton equations*

$$\frac{\mathrm{d}q^i}{\mathrm{d}t} = \frac{\partial H}{\partial p_i}, \quad \frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial H}{\partial q^i}, \quad 1 \le i \le n. \tag{B.5}$$

B.2.2 Poisson bracket

Let (M^{2n}, ω) be a symplectic manifold. The *Poisson bracket* of two functions $f, g \in \mathcal{F}(M^{2n})$ is defined as

$$\{f, g\} := \omega(X_f, X_g) = (i_{X_f}\omega)(X_g) = i_{X_g} i_{X_f}\omega, \tag{B.6}$$

where X_f and X_g are the Hamiltonian vector fields associated with the functions f and g, respectively. Since $(i_{X_f}\omega)(Y) = (\mathrm{d}f)Y$, then $\omega(X_f, Y) = Y(f)$. In particular, choosing $Y = X_g$, we get $\mathcal{L}_{X_g} f = X_g(f) = \omega(X_f, X_g) = \{f, g\}$.

The Poisson bracket satisfies, for all $f, g, h \in \mathcal{F}(M^{2n})$: (i) $\{f, g\} = -\{g, f\}$; (ii) $\{f, gh\} = \{f, g\}h + g\{f, h\}$; (iii) $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$ (Jacobi identity), as a result of the fact that ω is exact; (iv) $\{af, g\} = a\{f, g\}$, $\forall\, a \in \mathbb{R}$; (v) $\{f + g, h\} = \{f, h\} + \{g, h\}$. This operation turns the real vector space $\mathcal{F}(M^{2n})$ into a Lie algebra with the Poisson bracket as the product. By virtue of the Jacobi identity (iii), it is immediate to check that $X_{\{f,g\}} = -[X_f, X_g]$, $f, g \in \mathcal{F}(M^{2n})$, where we have defined the Lie bracket $[X,Y](f) := X(Y(f)) - Y(X(f))$, $X, Y \in \mathfrak{X}(M^{2n})$, i.e., the map $f \mapsto X_f$ associating to f its corresponding Hamiltonian vector field X_f takes Poisson brackets of pairs of functions to Lie commutators of vector fields.

Taking canonical coordinates (q^i, p_i) in M^{2n}, and making use of (B.4), the Poisson bracket (B.6) is given by

$$\{f,g\} = \mathcal{L}_{X_g} f = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i} \right) . \tag{B.7}$$

In particular, we obtain the Poisson brackets of the canonical coordinates,

$$\{q^i, q^j\} = \{p_i, p_j\} = 0 \,, \quad \{q^i, p_j\} = \delta^i_j \,, \quad 1 \le i, j \le n \,.$$

Furthermore, Hamilton equations (B.5) can be rewritten as

$$\frac{\mathrm{d}q^i}{\mathrm{d}t} = \{q^i, H\} \,, \;\; \frac{\mathrm{d}p_i}{\mathrm{d}t} = \{p_i, H\} \,, \;\; 1 \le i \le n \,. \tag{B.8}$$

It is easy to show that the Poisson bracket is invariant under the action of a canonical transformation $\phi : M^{2n} \to M^{2n}$, i.e., $\phi^*\{f,g\} = \{f,g\} \circ \phi = \{f \circ \phi, g \circ \phi\} = \{\phi^* f, \phi^* g\}$. As a consequence, canonical transformations preserve the form of the Hamilton equations (B.8). Indeed, if $\phi : (q^i, p_i) \to (\tilde{q}^i, \tilde{p}_i)$, where (q^i, p_i) and $(\tilde{q}^i, \tilde{p}_i)$ are canonical coordinates, we have

$$\begin{aligned} \phi^*\{q^i, H\} &= \{q^i \circ \phi, H \circ \phi\} = \{\tilde{q}^i, \tilde{H}\} = \frac{\mathrm{d}\tilde{q}^i}{\mathrm{d}t} \,, \\ \phi^*\{p_i, H\} &= \{p_i \circ \phi, H \circ \phi\} = \{\tilde{p}_i, \tilde{H}\} = \frac{\mathrm{d}\tilde{p}_i}{\mathrm{d}t} \,, \;\; 1 \le i \le n \,, \end{aligned}$$

with $\tilde{H} := \phi^* H = H \circ \phi$.

B.2.3 Cosymplectic manifolds

Let V be a $(2n+1)$-dimensional real vector space, $\eta \in \Lambda^1(V)$ a 1-form, and $\omega \in \Lambda^2(V)$ a 2-form on V, respectively. The triplet (V, η, ω) is called a *cosymplectic vector space* if $\eta \wedge \omega^n \neq 0$. Consider the linear map $\chi_{\eta,\omega} : V \to V^*$, where V^* denotes the dual space of V,

$$\chi_{\eta,\omega}(v) := i_v\omega + (\eta(v))\eta \,, \quad \forall\, v \in V \,.$$

This map defines a linear isomorphism iff: (i) (V, η, ω) is a cosymplectic vector space in the case when $\dim V$ is an odd number, or (ii) (V, ω) is a symplectic vector space in the case when V is even dimensional. Therefore, as for a cosymplectic vector space (V, η, ω), there exists a unique $\mathcal{R} \in V$, called the *Reeb vector* of the cosymplectic vector space, such that $\eta(\mathcal{R}) = 1$ and $i_{\mathcal{R}}\omega = 0$, i.e., $\mathcal{R} = \chi^{-1}_{\eta,\omega}(\eta)$.

Let M^{2n+1} be a smooth (2n+1)-dimensional manifold. M^{2n+1} is said to be an *almost cosymplectic manifold* if there exist $\eta \in \Lambda^1(M^{2n+1})$ and $\omega \in \Lambda^2(M^{2n+1})$ such that, for all $x \in M^{2n+1}$, the triplet $(T_x(M^{2n+1}), \eta_x, \omega_x)$ is a cosymplectic vector space. If the p-forms η and ω are also closed, M^{2n+1} is called *cosymplectic*.

Let (M^{2n+1}, η, ω) be an almost cosymplectic manifold, $\mathcal{R}$ its Reeb vector field, and $\chi_{\eta,\omega} : \mathfrak{X}(M^{2n+1}) \to \Lambda^1(M^{2n+1})$ its corresponding isomorphism. Denote by $\mathcal{F}(M^{2n+1})$ the ring of differentiable real functions on M^{2n+1}. By virtue of the isomorphism $\chi_{\eta,\omega}$, every function $f \in \mathcal{F}(M^{2n+1})$ has a unique associated vector field $X_f \in \mathfrak{X}(M^{2n+1})$, called the *Hamiltonian vector field with energy function* f, defined by

$$X_f := \chi_{\eta,\omega}^{-1}(\mathrm{d}f - \mathcal{R}(f)\eta) \Leftrightarrow i_{X_f}\eta = 0\,, \quad i_{X_f}\omega = \mathrm{d}f - \mathcal{R}(f)\eta\,.$$

Clearly, this construction generalizes the one corresponding to Hamiltonian vector fields on symplectic manifolds. The *evolution vector field* associated with $f \in \mathcal{F}(M^{2n+1})$ is given by

$$E_f := \mathcal{R} + X_f\,.$$

Let (M^{2n+1}, η, ω) be a cosymplectic manifold. It is then possible to define a *Poisson bracket* on $\mathcal{F}(M^{2n+1})$ by $\{f, g\} := \omega(X_f, X_g) = \mathcal{L}_{X_g} f$, with $f, g \in \mathcal{F}(M^{2n+1})$. In this way, note that $E_f(g) = \mathcal{R}(g) + \{g, f\}$, $g \in \mathcal{F}(M^{2n+1})$.

B.2.4 Nonautonomous Hamiltonian systems

Let (M^{2n}, ω) be a $2n$-dimensional symplectic manifold. Consider the product manifold $\mathbb{R} \times M^{2n}$ and denote by $\pi : \mathbb{R} \times M^{2n} \to M^{2n}$ the canonical projection $\pi(t, x) = x$ on the second factor, where $t \in \mathbb{R}$ and $x \in M^{2n}$, with t being a global coordinate on $\mathbb{R}$. Define $\tilde{\omega} := \pi^*\omega$ and $\eta := \mathrm{d}t$; then, the triplet $(\mathbb{R} \times M^{2n}, \mathrm{d}t, \tilde{\omega})$ is a cosymplectic manifold.

Take a function $H \in \mathcal{F}(\mathbb{R} \times M^{2n})$ with $X_H \in \mathfrak{X}(\mathbb{R} \times M^{2n})$ being its associated Hamiltonian vector field, univocally characterized by the relations

$$i_{X_H}\tilde{\omega} = \mathrm{d}H - \frac{\partial H}{\partial t}\mathrm{d}t\,, \quad i_{X_H}\mathrm{d}t = 0\,,$$

where we have taken into account that the Reeb vector field is given in this case by $\partial/\partial t$. The 4-tuple $(\mathbb{R} \times M^{2n}, \mathrm{d}t, \tilde{\omega}, H)$ is said to define a *nonautonomous Hamiltonian system*. It provides the proper geometric description for the generalized phase space of a time-dependent classical Hamiltonian system. Let (q^i, p_i) be canonical coordinates in M^{2n}; (t, q^i, p_i) are then the induced coordinates in $\mathbb{R} \times M^{2n}$. Since $\omega = \sum_{i=1}^n \mathrm{d}q^i \wedge \mathrm{d}p_i$, $\tilde{\omega}$ takes the same expression, $\tilde{\omega} = \sum_{i=1}^n \mathrm{d}q^i \wedge \mathrm{d}p_i$. The corresponding evolution vector field (see the *figure B.1*) is given by

$$E_H = \frac{\partial}{\partial t} + X_H = \frac{\partial}{\partial t} + \sum_{i=1}^{n} \left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial q^i} - \frac{\partial H}{\partial q^i}\frac{\partial}{\partial p_i} \right). \tag{B.9}$$

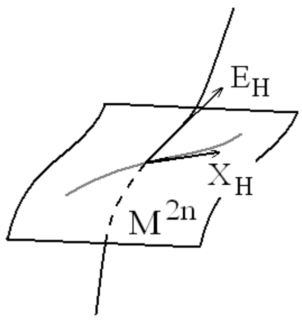

Figure B.1: Evolution vector field E_H corresponding to the Hamiltonian function H.

It is important to highlight that, by introducing the (closed) 2-form on $\mathbb{R} \times M^{2n}$

$$\omega_H := \tilde{\omega} + \mathrm{d}H \wedge \mathrm{d}t \,, \tag{B.10}$$

E_H is the unique vector field on $\mathbb{R} \times M^{2n}$ satisfying

$$i_{E_H}\omega_H = 0 \,, \;\; i_{E_H}\mathrm{d}t = 1 \,.$$

Note that the 2-form (B.10) has the feature that the time parameter t plays a role analogous to the one played by the generalized coordinates q^i, but with minus the Hamiltonian as its associated canonical conjugate momentum (see the next section for a definition of these concepts).

The integral curves of E_H, in local coordinates $\sigma(t) = (a(t), q^i(t), p_i(t))$, $\dot{\sigma}(t) = E_H|_{\sigma(t)}$, satisfy the equations $\mathrm{d}a/\mathrm{d}t = 1$, i.e., $a(t) = t + c$, $c \in \mathbb{R}$, and

$$\frac{\mathrm{d}q^i}{\mathrm{d}t} = \{q^i, H\} = \frac{\partial H}{\partial p_i} \,, \quad \frac{\mathrm{d}p_i}{\mathrm{d}t} = \{p_i, H\} = -\frac{\partial H}{\partial q^i} \,, \;\; 1 \leq i \leq n \,.$$

The above relations are called the *Hamilton equations* for the nonautonomous Hamiltonian H. Here, $\mathcal{L}_{E_H} H = \partial H/\partial t \neq 0$ and, hence, the energy is not a constant quantity for this type of (dissipative) systems.

B.3 Autonomous Lagrangian systems

Let $\mathscr{C}$ be a n-dimensional manifold and $(T\mathscr{C}, \tau_{\mathscr{C}}, \mathscr{C})$ its tangent bundle, with $\tau_{\mathscr{C}} : T\mathscr{C} \to \mathscr{C}$ being the canonical projection; this is the so-called *phase space of velocities* associated with the *configuration space* $\mathscr{C}$. Taking local coordinates q^i in $\mathscr{C}$, let (q^i, v^i), $1 \leq i \leq n$, be the induced coordinates in $T\mathscr{C}$ (i.e., any vector X can be expressed $X = \sum_{i=1}^{n} v^i(\partial/\partial q^i)$). Consider an (autonomous) *Lagrangian function* $L \in \mathcal{F}(T\mathscr{C})$. We introduce the following associated (closed) 2-form on $T\mathscr{C}$,

$$\omega_L := -\mathrm{d}\mathrm{d}_J L \,,$$

where J denotes the *canonical almost tangent structure* on $T\mathscr{C}$, locally given by $J = (\partial/\partial v^i) \otimes (\mathrm{d}q^i)$, and d_J is the *vertical differentiation* on $T\mathscr{C}$, in local coordinates $d_J L = \sum_{i=1}^n (\partial L/\partial v^i)\mathrm{d}q^i$, with $\mathrm{d}_J(\mathrm{d}q^i) = \mathrm{d}_J(\mathrm{d}v^i) = 0$. Thus, locally,

$$\omega_L = \sum_{i,j=1}^n \left(\frac{\partial^2 L}{\partial q^i \partial v^j} \mathrm{d}q^i \wedge \mathrm{d}q^j + \frac{\partial^2 L}{\partial v^i \partial v^j} \mathrm{d}q^i \wedge \mathrm{d}v^j \right) . \tag{B.11}$$

The form ω_L is a symplectic form on $T\mathscr{C}$ iff the Lagrangian function L is *regular* (or nondegenerate), i.e., iff the Hessian matrix

$$\left[\frac{\partial^2 L}{\partial v^i \partial v^j} \right]_{i,j=1}^n$$

is invertible (of maximal rank) for any coordinate system[3] (q^i, v^i). Otherwise, the function L is said to be *singular*.

We define the *energy function* associated with the Lagrangian function L by

$$E_L := C(L) - L\,, \tag{B.12}$$

where C denotes the *Liouville vector field* on $T\mathscr{C}$; in terms of the induced coordinates, it is given by $C = \sum_{i=1}^n v^i(\partial/\partial v^i)$. Consider now the equation

$$i_X \omega_L = \mathrm{d}E_L\,. \tag{B.13}$$

If L is a regular Lagrangian function, then equation (B.13) admits a unique solution $X = \xi_L$ (for ω_L is symplectic) called the *Euler-Lagrange vector field*. Furthermore, this field is a *second order differential equation*, i.e., $J\xi_L = C$, so that it can be written

$$\xi_L = \sum_{i=1}^n \left(v^i \frac{\partial}{\partial q^i} + \xi^i \frac{\partial}{\partial v^i} \right) . \tag{B.14}$$

Let $\dot{c}(t) = (q^i(t), \dot{q}^i(t))$ be an integral curve of ξ_L, with $c(t) = (q(t))$ its projection in $\mathscr{C}$ (the dot denotes time derivative). According to (B.11)-(B.14), $c(t)$ verifies the *Euler-Lagrange equations*

$$\frac{\partial L}{\partial q^i} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}^i} \right) = 0\,, \;\; 1 \leq i \leq n\,. \tag{B.15}$$

Let $L \in \mathcal{F}(T\mathscr{C})$ be a Lagrangian function. Fix two points q_1, q_2 of $\mathscr{C}$ and some interval $[a,b] \subset \mathbb{R}$. We define the *path space* from q_1 to q_2 by

$$\Omega(q_1, q_2, [a,b]) := \left\{ c : [a,b] \to \mathscr{C} \mid c \text{ is a } \mathrm{C}^\infty \text{ curve}, \, c(a) = q_1, \, c(b) = q_2 \right\} . \tag{B.16}$$

[3]Indeed, under this assumption $\omega_L^n = c \det(\partial^2 L/\partial v^i \partial v^j)\mathrm{d}q^1 \wedge \ldots \wedge \mathrm{d}q^n \wedge \mathrm{d}v^1 \wedge \ldots \wedge \mathrm{d}v^n$, $c \in \mathbb{R}_+$, becomes a volume form for $T\mathscr{C}$.

It can be shown that (B.16) defines a smooth infinite-dimensional manifold. Consider the map $\mathrm{J} : \Omega(q_1, q_2, [a, b]) \to \mathbb{R}$ given by

$$\mathrm{J}(c) = \int_a^b \mathrm{d}t \, L(\dot{c}(t)) \, , \;\; c \in \Omega(q_1, q_2, [a, b]) \, ,$$

where $\dot{c}(t) = (q(t), \dot{q}(t))$ is the natural prolongation to $T\mathscr{C}$ of a curve $c(t) = (q(t))$ in $\mathscr{C}$. In this context, q^i and $\dot{q}^i$ are called *generalized coordinates* and *velocities*, respectively. Then, we can state the well-known *variational principle* of Hamilton [2], which becomes the main result of Analytical Mechanics is terms of calculus of variations:

Theorem B.3.1 (Hamilton's variational principle)**.** *Let $L \in \mathcal{F}(T\mathscr{C})$ be a Lagrangian function and $c_0 \in \Omega(q_1, q_2, [a, b])$ a smooth curve joining $q_1 = c_0(a)$ to $q_2 = c_0(b)$; c_0 satisfies the Euler-Lagrange equations (B.15) iff it is a* critical point *of the function* $\mathrm{J} : \Omega(q_1, q_2, [a, b]) \to \mathbb{R}$*, i.e.,* $\mathrm{dJ}(c_0) = 0$*. For regular Lagrangian functions, this condition amounts to demanding that $\dot{c}_0$ be an integral curve of the field ξ_L.*

The Euler-Lagrange equations (B.15) may be written

$$V_i(q, \dot{q}) - \sum_{j=1}^{n} W_{ij}(q, \dot{q}) \ddot{q}^j = 0 \, , \;\; 1 \leq i \leq n \, ,$$

where we have defined

$$V_i := \frac{\partial L}{\partial q^i} - \sum_{j=1}^{n} \frac{\partial^2 L}{\partial \dot{q}^i \partial q^j} \dot{q}^j \, , \quad W_{ij} := \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} \, , \;\; 1 \leq i, j \leq n \, .$$

Note that the *generalized accelerations* $(\ddot{q}^i)$ at a given time are uniquely determined as functions of the generalized coordinates and velocities $(q^i, \dot{q}^i)$, provided that L is regular. This is not the case for singular Lagrangian systems.

B.3.1 Legendre transformation

Let $(T^*\mathscr{C}, \pi_{\mathscr{C}}, \mathscr{C})$ be the cotangent bundle of the configuration space $\mathscr{C}$, with $\pi_{\mathscr{C}}$ being its canonical projection; this is the so-called *phase space* (of momenta) associated with $\mathscr{C}$. Let (q^i, p_i), $1 \leq i \leq n$, be induced coordinates on $T^*\mathscr{C}$ (i.e., every 1-form α takes the local expression $\alpha = \sum_{i=1}^n p_i \mathrm{d}q^i$). The manifold $T^*\mathscr{C}$ is endowed with a natural symplectic form,

$$\omega_{\mathscr{C}} := \sum_{i=1}^{n} \mathrm{d}q^i \wedge \mathrm{d}p_i \, , \tag{B.17}$$

so that the induced coordinates on $T^*\mathscr{C}$ are canonical. As a concrete example, the phase space of a simple pendulum is given by the cotangent bundle of $\mathbb{S}^1$, $\mathbb{S}^1 \times \mathbb{R}$, with pairs (θ, p_θ), $\theta \in \mathbb{S}^1$, $p_\theta \in \mathbb{R}$; the symplectic form is simply given in this case by $\omega = \mathrm{d}\theta \wedge \mathrm{d}p_\theta$.

We will analyze now the relation between the Lagrangian formulation on $T\mathscr{C}$ and a suitable Hamiltonian formulation on $T^*\mathscr{C}$. Consider a regular Lagrangian function $L \in \mathcal{F}(T\mathscr{C})$ and let (q^i, v^i) and (q^i, p_i) be induced coordinates on $T\mathscr{C}$ and $T^*\mathscr{C}$, respectively. For each tangent vector $v \in T_x\mathscr{C}$, $x \in \mathscr{C}$, let us introduce the natural identifications (isomorphisms) $\varphi_v : T_x\mathscr{C} \to T_v(T_x\mathscr{C})$, $\varphi_v^* : T_x^*\mathscr{C} \to T_v^*(T_x\mathscr{C})$, given by

$$\varphi_v((\partial/\partial q^i)_x) = (\partial/\partial q^i)_v\,, \quad \varphi_v^*((\mathrm{d}q^i)_x) = (\mathrm{d}q^i)_v\,. \tag{B.18}$$

Denote by $L_x : T_x\mathscr{C} \to \mathbb{R}$ the restriction of L to $T_x\mathscr{C}$. The *Legendre transformation* (or *fiber derivative*) determined by the Lagrangian function L is the mapping $Leg_L : T\mathscr{C} \to T^*\mathscr{C}$ such that

$$Leg_L(v) := (\varphi_v^*)^{-1}(\mathrm{d}L_x(v))\,. \tag{B.19}$$

Thus, from (B.18), we have

$$Leg_L(q^i, v^i) = (q^i, p_i) = (q^i, \partial L/\partial v^i)\,.$$

It follows that $\omega_L = (Leg_L)^*\omega_{\mathscr{C}}$, with the 2-forms ω_L and $\omega_{\mathscr{C}}$ given by (B.11) and (B.17), respectively. The Legendre transformation (B.19) defines a local diffeomorphism iff L is regular. In particular, L is said to be *hyperregular* if Leg_L is a global diffeomorphism.

Let $c(t) = (q(t))$ be a smooth curve on $\mathscr{C}$ and $\dot{c}(t) = (q(t), \dot{q}(t))$ its natural prolongation to $T\mathscr{C}$. Along $\dot{c}$, we have $p_i = \partial L/\partial \dot{q}^i$; in this context, p_i is called the *momentum canonically conjugate to* q^i.

Consider a hyperregular Lagrangian function $L \in \mathcal{F}(T\mathscr{C})$ and define its associated Hamiltonian $H : T^*\mathscr{C} \to \mathbb{R}$ by

$$H := E_L \circ Leg_L^{-1}\,.$$

Let X_H be the corresponding Hamiltonian vector field. Then, $(Leg_L)_*\xi_L = X_H$. The integral curves of ξ_L are mapped by Leg_L onto integral curves of X_H satisfying the Hamilton equations (B.5) corresponding to H. Furthermore, these curves have the same projections on $\mathscr{C}$. The Lagrangian and Hamiltonian formalisms are, thus, globally equivalent in the hyperregular case,[4] being transformed one into the other by the Legendre transformation.

B.3.2 Dirac-Bergmann algorithm

If the Lagrangian function L is singular (i.e., degenerate or non-regular), Leg_L does not define a local diffeomorphism. Let us assume by hypothesis that the image $\Gamma_p := Leg_L(T\mathscr{C}) \subset T^*\mathscr{C}$ is an embedded submanifold of $T^*\mathscr{C}$, called the *primary constraint surface*, and that the rank of the Hessian matrix $(\partial^2 L/\partial v^i \partial v^j)$ is constant and equal

[4]This equivalence is just local for regular functions.

to $R = n - M$ on $T\mathscr{C}$. Then, there are $M = n - R$ independent equations, called the *primary constraints*, that locally describe the $(2n - M)$-dimensional surface Γ_p,

$$\phi_m(q^i, p_i) = 0\,,\ \ 1 \leq m \leq M\,. \tag{B.20}$$

These relations directly follow from the definition of the conjugate momenta, in the sense that when the momenta p_i are replaced by their definitions $p_i = \partial L/\partial \dot{q}_i$ in terms of generalized coordinates and velocities the previous equations are identically satisfied.

Given the energy function E_L associated with L, the map Leg_L projects a function h on Γ_p such that $h(Leg_L(x)) \equiv E_L(x)$, $\forall\, x \in T\mathscr{C}$. If H is an arbitrary extension of h to $T^*\mathscr{C}$, all the Hamiltonian functions of the form $\tilde{H} = H + \sum_{m=1}^{M} u^m \phi_m$, with u^m being Lagrange multipliers, are weakly equal[5] on Γ_p, i.e., $\tilde{H} \approx H \approx h$. The corresponding equations of motion are given by

$$\dot{q}^i \;=\; \mathcal{L}_{X_{\tilde{H}}}(q^i) = \{q^i, \tilde{H}\}\,, \tag{B.21}$$

$$\dot{p}_i \;=\; \mathcal{L}_{X_{\tilde{H}}}(p_i) = \{p_i, \tilde{H}\}\,,\ \ 1 \leq i \leq n\,, \tag{B.22}$$

$$\phi_m \;=\; 0\,,\ \ 1 \leq m \leq M\,, \tag{B.23}$$

i.e.,

$$\dot{F} = \mathcal{L}_{X_{\tilde{H}}}(F) = \{F, \tilde{H}\}\,,\ \ \phi_m = 0\,,\ \ 1 \leq m \leq M\,, \tag{B.24}$$

for any function $F \in \mathcal{F}(T^*\mathscr{C})$, where $X_{\tilde{H}}$ is the Hamiltonian vector field of $\tilde{H}$. We clearly see that there is an ambiguity in the description of the dynamics, characterized by the multipliers u^m, $1 \leq m \leq M$; by using them, it is possible to define an invertible mapping from the $2n$-dimensional phase space of velocities $T\mathscr{C}$ to the $2n$-dimensional $\Gamma_p \times \{u^m\}$ space,

$$q^i = q^i\,,\ \ p_i = \frac{\partial L}{\partial \dot{q}^i}(q^{i'}, \dot{q}^{i'})\,,\ \ u^m = u^m(q^i, \dot{q}^i)\,,\ \ 1 \leq i \leq n,\ \ 1 \leq m \leq M\,,$$

with inverse transformation

$$q^i = q^i\,,\ \ \dot{q}^i = \frac{\partial H}{\partial p_i} + u^m \frac{\partial \phi_m}{\partial p_i}\,,\ \ \phi_m(q^i, p_i) = 0\,,\ \ 1 \leq i \leq n,\ \ 1 \leq m \leq M\,.$$

A basic consistency requirement for the dynamics is that the primary constraints be preserved under the time evolution. That is, given an initial condition (q^i, p_i) in Γ_p, the dynamical trajectory should remain there at later times. We thus impose $X_{\tilde{H}}(\phi_m) \approx 0$, $\forall\, m$, so that $X_{\tilde{H}}$ is tangential to Γ_p,

$$\{\phi_m, H\} + \{\phi_m, \phi_{m'}\} u^{m'} \approx 0\,,\ \ 1 \leq m \leq M\,. \tag{B.25}$$

[5] A function f defined in the neighborhood of Γ_p is said to be *weakly zero* if its restriction on Γ_p vanishes, $f|_{\Gamma_p} = 0$. This condition is usually denoted as $f \approx 0$.

For inadmissable Lagrangian functions (for instance, $L = \dot{q} - q$), these relations will be inconsistent (in the previous example, $H = q$, $\phi = p - 1$, so that $1 \approx 0$). The vanishing of (B.25) can yield two types of consequences: (i) some of the arbitrary functions u^m is determined or (ii) a new independent constraint arises. The new constraints so obtained are called *secondary constraints*; they are consequence of the definition of the momenta and of the equations of motion as well. Again, the secondary constraints should be preserved under the dynamics, so we must impose new consistency conditions. This process, called the *Dirac-Bergmann algorithm* [4], is iteratively applied until a final surface defined by primary and secondary constraints is obtained, where consistent solutions exist. A different classification of constraints is introduced at this point, playing a central role in the theory of constrained dynamical systems; namely, a constraint function is said to be of *first class* if its Poisson brackets with all the remaining constraints weakly vanish. Otherwise, it is said to be of *second class*. In the next section we will focus on purely *first class systems*, where all primary and secondary constraints are of first class, since this is the situation of interest in this thesis.

B.4 First class constrained manifolds

Let V be a finite-dimensional vector space, $\omega \in \Lambda^2 V$ a 2-form, and K a subspace of V. The subspace $K^\perp := \{u \in V \,|\, \omega(u, v) = 0, \forall\, v \in K\}$ is called the *orthocomplement of K in V with respect to ω*. Given a vector $v \in V$, we define $v^\perp := \{u \in V \,|\, \omega(u, v) = 0\}$. One has: (i) $\ker\chi_\omega = V^\perp$, which implies $\mathrm{corank}\,\omega = \dim V^\perp$ –see equation (B.1)–; (ii) $\dim V + \dim(V^\perp \cap K) = \dim K + \dim K^\perp$; in particular, if ω is a symplectic form, then $\dim V = \dim K + \dim K^\perp$.

Consider a symplectic vector space (V, ω). A subspace $K \subset V$ is said to be *isotropic*, resp. *coisotropic*, resp. *Lagrangian*, resp. *symplectic* in V if $K \subset K^\perp$, resp. $K^\perp \subset K$, resp. K is a maximal isotropic subspace[6] of (V, ω), resp. $K \cap K^\perp = 0$.

Let (M^{2n}, ω) be a symplectic manifold. A submanifold $K \subset M^{2n}$ is called *isotropic*, resp. *coisotropic*, resp. *Lagrangian*, resp. *symplectic* in (M^{2n}, ω) if, for each $x \in K$, $T_x K \subset (T_x K)^\perp$, resp. $(T_x K)^\perp \subset T_x K$, resp. K is a maximal isotropic submanifold of M^{2n}, resp. $(T_x K) \cap (T_x K)^\perp$. Here, $(T_x K)^\perp$ denotes the orthocomplement of $T_x K$ in $T_x M^{2n}$ with respect to $\omega(x) \in \Lambda^2(T_x M^{2n})$. If K is isotropic, then $\dim K \leq n$; if it is coisotropic, $\dim K \geq n$, and if it is Lagrangian, $\dim K = n$.

A set of smooth functions $f_1, \ldots, f_k \in \mathcal{F}(M^{2n})$ is said to be *independent* if the corresponding Hamiltonian vector fields $X_{f_1}, \ldots, X_{f_k}$ are linearly independent (or equivalently, if the 1-forms $\mathrm{d}f_1, \ldots, \mathrm{d}f_k$ are linearly independent). It is then possible to prove the following theorem.

Theorem B.4.1. *Let K be a $(2n-k)$-dimensional submanifold of M^{2n}, locally defined by the independent functions $f_1 = \ldots = f_k = 0$, $k \leq n$. K is coisotropic iff $\{f_i, f_j\} = 0$ on*

[6] This amounts to demanding $K = K^\perp$.

K, for all $1 \leq i,j \leq k$. This implies that there exist functions ${t_{ij}}^l$ on M^{2n}, $1 \leq i,j,l \leq k$, called structure functions*, such that $\{f_i, f_j\} = \sum_{l=1}^{k} {t_{ij}}^l f_l$.*

We can reformulate this result by saying that K is coisotropic iff the functions f_i, $1 \leq i \leq k$, weakly commute, $\{f_i, f_j\} \approx 0\,,\ \forall\, i,j$. A coisotropic submanifold corresponds to a *fist class constrained manifold* in Dirac's terminology, the f_i functions being *first class constraints* in this context. If $\varphi : K \to M^{2n}$ denotes the embedding, then the symplectic form ω induces a 2-form $\bar{\omega}$ on K, $\bar{\omega} = \varphi^* \omega$, whose rank will be assumed to be constant along K. Let X_{f_i} be the Hamiltonian vector fields corresponding to the functions f_i; these fields are linearly independent and tangential to K by definition. Note that, since the exterior derivative commutes with the pull-back action, the induced 2-form is closed, although possibly degenerate. The pair $(K, \bar{\omega})$ is said to define a *presymplectic* manifold. In fact, it is possible to show that the induced 2-form $\bar{\omega}$ is, in this case, maximally degenerate (rank$\bar{\omega} = 2n - 2k$), with its kernel generated by the X_{f_i} vector fields.

At each point $x \in K$, the vector fields X_{f_i} span a k-dimensional subspace $\mathcal{G}_x \subset T_x(K)$, assumed to vary smoothly with x in the sense that for each $x \in K$ there exists an open neighborhood $U \ni x$, such that, in U, $\mathcal{G}$ is generated by C^∞ vector fields. Denote by $\mathcal{G}$ the collection of subspaces $\mathcal{G}_x$. According to the Frobenius integrability theorem, $\mathcal{G}$ possesses integral submanifolds –i.e., through each point $x \in K$ we can find an embedded submanifold S such that the tangent space to this submanifold at each $y \in S$ coincides with $\mathcal{G}$– iff $\mathcal{G}$ is involutive, i.e., $[Y_1, Y_2] \in \mathcal{G}$, $\forall\, Y_1, Y_2 \in \mathcal{G}$. This is precisely our case, since by virtue of the Jacobi identity, $[X_{f_i}, X_{f_j}] = -X_{\{f_i, f_j\}} = -\sum_{l=1}^{k} {t_{ij}}^l X_{f_l}$, with the structure functions defined as in *Theorem B.4.1*. Vector fields in $\mathcal{G}$ are called *constraints vector fields*. As Dirac pointed out, motion along these directions corresponds, within the context of the analysis of constrained dynamical systems, to *gauge transformations* of the physical system, i.e., transformations that do not alter the physical state of the system [5, 6].

One can recover a symplectic form from the degenerate $\bar{\omega}$ by taking the space of orbits of the gauge diffeomorphisms $\Gamma_R := K/\mathcal{G}$ (this is possible because $\mathcal{G}$ is integrable and $\mathcal{L}_{X_{f_i}} \omega = 0 \Rightarrow \mathcal{L}_{X_{f_i}} \bar{\omega} = 0$), called the *reduced phase space*. As a different alternative, one can also proceed to perform a *gauge fixing process* by defining a global section $\Gamma_G \subset K$ intersecting the gauge orbits on K once and only once (see the figure *B.2*). The number of independent gauge fixing conditions $C_a = 0$ describing Γ_G together with $f_i = 0$, $1 \leq i \leq k$, must be equal to the number k of (independent) first class constraints. The type of intersections mentioned above is locally guaranteed if [6]

$$\det\big[\{C_i, f_j\}\big] \neq 0 \tag{B.26}$$

on the gauge surface Γ_G. We may then restrict ourselves to states lying on that surface, with the pull-back of the 2-form $\bar{\omega}$ being nondegenerate. It should be taken into

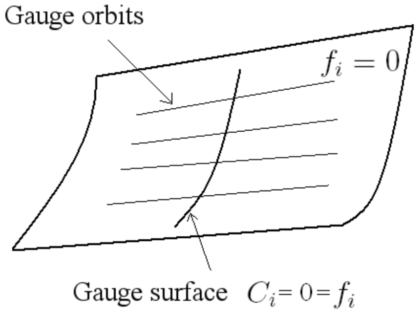

Figure B.2: Gauge fixing surface $C_i = 0 = f_i$ intersecting the gauge orbits once and only once.

account, however, that such a global cross-section need not always exists, depending on the geometry of the constraint surface and of the gauge orbits. This problem is usually referred to as the *Gribov obstruction*. In such a situation, even if the local condition (B.26) is fulfilled, the gauge surface would intersect some orbits (at least) twice, or would not intersect some others.

References

1 M. de León and P. R. Rodrigues, *Methods of Differential Geometry in Analytical Mechanics*, North Holland, Mathematics Studies 158, 1989.

2 R. Abraham and J. E. Marsden, *Foundations of Mechanics*, 2ª ed., Benjamin, New York, 1978.

3 P. R. Chernoff and J. E. Marsden, *Properties of Infinite Dimensional Hamiltonian Systems*, Springer-Verlag, 1974.

4 M. J. Gotay, J.M. Nester, and G. Hinds, J. Math. Phys. **19**, 2388 (1978).

5 P. A. M. Dirac, *Lectures on Quantum Mechanics*, Belfer Graduate School of Science Monograph, Yeshiva University, New York, 1964; Proc. Roy. Soc. (London) A **246**, 333 (1958); Phys. Rev. **114**, 924 (1959).

6 M. Henneaux and C. Teitelboim, *Quantization of Gauge Systems*, Princeton University Press, 1994.

7 N. M. J. Woodhouse, *Geometric quantization*, Oxford University Press, USA; 2nd edition (1997).

Appendix C

Mathematical Structure of Physical Theories

In this appendix, we briefly revise the algebraic formulation of (classical and quantum) physical systems in terms of C^*-algebras. In our opinion, in the case of atomic systems, this description is actually better motivated than the usual Dirac-von Neumann axiomatic structure of quantum theory [1], which becomes nearly inevitable in this context –except for the so-called measurement problem and the reduction of the wave packet, concerning the interaction between the quantum system and the measuring apparatus, which will not be analyzed here. For a more detailed study, the reader is strongly suggested to consult the bibliography given at the end of this appendix and references therein.

C.1 Observables and states

In any physical system it is necessary to properly distinguish between the measuring instruments and the objects on which the measurements are performed [2]. Denote by Q the measuring apparatus properly prepared into definite initial conditions and by ω a *preparation state* of the object under study.[1] Suppose that we perform N replicated measurements of ω by the instrument Q, in such a way that the *measured value* $q \in D_Q \subset \mathbb{R}$ is obtained $n(q)$ times. For simplicity, D_Q is assumed to be a discrete set. Of course, it is possible to reformulate this analysis in terms of continuous random variables and their associated probability density functions. Nevertheless, it suffices to consider the discrete version in order to explain the concepts of observables and states of a system in a simple way. The foundations of experimental physics assume the existence of the limit of the ratio $n(q)/N$ as $N \to +\infty$,

$$P_\omega^Q(q) = \lim_{N\to+\infty} \frac{n(q)}{N} \,,$$

[1]It is still under discussion if the word *state* refers to an individual system or an ensamble. This topic is beyond the scope of this appendix.

interpreted as the probability that the physical measurement of Q has the value q in the preparation state ω. By definition, this quantity satisfies the usual probabilistic properties

$$P^Q_\omega(q) \in [0,1] \quad \text{and} \quad \sum_q P^Q_\omega(q) = 1\,,$$

where the sum must be extended over all possible measured values q. Clearly, if for all preparation states ω and experimental results q one obtains the same probabilities $P^{Q_1}_\omega(q) = P^{Q_2}_\omega(q)$ for two different instruments Q_1 and Q_2, then they must be identified since they measure the same physical quantity. This introduces an equivalence relation between the measuring instruments; the set of all equivalent classes is denoted by $\mathcal{O}$ and its elements are again identified by the letter Q, being called the *observables* of the system. Similarly, two preparation states ω_1 and ω_2 cannot be distinguished by any measurement if the relation $P^Q_{\omega_1}(q) = P^Q_{\omega_2}(q)$ holds for all Q and q. Again, this defines an equivalence relation called a *state* of the system, also denoted by ω.

Given a real function $f:\mathbb{R}\to\mathbb{R}$ and two observables $Q, Q' \in \mathcal{O}$, if for all states ω and measured values q' the equation

$$P^{Q'}_\omega(q') = \sum_{q\,:\,f(q)=q'} P^Q_\omega(q)$$

is satisfied, then the observable Q' is said to be a function of Q, being denoted as $Q' = f(Q)$. For instance, $f(q) = cq$ defines a rescaling of the apparatus by $c \in \mathbb{R}$. Note that Q and Q' are then *simultaneously measurable* observables, since that by measuring Q the experimental value of Q' is known at the same time. More generally, consider a finite set of simultaneously measurable observables $\{Q_k\}^n_{k=1}$, all of them functions of a single observable $Q \in \mathcal{O}$, i.e., $Q_k = f_k(Q)$, $(k = 1,\ldots,n)$. The *joint probability* of getting the values $\{q_k\}^n_{k=1}$ when these observables are measured for the state ω is given by

$$P^Q_\omega\left(\{q_k\}^n_{k=1};\{Q_k\}^n_{k=1}\right) = \sum_{q\,:\,f_k(q)=q_k,\,k=1,\ldots,n} P^Q_\omega(q)\,. \tag{C.1}$$

A (non necessarily finite) set of observables $\mathcal{C} \subset \mathcal{O}$ is said to be a *full system of compatible simultaneous measurable observables* if the following three conditions are verified: (i) Any finite number of observables belonging to $\mathcal{C}$ can be expressed as functions of a (probably non-unique) observable $Q \in \mathcal{C}$; (ii) any function $f(Q)$ of $Q \in \mathcal{C}$ is in $\mathcal{C}$; (iii) the joint probability (C.1) is independent of the observable Q in terms of which the Q_k observables can be written.

The *expectation value* of an observable $Q \in \mathcal{O}$ in the state ω, denoted $\omega(Q)$, is defined as the average over the results of measurements

$$\omega(Q) := \sum_q q P^Q_\omega(q)\,. \tag{C.2}$$

Obviously, the state ω is fully characterized by all the expectation values $\omega(Q)$ as Q varies over $\mathcal{O}$. Taking into account that, for simultaneously measurable observables, the relation

$$\omega\left(\sum_{k=1}^{n} c_k Q_k\right) = \sum_{k=1}^{n} c_k \omega(Q_k)$$

is verified, we conclude that any state of a physical system can be interpreted as a *real linear functional* on the set of observables $\mathcal{O}$. In addition, this functional is *positive*, since that $\omega(Q) \geq 0$ for any positive observable $Q \in \mathcal{O}$, i.e., an observable for which all the results of measurements are positive real numbers; Q is then of the form $Q = \tilde{Q}^2$, $\tilde{Q} \in \mathcal{O}$. Note that, by definition of observables and states, $\omega(Q_1) = \omega(Q_2)$ for all states ω implies $Q_1 = Q_2$ (the states separate the observables), and conversely $\omega_1(Q) = \omega_2(Q)$, $\forall\, Q \in \mathcal{O}$, implies $\omega_1 = \omega_2$ (the observables separate the states).

Finally, it is important to distinguish between two disjoint classes of states, the so-called *pure* and *mixed states*, the first of them being states that cannot be expressed as nontrivial convex combinations of two different states, i.e., $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$, $\lambda \in \mathbb{R}$, is pure iff $\lambda \in \{0,1\}$ or $\omega_1 = \omega_2$ (λ arbitrary). Any state that is not pure is called a mixed state.

C.2 Segal systems

From a purely operational point of view, and making use of generic arguments regarding the physical properties of states and observables, Segal established the mathematical basis for the description of any (classical or quantum) physical system [3]. Concretely, the set of conditions that the observables in $\mathcal{O}$ should satisfy can be enunciated as follows: (i) $(\mathcal{O}, \|\cdot\|)$, with the norm $\|Q\| := \sup_\omega |\omega(Q)|$, is a real Banach space (thus, it is assumed in particular that $\mathcal{O}$ is linear); (ii) the square $Q \mapsto Q^2$ is continuous in the norm; (iii) $\|Q^2\| = \|Q\|^2$ and $\|Q_1^2 - Q_2^2\| \leq \max(\|Q_1\|^2, \|Q_2\|^2)$, $\forall\, Q, Q_1, Q_2 \in \mathcal{O}$. Note that, following the operational description of the system, only bounded observables ($\|Q\| < +\infty$) are considered as basic, since any measurement of an observable Q must belong to a bounded set of real numbers, given the intrinsic limitations of the measuring instruments.

A Segal system is called *special* if there exists a C^*-algebra $\mathfrak{A}$ with identity $\mathbf{1}$ generated by (complex linear combination of elements of) $\mathcal{O}$, with $\mathcal{O}$ identified as the subset of $*$-invariant elements of $\mathfrak{A}$ (i.e., elements satisfying $Q = Q^*$, usually referred to as *self-adjoint*). The system is called *exceptional* otherwise. Since it is quite difficult to construct concrete examples of this last class of Segal systems, and it is not clear their physical usefulness either, we will focus our attention in the special case only.

A self-adjoint element $A \in \mathfrak{A}$ is said to be *positive* if $A = B^2$ for some self-adjoint $B \in \mathfrak{A}$. It is possible to show that any positive element of the C^*-algebra is of the form

A^*A. Any *state*[2] is defined as a linear functional $\omega : \mathfrak{A} \to \mathbb{C}$ satisfying: (i) ω is *normalized*, in the sense that $\omega(\mathbf{1}) = 1$; (ii) ω is *positive* on positive elements, $\omega(A^*A) \geq 0$, $\forall\, A \in \mathfrak{A}$. Positivity implies $\omega(A^*) = \overline{\omega(A)}$, where the bar denotes complex conjugation, and also that ω is continuous, so that ω belongs to the dual $\mathfrak{A}^*$ of $\mathfrak{A}$.

Let us now recall the abstract definition of a C^*-algebra:

Definition C.2.1. *A set $\mathfrak{A}$ is called a C^*-algebra (with identity) if the following properties are satisfied:*

1. *$\mathfrak{A}$ is an associative algebra (with identity) with complex numbers $\mathbb{C}$ as the coefficient field.*
2. *A bijection $* : A \in \mathfrak{A} \mapsto A^* \in \mathfrak{A}$ is defined on $\mathfrak{A}$, satisfying $(c_1A_1 + c_2A_2)^* = \bar{c}_1A_1^* + \bar{c}_2A_2^*$, $(A_1A_2)^* = A_2^*A_1^*$, and $(A^*)^* = A$, for all $A_k \in \mathfrak{A}$, $c_k \in \mathbb{C}$. Here, the bar denotes complex conjugation. Such a mapping is called an* involution, *and $\mathfrak{A}$ becomes a $*$-algebra.*
3. *A norm $\|\cdot\|$ is defined on $\mathfrak{A}$, with respect to which the product is continuous, $\|AB\| \leq \|A\|\|B\|$, and $\mathfrak{A}$ is complete respect to the metric topology defined by the norm, referred to as the* uniform topology*: A neighborhood basis of an element $A \in \mathfrak{A}$ is given by the sets $\mathscr{U}(A;\epsilon) = \{B \in \mathfrak{A} : \|B-A\| < \epsilon\}$, $\epsilon > 0$. Furthermore, the normed algebra is assumed to verify $\|A\| = \|A^*\|$, $\forall\, A \in \mathfrak{A}$, so that $\mathfrak{A}$ is a Banach $*$-algebra.*
4. *The norm verifies the so-called* C^*-condition*: $\|A^*A\| = \|A\|^2$, for all $A \in \mathfrak{A}$.*

Next, we will look for suitable realizations of this abstract structure in order to facilitate concrete physical calculations. For this purpose, taking advantage of the fact that the set of all bounded linear operators on a Hilbert space $\mathfrak{H}$, denoted $\mathscr{B}(\mathfrak{H})$, defines a C^*-algebra with identity,[3] we introduce the concept of *representation* as follows:

Definition C.2.2. *A* representation *π of a C^*-algebra $\mathfrak{A}$ with identity in a Hilbert space $\mathfrak{H}$ is a $*$-homomorphism of $\mathfrak{A}$ into the C^*-algebra $\mathscr{B}(\mathfrak{H})$ of bounded linear operators in $\mathfrak{H}$, i.e., a linear mapping $\pi(c_1A_1 + c_2A_2) = c_1\pi(A_1) + c_2\pi(A_2)$, $*$-preserving $\pi(A^*) = (\pi(A))^*$, and multiplicative $\pi(A_1A_2) = \pi(A_1)\pi(A_2)$, $\pi(\mathbf{1}_{\mathfrak{A}}) = \mathbb{I}_{\mathfrak{H}}$, with $\mathbb{I}_{\mathfrak{H}}$ being the identity operator. The representation is called* faithful *if it is injective (i.e.,* $\ker(\pi) =$

[2]It is possible to prove that the set of positive linear functionals on a C^*-algebra $\mathfrak{A}$ keeps separating the elements of the algebra [4]. However, one can think in the possibility that the states with physical interpretation (*physical states*) is smaller than the set of all positive linear functional on $\mathfrak{A}$; in this case, the set of physical states must separate the observables (and, conversely, the observables separate the states).

[3]The sums and products of elements of $\mathscr{B}(\mathfrak{H})$ are defined in the standard manner, and the set is equipped with the operator norm $\|A\| := \sup\{\|A\Psi\|_{\mathfrak{H}}\,;\, \Psi \in \mathfrak{H}\,,\, \|\Psi\|_{\mathfrak{H}} = 1\}$, with $\|\cdot\|_{\mathfrak{H}}$ being the norm defined by the inner product. The Hilbert space adjoint operation defines an involution on $\mathscr{B}(\mathfrak{H})$, which becomes a C^*-algebra.

$\{\Psi \in \mathfrak{H} \,:\, \pi(A)\Psi = 0\,,\, \forall\, A \in \mathfrak{A}\} = \{0\}$*; π is called a $*$-isomorphism in this case). The representation is* irreducible *if $\{0\}$ and $\mathfrak{H}$ are the only closed subspaces invariant under π; in this case, every vector $\Psi \in \mathfrak{H}$ is* cyclic*, i.e., $\pi(\mathfrak{A})\Psi := \{\pi(A)\Psi\,;\, A \in \mathfrak{A}\}$ is dense in $\mathfrak{H}$. Two representations of the same algebra $\mathfrak{A}$, $\pi_i : \mathfrak{A} \to \mathscr{B}(\mathfrak{H}_i)$, (i=1,2), are said to be* unitarily equivalent *if there exists a unitary transformation $U : \mathfrak{H}_1 \to \mathfrak{H}_2$ verifying $U\pi_1(A)U^{-1} = \pi_2(A)$, $\forall\, A \in \mathfrak{A}$.*

Now, we can enunciate the following fundamental result due to Gel'fand, Naimark, and Segal (see [4] for a proof):

Theorem C.2.1 (GNS construction)**.** *Given a state ω over a C^*-algebra $\mathfrak{A}$ with identity, there exist a Hilbert space $\mathfrak{H}_\omega$ and a representation $\pi_\omega : \mathfrak{A} \to \mathscr{B}(\mathfrak{H}_\omega)$ such that:*

1. *$\mathfrak{H}_\omega$ contains a cyclic vector Ψ_ω, i.e., $\overline{\pi(\mathfrak{A})\Psi_\omega} = \mathfrak{H}_\omega$, with the bar denoting closure.*
2. *$\omega(A) = \langle \Psi_\omega \,|\, \pi_\omega(A)\Psi_\omega\rangle_{\mathfrak{H}_\omega}$, for all $A \in \mathfrak{A}$, where $\langle\cdot|\cdot\rangle_{\mathfrak{H}_\omega}$ denotes the inner product in $\mathfrak{H}_\omega$.*
3. *Every other representation π in a Hilbert space $\mathfrak{H}$ with a cyclic vector Ψ such that $\omega(A) = \langle \Psi \,|\, \pi(A)\Psi\rangle_{\mathfrak{H}}$, $\forall\, A \in \mathfrak{A}$, is unitarily equivalent to π_ω, i.e., there exists a unitary transformation $U : \mathfrak{H} \to \mathfrak{H}_\omega$ satisfying $U\pi(A)U^{-1} = \pi_\omega(A)$, $\forall\, A \in \mathfrak{A}$, and $U\Psi = \Psi_\omega$.*

The set $(\mathfrak{H}_\omega, \pi_\omega, \Psi_\omega)$ satisfying these conditions is called the GNS triplet*, containing the* cyclic representation space *$\mathfrak{H}_\omega$, the* cyclic representation *π_ω, and the* cyclic vector *Ψ_ω associated with the state ω.*

Note that every *unit* vector Φ of the cyclic representation space $\mathfrak{H}_\omega$ defines a state ω_Φ on $\mathfrak{A}$ through the formula $\omega_\Phi(A) := \langle \Phi \,|\, \pi(A)\Phi\rangle_{\mathfrak{H}_\omega}$, $\forall\, A \in \mathfrak{A}$; indeed, this is a positive normalized linear functional on $\mathfrak{A}$. The GNS construction then provides a mapping between states and Hilbert space vectors, usually called *state vectors* in this context. If Φ is a cyclic vector, then according to *point 3* of GNS theorem, the representation π_ω is unitarily equivalent to the cyclic representation defined by the state ω_Φ. It is possible to prove the following result [4]:

Theorem C.2.2. *The cyclic representation π_ω is irreducible iff the state ω is pure.*

It easily follows from the above theorem that, when dealing with an irreducible GNS construction, any state vector Φ of the cyclic representation space $\mathfrak{H}_\omega$ defines a pure state ω_Φ on $\mathfrak{A}$. In such a situation, it is not possible to represent a mixed state by a state vector, but rather by a *density operator*: Given a positive trace class operator D on $\mathfrak{H}_\omega$ ($\mathrm{Tr}(|D|) < +\infty$), with trace equal to one ($\mathrm{Tr}(D) = 1$), the formula

$$\omega_D(A) := \mathrm{Tr}(D\pi_\omega(A))\,, \;\; \forall\, A \in \mathfrak{A}\,, \tag{C.3}$$

defines a state on $\mathfrak{A}$. The set $\mathfrak{F}(\pi_\omega)$ of all states of this form (called *normal states*) defines the *folium of the representation* π_ω. Pure states are included in this class if D

is a one-dimensional projection.

A state ω is *faithful* if $\omega(A^*A) > 0$, $\forall\, A \neq 0$, and then the corresponding GNS representation is also faithful. In general, the GNS realization of a C^*-algebra $\mathfrak{A}$ as a family of operators in a Hilbert space may not be a $*$-isomorphism. Nevertheless, the Gel'fand-Naimark theorem guarantees the existence of at least one faithful representation [4]:

Theorem C.2.3 (Gel'fand-Naimark characterization of C^*-algebras)**.** *A C^*-algebra is isomorphic to an algebra of bounded operators in a Hilbert space.*

This result encodes the Dirac-von Neumann quantum theory axiom according to which the observables of any quantum system are realized as bounded operators in a Hilbert space. Only for *abelian* (or *commutative*) algebras (as characteristic of classical systems) this representation is equivalent to a description in terms of continuous functions, the states acting in this case as probability measures (see next section) [4]:

Theorem C.2.4 (Gel'fand-Naimark characterization of abelian C^*-algebras)**.** *Let $\mathfrak{A}$ be an abelian C^*-algebra with identity. A* character *of $\mathfrak{A}$ is a nonzero linear map $\omega : \mathfrak{A} \to \mathbb{C}$ such that $\omega(AB) = \omega(A)\omega(B)$, $\forall\, A, B \in \mathfrak{A}$. The* Gel'fand spectrum *of $\mathfrak{A}$, denoted $sp(\mathfrak{A})$, is defined as the set of all characters on $\mathfrak{A}$. It is a subset of the dual $\mathfrak{A}^*$ of $\mathfrak{A}$. It is proved that a state ω is pure iff it is a character. The set $sp(\mathfrak{A})$, endowed with the weak* topology[4] inherited from the dual $\mathfrak{A}^*$ of $\mathfrak{A}$, is a compact Hausdorff topological space. Moreover, $\mathfrak{A}$ is isometrically isomorphic to the C^*-algebra of continuous functions over $sp(\mathfrak{A})$.*

Given a state ω (i.e., a normalized positive linear functional) on the C^*-algebra $\mathfrak{A}$, the Riesz-Markov representation theorem then ensures the existence of a unique associated probability measure μ_ω on $sp(\mathfrak{A})$ such that

$$\omega(A) = \int_{sp(\mathfrak{A})} f_A \, \mathrm{d}\mu_\omega \,, \quad \mu_\omega(sp(\mathfrak{A})) = \omega(\mathbf{1}) = 1 \,,$$

where f_A is the *Gel'fand transform* of $A \in \mathfrak{A}$ assigned by the isomorphism.

C.2.1 Classical systems

Let us consider a classical system described by a phase space Γ, that will be assumed to be compact in order to facilitate subsequent discussions.[5] This is the case if the system under study is confined into a finite spatial region and its energy is also bounded.

[4]In the weak* topology, a neighborhood basis of an element $\omega \in \mathfrak{A}^*$ is indexed by finite sets of elements $A_1, \ldots, A_n \in \mathfrak{A}$, and $\epsilon > 0$; one has the sets $\mathscr{U}(\omega; A_1, \ldots, A_n; \epsilon) = \{\omega' \in \mathfrak{A} : |\omega'(A_i) - \omega(A_i)| < \epsilon\,,\ i = 1, \ldots, n\}$.

[5]Note, however, that this excludes phase spaces characterized by cotangent bundles. The possibility to consider these cases will be discussed later.

The classical observables will belong to a proper class of functions on Γ, for instance the continuous real functions $\mathcal{O}_c = C(\Gamma;\mathbb{R})$. It is then straightforward to define an *abelian* C^*-algebra $\mathfrak{A}_c$ with identity by considering the complex continuous functions $C(\Gamma;\mathbb{C})$ (the algebraic product being the pointwise composition of functions), where the identity $\mathbf{1}$ is the unit function[6] $f = 1$, the $*$ bijection is given by the standard complex conjugation $\bar{\ }: \mathbb{C} \to \mathbb{C}$, and the norm for elements $f \in \mathfrak{A}_c$ is defined as $\|f\| := \sup_{x\in\Gamma} |f(x)|$. The product is continuous in the norm topology since $\|fg\| \leq \|f\|\|g\|$, and the C^*-condition $\|f^*f\| = \|f\|^2$ is obviously verified. $\mathcal{O}_c$ coincides with the class of functions satisfying $f = \bar{f} = f^*$, and we clearly deal with a special Segal system.

Given a state ω on the abelian C^*-algebra $\mathfrak{A}_c$ of continuous functions on the compact (Hausdorff) phase space Γ, the Riesz-Markov representation theorem guarantees the existence of a unique associated probability measure μ_ω on Γ such that

$$\omega(f) = \int_\Gamma f(x)\,\mathrm{d}\mu_\omega(x)\,, \quad f \in \mathcal{O}_c\,,$$

with $\mu_\omega(\Gamma) = \omega(\mathbf{1}) = 1$. Conversely, every probability measure μ defines a state ω_μ on $\mathfrak{A}_c$ through the formula $\omega_\mu(f) = \int_\Gamma f(x)\,\mathrm{d}\mu(x)$ and, thus, we can identify the classical space of states with the space of probability measures on Γ. In particular, pure states –those that cannot be expressed as convex linear combinations of other states– correspond to singular δ measures, i.e., probability measures concentrated on definite points $x_0 \in \Gamma$, in such a way that $\omega_{x_0}(f) = f(x_0)$. Note that for this class of states the mean square deviation or *variance* relative to ω_{x_0} of *any* observable $f \in \mathcal{O}_c$,

$$\Delta^2_{\omega_{x_0}}(f) := \omega_{x_0}(f^2) - \omega_{x_0}(f)^2\,,$$

is identically zero. This is the reason why these states are also called *dispersion free states*. The idealized nature of such states is a consequence not only of the experimental impossibility to determine with infinite precision the position and momentum of particles, but also of the need to perform some type of statistical description when the number of degrees of freedom of the system is too large, typically $\sim 10^{23}$, owing to the unfeasibility of setting out an initial value problem in this case. The realistic states define, in this way, probability distributions on the *random variables* describing the observables of the system. From a theoretical point of view, however, there is no obstruction to closely approximate the idealized pure states, obtaining states for which the dispersion of the configuration and momentum variables are arbitrarily small. This fact lies on the assumption that the algebra of observables is commutative, as will be clarified in the next section.

[6]For noncompact phase spaces, the continuous functions are restricted to vanish at infinity, so that $f = 1$ is not an observable and the resulting C^*-algebra is not unital. The absence of an identity can to a large extent be avoided, however, by embedding this algebra into another suitable one with identity [5].

C.2.2 Quantum systems

The following theorem is easily shown to be true for any noncommutative C^*-algebra $\mathfrak{A}$ (the result is trivial for the abelian case):

Theorem C.2.5 (Heisenberg uncertainty relations)**.** *Given two observables $A, B \in \mathfrak{A}$, ($A = A^*$, $B = B^*$), the inequality*

$$\Delta_\omega(A) \cdot \Delta_\omega(B) \geq \frac{1}{2}|\omega([A, B])|$$

holds for any state ω on $\mathfrak{A}$, where $\Delta_\omega(A) = (\omega(A^2) - \omega(A)^2)^{1/2}$ denotes the variance of A respect to ω, and $[A, B] := AB - BA$ is the commutator *of the observables.*

Proof. Define the observables $A' := A - \omega(A)\mathbf{1}$ and $B' := B - \omega(B)\mathbf{1}$. Given the positivity of $(A' - i\lambda B')(A' + i\lambda B')$, $\forall\, \lambda \in \mathbb{R}$, one has $\omega(A'^2) + \lambda^2\omega(B'^2) + \lambda\omega(i[A', B']) \geq 0$; the positive-definiteness of this quadratic form in λ requires $4\omega(A'^2)\omega(B'^2) \geq |\omega(i[A', B'])|^2$, so that $\Delta_\omega(A) \cdot \Delta_\omega(B) \geq |\omega([A, B])|/2$. Here, we have made use of the equivalent expression $\Delta_\omega(A)^2 = \omega((A - \omega(A)\mathbf{1})^2)$ and the fact that $[A', B'] = [A, B]$. □

Using convincing physical arguments, Heisenberg showed that it is not possible to measure the position X of an atomic particle without affecting its momentum P, in such a way that the uncertainties of the components of these observables in definite spatial directions are subject to verify the inequalities[7] $\Delta_\omega(X_k) \cdot \Delta_\omega(P_{k'}) \geq (\hbar/2)\delta(k, k')$, for all physical states. According to the theorem proved above, it is then expected that the commutator of these quantities satisfies the *Heisenberg commutation relations*[8]

$$[X_k, P_{k'}] = i\hbar\delta(k, k')\mathbf{1}\,.$$

Thus, the atomic particles are characterized by noncommutative algebras. Only in the classical limit $\hbar \to 0$, where the perturbing effects of the measurement processes can be ignored, we recover the abelian algebras.

In order to analyze the probabilistic interpretation of quantum physics, take a *normal* element $A \in \mathfrak{A}$, (by definition, A and A^* are assumed to commute) and construct the abelian C^*-algebra $\mathfrak{A}(A)$ generated by $\{\mathbf{1}, A, A^*\}$. The Gel'fand spectrum $sp(\mathfrak{A}(A))$ coincides in this case with the spectrum[9] $\sigma(A)$ of A, i.e.,

$$sp(\mathfrak{A}(A)) \equiv \sigma(A) := \{\lambda \in \mathbb{C} \,:\, (\lambda\mathbf{1} - A) \text{ does not have a two sided inverse in } \mathfrak{A}\}\,.$$

[7] Here, subscript denotes the component of the observables in the k-th spatial direction.

[8] On the contrary, it is possible to measure any two components of the position (or the momentum) simultaneously, so that the corresponding commutators must vanish, $[X_k, X_{k'}] = 0 = [P_k, P_{k'}]$.

[9] More generally, if $\mathfrak{A}$ is an abelian C^*-algebra generated by $\{\mathbf{1}, A_i, A_i^*\}_{i=1,\ldots,n}$ (the set assumed to be algebraically independent), then the Gel'fand spectrum of $\mathfrak{A}$ is given by the Cartesian product $sp(\mathfrak{A}) = \times_{i=1}^n \sigma(A_i)$.

According to *Theorem C.2.4* and the discussion below it, given a generic state ω on $\mathfrak{A}(A)$ there exists a probability measure $\mu_{\omega,A}$ supported on $\sigma(A)$ such that

$$\omega(B) = \int_{\sigma(A)} f_B(\lambda)\,\mathrm{d}\mu_{\omega,A}(\lambda)\,, \quad B \in \mathfrak{A}(A)\,,$$

where f_B denotes the Gel'fand transform of B. In particular,

$$\omega(A) = \int_{\sigma(A)} \lambda\,\mathrm{d}\mu_{\omega,A}(\lambda)\,.$$

If the element A is an observable ($A = A^*$), then it can be shown that[10] $\sigma(A) \subseteq [-\|A\|, \|A\|] \subset \mathbb{R}$, and the (Born) probabilistic interpretation of measurements on A is the following: The possible measured values of the observable A belong to its spectrum $\sigma(A)$, and the probability that the observable takes values within the Borel set $\Delta \in \mathrm{Bor}(\mathbb{R})$ when the system is in the state ω is given by $\mu_{\omega,A}(\Delta)$; compare this with equation (C.2). In the GNS construction context, $\mu_{\omega,A}(\Delta) = \langle \Psi_\omega \,|\, E^{\pi_\omega(A)}(\Delta)\Psi_\omega\rangle_{\mathfrak{H}_\omega}$, where $E^{\pi_\omega(A)}$ denotes the unique spectral measure associated with the (bounded and self-adjoint) operator $\pi_\omega(A)$. The two main differences of noncommutative algebras with respect to the abelian case are the following: (i) The probability measure $\mu_{\omega,A}$ depends on the observable A; as a consequence of this, the algebra of observables $\mathfrak{A}$ cannot be realized as an algebra of random variables on a single probability space. This can be done for any abelian subalgebra of $\mathfrak{A}$, but the probability spaces associated with noncommuting observables will in fact be different; (ii) the probability measure associated with pure states are not δ measures, i.e., the statistical interpretation cannot be avoided even if restricting our considerations to pure states; the statistical description is, thus, intrinsic to any quantum system.

For a concrete example, let us consider the simplest physical system consisting of a single spinless point particle moving along the real line (this study can be easily generalized to higher dimensions). The basic classical observables are the position X and the momentum P of the particle. Tentatively, one could propose as quantum algebra of observables that generated by $\{\mathbf{1}, X, P\}$ satisfying the Heisenberg commutation relations (from now on we will consider units such that $\hbar = 1$)

$$[X, P] = i\mathbf{1}\,, \quad [X, X] = 0 = [P, P]\,. \tag{C.4}$$

This *Heisenberg algebra*, however, does not fall into the Segal scheme, because it is a well-known fact that any X and P satisfying (C.4) cannot be realized as bounded self-adjoint elements of a C^*-algebra.[11] This is not a surprise from the operational

[10]For a positive element, $\sigma(A)$ is a subset of the positive half-line, $\sigma(A) \subseteq [0, \|A\|] \subset \mathbb{R}_+$.

[11]Indeed, by induction one gets $[X, P^n] = inP^{n-1}$, $n \in \mathbb{N}$, which implies $n\|P^{n-1}\| \leq \|XP^n\| + \|P^nX\| \leq 2\|X\|\|P\|\|P^{n-1}\|$ for some C^*-norm. Since $\|P^{n-1}\| \neq 0$ –otherwise, $P = 0$ and, hence, (C.4) is not verified–, one finally obtains $\|X\|\|P\| \geq n/2$, $\forall\, n \in \mathbb{N}$.

point of view: The technical limitations of the measuring apparatuses imply that only bounded functions of X and P can be measured. Of course, one could try to obtain a representation of the Heisenberg algebra in terms of unbounded self-adjoint operators X and P with dense domains in a certain Hilbert space $\mathfrak{H}$, but this would not follow the operational description given in this section. Nevertheless, this problem can be easily overcome by introducing the so-called *Weyl algebra* –in fact, this will allow us to recover the Heisenberg algebra in a definite sense at the end of this section. Consider the bounded formal functions of X and P, called *Weyl operators*,

$$U(\alpha) := \exp(i\alpha X)\,, \quad V(\beta) := \exp(i\beta P)\,, \quad \alpha, \beta \in \mathbb{R}\,. \tag{C.5}$$

The Heisenberg commutation relations (C.4) are now replaced by the *Weyl relations*

$$\begin{aligned} &U(\alpha)V(\beta) = V(\beta)U(\alpha)\exp(-i\alpha\beta)\,, \\ &U(\alpha)U(\beta) = U(\alpha+\beta)\,, \quad V(\alpha)V(\beta) = V(\alpha+\beta)\,, \end{aligned}$$

formally obtained from (C.4) and (C.5) by applying the Baker-Campbell-Hausdorff formula $\exp(A)\exp(B) = \exp(A + B + [A, B]/2)$, with $[A, B]$ assumed to be a c-number. There is a natural $*$-operation on the Weyl algebra generated by linear complex combinations and products of these basics elements, as suggested by the self-adjointness of X and P,

$$U(\alpha)^* = U(-\alpha)\,, \quad V(\beta)^* = V(-\beta)\,,$$

so that $U(\alpha)$ and $V(\beta)$ are unitary, i.e., $U(\alpha)^*U(\alpha) = U(\alpha)U(\alpha)^* = \mathbf{1}$, and similarly for $V(\beta)$. It is possible to prove the existence of a unique C^*-norm such that the completion of the Weyl algebra in this norm is a (non commutative) C^*-algebra [4], called the Weyl C^*-algebra and denoted $\mathfrak{A}_{\mathrm{Weyl}}$. According to the C^*-condition, we have $\|U(\alpha)\| = \|V(\beta)\| = \|U(\alpha)V(\beta)\| = 1$, $\forall\,\alpha, \beta \in \mathbb{R}$. One faces now the problem of finding suitable representations for this algebra. The following theorem was rigorously proved for the first time by von Neumann [1]:

Theorem C.2.6 (von Neumann)**.** *All regular irreducible representations of the Weyl C^*-algebra $\mathfrak{A}_{\mathrm{Weyl}}$ in a separable Hilbert space are unitarily equivalent.*

Here, a representation $\pi : \mathfrak{A}_{\mathrm{Weyl}} \to \mathscr{B}(\mathfrak{H})$ into a separable Hilbert space $\mathfrak{H}$ is said to be *regular* if $\pi(U(\alpha))$ and $\pi(V(\beta))$ are (one-parameter unitary groups) strongly continuous in the real α and β parameters, respectively. Thus, it suffices to find one regular irreducible representation to univocally characterize all the representations of this class; concretely, a well-known solution is given by the *Schrödinger representation* π_s into the separable Hilbert space $\mathfrak{H}_s = L^2(\mathbb{R}, \mathrm{d}x)$, where for all pure states (L^2-functions) $\Psi \in \mathfrak{H}_s$,

$$\left(\pi_s(U(\alpha))\Psi\right)(x) = \exp(i\alpha x)\Psi(x)\,, \quad \left(\pi_s(V(\beta))\Psi\right)(x) = \Psi(x+\beta)\,.$$

It is easy to check the regularity and irreducibility of this representation. Note that the strong continuity in the α and β parameters ensures, by virtue of Stone's theorem, the existence of (unbounded) self-adjoint generators X and P with dense domain in $\mathfrak{H}_s$. In particular, the Schwartz space $\mathscr{S}(\mathbb{R})$ of smooth rapidly decreasing functions in $\mathbb{R}$ is a common invariant dense domain of essential self-adjointness for X and P, where the Heisenberg commutation relations (C.4) are satisfied. For all $\Psi \in \mathscr{S}(\mathbb{R})$,

$$(X\Psi)(x) = x\Psi(x)\,, \quad (P\Psi)(x) = -i\Psi'(x)\,,$$

where the prime denotes derivative. Therefore, thanks to regularity, the Heisenberg algebra can be recovered in a definite sense from the Weyl C^*-algebra.

C.3 Algebraic dynamics

Consider a C^*-algebra of observables, $\mathfrak{A}$. An autonomous (algebraic) dynamical system is a triplet $(\mathfrak{A}, I \subseteq \mathbb{R}, \alpha_t)$, with α_t, $t \in I$, being a (weakly) continuous one-parameter group of $*$-automorphisms (i.e., $*$-isomorphisms of $\mathfrak{A}$ into itself). An (irreducible) representation of the algebra $\pi : \mathfrak{A} \to \mathscr{B}(\mathfrak{H})$ is called *stable under time evolution* if π and $\pi \circ \alpha_t$ (equivalently $\pi \circ \alpha_t^{-1}$) are unitarily equivalent for all $t \in I$. In this case, there exists a unitary operator-valued function $U(t) : \mathfrak{H} \to \mathfrak{H}$, called the *time-evolution operator*, such that

$$\pi(\alpha_t(A)) = U(t)^{-1}\pi(A)U(t)\,, \quad \forall\, A \in \mathfrak{A}\,. \tag{C.6}$$

Furthermore, the weak continuity of α_t ensures the weak continuity of $U(t)$, so that by Stone's theorem we can write

$$U(t) = \exp(-itH)\,, \quad t \in \mathbb{R}\,,$$

where the generator H, called the *Hamiltonian operator*, is a self-adjoint operator with dense domain $\mathscr{D}_H \subset \mathfrak{H}$. It is obtained as the strong limit $s-\lim_{t\to 0} t^{-1}(U(t) - \mathbb{I})\Psi = -iH\Psi$, $\Psi \in \mathscr{D}_H$. Note that the H operator is unbounded in general –so it does not belong to the C^*-algebra of physical observables– and its expression depends on the concrete representation π. It is also important to realize that the relations (C.6) determine $U(t)$ univocally modulo a complex phase, so that the quantum Hamiltonian is unique up to an (irrelevant) real term proportional to the identity. Let $\Psi_0 \in \mathscr{D}_H$ be a state vector of the stable representation π, and let ω_0 be the pure state defined by it. Then, we have

$$\omega_0(\alpha_t(A)) = \langle \Psi_0 \,|\, U(t)^{-1}\pi(A)U(t)\Psi_0\rangle_{\mathfrak{H}} = \langle U(t)\Psi_0 \,|\, \pi(A)U(t)\Psi_0\rangle_{\mathfrak{H}} =: \omega_t(A)\,,$$

where ω_t is the pure state defined by $U(t)\Psi_0 =: \Psi(t) \in \mathfrak{H}$. This is an algebraic representation of the evolution of states in the Schrödinger picture. $\mathscr{D}_H$ contains a dense subdomain $\mathscr{D} \subset \mathscr{D}_H$ invariant under the action of $U(t)$, in which the Hamiltonian is essentially self-adjoint. For $\Psi_0 \in \mathscr{D}$, differentiating the state vector $\Psi(t)$ with respect to the time parameter t, we obtain the *Schrödinger equation*

$$i\frac{\mathrm{d}}{\mathrm{d}t}\Psi(t) = H\Psi(t)\,, \quad \Psi(0) = \Psi_0\,.$$

The time evolution can be equivalently formulated in terms of observables. Indeed, the $*$-automorphism $A \mapsto \alpha_t \circ A$, $\forall\, A \in \mathfrak{A}$ with $A = A^*$, can be interpreted as the algebraic representation of the evolution of observables in the Heisenberg picture. Denoting $A(t) := \pi(\alpha_t A) = U(t)^{-1}\pi(A)U(t)$ (see equation (C.6)), and differentiating this relation with respect to t, one finally obtains the *Heisenberg equation*

$$\frac{\mathrm{d}}{\mathrm{d}t}A(t) = i[H, A(t)]\,, \quad A(0) = \pi(A)\,.$$

References

1 J. Von Neumann, *Mathematical Foundations of Quantum Mechanics*, Princeton University Press (1964).

2 H. Araki, *Mathematical Theory of Quantum Fields*, The International Series of Monographs on Physics, Vol. 101, Oxford University Press (1999).

3 I. E. Segal, "Postulates for General Quantum Mechanics", The Annals of Mathematics **48**, 930-948 (1947); *Mathematical Problems of Relativistic Physics*, Lectures in Applied Mathematics Series, American Mathematical Society (1967).

4 F. Strocchi, *An Introduction to the Mathematical Structure of Quantum Mechanics. A Short Course for Mathematicians*, Advanced Series in Mathematical Physics, Vol. 27, World Scientific (2005).

5 O. Bratteli and D. W. Robinson, *Operator Algebras and Quantum Statistical Mechanics I. C^*- and W^*-Algebras. Symmetry Groups. Decomposition of States*, 2ª ed., Springer (1997).

6 C. Isham, *Lectures on Quantum Theory: Mathematical and Structural Foundations*, World Scientific (1995).

7 G. W. Mackey, *The Mathematical Foundations of Quantum Mechanics*, W. A. Benjamin Inc., New York (1963).

8 B. Simon, *Quantum Mechanics for Hamiltonians Defined as Quadratic Forms*, Princeton Univ. Press. Princeton, N. J. (1971).

Appendix D
The Time-dependent Harmonic Oscillator

D. G. Vergel and E. J. S. Villaseñor
Annals of Physics 324, 1360-1385 (2009)

In this appendix, we reformulate the quantum theory of a single one-dimensional time-dependent harmonic oscillator, summarizing some basic results concerning the unitary implementation of the dynamics. This is done by employing techniques different from those used so far to derive the Feynman propagator. In particular, we calculate the transition amplitudes for the usual harmonic oscillator eigenstates and define suitable semiclassical states for some physically relevant systems such as Gowdy-like oscillators.

D.1 Properties of the TDHO equation

We will review in this section some properties of the classical equation of motion of a single harmonic oscillator with time-dependent frequency, from now on referred to as the TDHO equation, and its connection with the so-called Ermakov-Pinney equation, which plays an auxiliary role in the calculation of invariants for nonquadratic Hamiltonian systems. The TDHO equation is given by

$$\ddot{u}(t) + \kappa(t)u(t) = 0\,, \quad t \in I = (t_-, t_+) \subseteq \mathbb{R}\,, \tag{D.1}$$

where $\kappa : I \rightarrow \mathbb{R}$ is a real-valued continuous function and time-derivatives are denoted by dots. Given an initial time $t_0 \in I$, let c_{t_0} and s_{t_0} be the independent solutions of (D.1) such that $c_{t_0}(t_0) = \dot{s}_{t_0}(t_0) = 1$ and $s_{t_0}(t_0) = \dot{c}_{t_0}(t_0) = 0$. These can be written in terms of any set of independent solutions to (D.1), say u_1 and u_2, as

$$c_{t_0}(t) = \frac{\dot{u}_2(t_0)u_1(t) - \dot{u}_1(t_0)u_2(t)}{W(u_1, u_2)}\,, \quad s_{t_0}(t) = \frac{u_1(t_0)u_2(t) - u_2(t_0)u_1(t)}{W(u_1, u_2)}\,, \tag{D.2}$$

where $(t_0, t) \in I \times I$ and $W(u_1, u_2) := u_1\dot{u}_2 - \dot{u}_1 u_2$ denotes the (time-independent) Wronskian of u_1 and u_2. In what follows, we will use the notation $c(t, t_0) := c_{t_0}(t)$, $\dot{c}(t, t_0) := \dot{c}_{t_0}(t)$, $s(t, t_0) := s_{t_0}(t)$, and $\dot{s}(t, t_0) := \dot{s}_{t_0}(t)$. Note that the s function belongs to the class $C^2(I \times I)$, whereas $c(\cdot, t_0) \in C^2(I)$ and $c(t, \cdot) \in C^1(I)$. As a concrete example, for the time-independent harmonic oscillator (TIHO) with constant frequency $\kappa(t) = \kappa_0 \in \mathbb{R}$, we simply get ($\omega > 0$)

$$\kappa_0 = \omega^2 , \quad c(t,t_0) = \cos((t-t_0)\omega) , \quad s(t,t_0) = \omega^{-1}\sin((t-t_0)\omega) ; \quad \text{(D.3)}$$

$$\kappa_0 = 0 , \quad c(t,t_0) = 1 , \quad s(t,t_0) = t - t_0 ; \quad \text{(D.4)}$$

$$\kappa_0 = -\omega^2 , \quad c(t,t_0) = \cosh((t-t_0)\omega) , \quad s(t,t_0) = \omega^{-1}\sinh((t-t_0)\omega) . \quad \text{(D.5)}$$

In fact, as well known from Sturm's theory, the c and s functions corresponding to arbitrary frequencies share several properties with the usual cosine and sine functions. Firstly, their Wronskian is normalized to unit, $W(c,s) = 1$. Hence, if one of them vanishes for some time $t = t_*$, then the other is automatically different from zero at that instant. In view of this condition and relations (D.2), their time-derivatives satisfy

$$\dot{s}(t,t_0) = c(t_0,t) , \quad \dot{c}(t,t_0) = \frac{c(t,t_0)c(t_0,t) - 1}{s(t,t_0)} , \quad \text{(D.6)}$$

where the last equation must be understood as a limit for those values of the time parameter t_* such that $s(t_*,t_0) = 0$. The odd character of the sine function translates into the condition $s(t_0,t) = -s(t,t_0)$. Finally, the well known formula for the sine of a sum of angles can be generalized as

$$s(t_2,t_1) = c(t_1,t_0)s(t_2,t_0) - c(t_2,t_0)s(t_1,t_0) . \quad \text{(D.7)}$$

It is well known that solutions to the TDHO equation (D.1) are related to certain non-linear differential equations. Here, we will restrict our attention to the so-called Ermakov-Pinney (EP) equation (see [1, 2]; the interested reader is strongly suggested to consult the historical account of [3] and references therein). Let

$$A = A^t = \begin{bmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{bmatrix} \in \mathrm{Mat}_{2\times 2}(\mathbb{R})$$

be a positive definite quadratic form with $\det A = 1$. Then, the (never vanishing) function $\rho : I \to (0, +\infty)$ defined as

$$\rho(t) := \sqrt{a_{11}c^2(t,t_0) + a_{22}s^2(t,t_0) + 2a_{12}s(t,t_0)c(t,t_0)} \quad \text{(D.8)}$$

verifies the EP equation

$$\ddot{\rho}(t) + \kappa(t)\rho(t) = \frac{1}{\rho^3(t)} , \quad t \in I . \quad \text{(D.9)}$$

According to (D.2), the most general analytic solution to (D.9) can be written as [4, 5]

$$\rho(t) = \sqrt{b_{11}u_1^2(t) + b_{22}u_2^2(t) + 2b_{12}u_1(t)u_2(t)} , \quad \text{(D.10)}$$

where, as a consequence of (D.8) and (D.9), the coefficients b_{11}, b_{12}, $b_{22} \in \mathbb{R}$ satisfy $W^2(u_1,u_2) = (b_{11}b_{22} - b_{12}^2)^{-1} > 0$. Conversely, given *any* solution to the EP equation it is possible to find the general solution to the TDHO equation. Indeed, it is straightforward to prove the following theorem.

Theorem D.1.1. *Let ρ be any solution to the EP equation (D.9); then, the c and s solutions to (D.1) are given by*

$$c(t,t_0) = \frac{\rho(t)}{\rho(t_0)}\cos\left(\int_{t_0}^{t}\frac{\mathrm{d}\tau}{\rho^2(\tau)}\right) - \rho(t)\dot{\rho}(t_0)\sin\left(\int_{t_0}^{t}\frac{\mathrm{d}\tau}{\rho^2(\tau)}\right), \tag{D.11}$$

$$s(t,t_0) = \rho(t)\rho(t_0)\sin\left(\int_{t_0}^{t}\frac{\mathrm{d}\tau}{\rho^2(\tau)}\right), \quad (t,t_0)\in I\times I\,. \tag{D.12}$$

Remark D.1.1. By using (D.11) and (D.12), it is possible to find other ρ-independent objects. For example, the combination

$$\frac{\rho(t_0)}{\rho(t)}\cos\left(\int_{t_0}^{t}\frac{\mathrm{d}\tau}{\rho^2(\tau)}\right) + \rho(t_0)\dot{\rho}(t)\sin\left(\int_{t_0}^{t}\frac{\mathrm{d}\tau}{\rho^2(\tau)}\right) = c(t_0,t) = \dot{s}(t,t_0)$$

and the zeros of $s(t,t_0)$, characterized by

$$\int_{t_0}^{t}\frac{\mathrm{d}\tau}{\rho^2(\tau)} \equiv 0 \pmod{\pi}\,,$$

are independent of the particular solution ρ to the EP equation. These results will be profusely applied along this appendix.

D.2 Unitary quantum time evolution

D.2.1 General framework

The *canonical* phase space description of the classical system under consideration consists of a nonautonomous Hamiltonian system $(I\times\mathbf{P},\mathrm{d}t,\boldsymbol{\omega},H(t))$. Here, $\mathbf{P}:=\mathbb{R}^2$ denotes the space of Cauchy data (q,p) endowed with the usual symplectic structure $\boldsymbol{\omega}((q_1,p_1),(q_2,p_2)) := p_1q_2 - p_2q_1$, $\forall\,(q_1,p_1),(q_2,p_2)\in\mathbf{P}$. The triplet $(I\times\mathbf{P},\mathrm{d}t,\boldsymbol{\omega})$ then has the mathematical structure of a cosymplectic vector space. The time-dependent Hamiltonian $H(t):\mathbf{P}\to\mathbb{R}$, $t\in I$, is given by

$$H(t,q,p) := \frac{1}{2}\Big(p^2+\kappa(t)q^2\Big)\,. \tag{D.13}$$

The solution to the corresponding Hamilton equations with initial Cauchy data (q,p) at time t_0 can be written down as

$$\begin{bmatrix} q_H(t,t_0) \\ p_H(t,t_0)\end{bmatrix} = \mathcal{T}_{(t,t_0)}\cdot\begin{bmatrix} q\\ p\end{bmatrix},\quad \mathcal{T}_{(t,t_0)} := \begin{bmatrix} c(t,t_0) & s(t,t_0)\\ \dot{c}(t,t_0) & \dot{s}(t,t_0)\end{bmatrix}. \tag{D.14}$$

Note that the properties stated in *section D.1* about the c and s solutions to the TDHO equation (D.1) guarantee that $\mathcal{T}_{(t,t_0)}\in SL(2,\mathbb{R}) = SP(1,\mathbb{R})$ for all $(t,t_0)\in I\times I$, i.e., the classical time evolution is implemented by symplectic transformations.

We now formulate the quantum theory of the TDHO by defining the corresponding Weyl C^*-algebra of quantum observables $\mathscr{W}(\mathbf{P})$ and choosing a suitable representation in terms of self-adjoint operators in some separable Hilbert space $\mathscr{H}$. As we pointed out in *appendix C*, the natural realization for this algebra is given by the well-known Schrödinger representation $(Q\psi)(q) = q\psi(q)$, $(P\psi)(q) = -i\psi'(q)$, $\psi \in L^2(\mathbb{R})$. Another possibility is to represent the canonical commutation relations (CCR) in the space $L^2(\mathbb{R}, \mathrm{d}\mu_\alpha)$ where, given some $\alpha \in \mathbb{C}\setminus\{0\}$, μ_α denotes the Gaussian probability measure

$$\mathrm{d}\mu_\alpha = \frac{1}{\sqrt{2\pi}|\alpha|} \exp\left(-\frac{q^2}{2|\alpha|^2}\right) \mathrm{d}q \,.$$

To each α there corresponds a family of unitary transformations $V_\alpha(\beta) : L^2(\mathbb{R}, \mathrm{d}q) \to L^2(\mathbb{R}, \mathrm{d}\mu_\alpha)$ connecting the standard Hilbert space with the new one in the form

$$\Psi(q) = \big(V_\alpha(\beta)\psi\big)(q) = \big(\sqrt{2\pi}|\alpha|\big)^{1/2} \exp\big(-i\bar{\beta}q^2/(2\bar{\alpha})\big)\psi(q) \,, \qquad \text{(D.15)}$$

where the complex numbers β must satisfy $\alpha\bar{\beta} - \beta\bar{\alpha} = i$. Note that the unitary transformations $V_\alpha(\beta)$ map the 'vacuum' state

$$\psi_0(q) = \big(\sqrt{2\pi}|\alpha|\big)^{-1/2} \exp\big(i\bar{\beta}q^2/(2\bar{\alpha})\big) \in L^2(\mathbb{R}, \mathrm{d}q)$$

onto the unit function $\Psi_0(q) = (V_\alpha(\beta)\psi_0)(q) = 1 \in L^2(\mathbb{R}, \mathrm{d}\mu_\alpha)$. In these cases, the position and momentum operators act on state vectors as

$$(Q\Psi)(q) = q\Psi(q) \quad \text{and} \quad (P\Psi)(q) = -i\Psi'(q) + \frac{\bar{\beta}}{\bar{\alpha}} q\Psi(q) \,,$$

where, with the aim of simplifying the notation, Q and P respectively denote the transformed operators $V_\alpha(\beta)QV_\alpha(\beta)^{-1}$ and $V_\alpha(\beta)PV_\alpha(\beta)^{-1}$ with common dense domain $V_\alpha(\beta)\mathscr{S}(\mathbb{R}) \subset L^2\big(\mathbb{R}, \mathrm{d}\mu_\alpha\big)$.

Any regular irreducible representation $\pi : \mathscr{W}(\mathbf{P}) \to \mathscr{B}(\mathscr{H})$ is stable under time evolution, i.e., there exists a unitary evolution operator $U(t, t_0) : \mathscr{H} \to \mathscr{H}$, $(t_0, t) \in I \times I$, implementing the quantum dynamics. It is important to notice at this point that, if the classical evolution has singularities at the boundary of the interval I, they also occur for the quantum dynamics, i.e., there is no resolution of classical singularities. The Heisenberg equations for Q and P can be solved just by the same expressions involved in the classical solutions (D.14), i.e.,

$$\left[\begin{array}{c} Q_H(t, t_0) \\ P_H(t, t_0) \end{array}\right] := U^{-1}(t, t_0) \left[\begin{array}{c} Q \\ P \end{array}\right] U(t, t_0) = \left[\begin{array}{cc} c(t, t_0) & s(t, t_0) \\ \dot{c}(t, t_0) & \dot{s}(t, t_0) \end{array}\right] \cdot \left[\begin{array}{c} Q \\ P \end{array}\right] . \qquad \text{(D.16)}$$

With more generality, given any well-behaved (analytic) classical observable $F : \mathbf{P} \to \mathbb{R}$ for the TDHO, the time evolution of its quantum counterpart in the Heisenberg picture $F_H(t, t_0) := U^{-1}(t, t_0)F(Q, P)U(t, t_0)$ is simply given by

$$F_H(t, t_0) = F(Q_H(t, t_0), P_H(t, t_0)) = F\big(c(t, t_0)Q + s(t, t_0)P, \dot{c}(t, t_0)Q + \dot{s}(t, t_0)P\big) \,. \qquad \text{(D.17)}$$

Hence, the matrix elements $\langle \Psi_2 \,|\, U^{-1}(t_2,t_1)F(Q,P)U(t_2,t_1)\Psi_1\rangle$, $\Psi_1,\Psi_2 \in \mathscr{H}$, can be computed without the explicit knowledge of the unitary evolution operator. This is also the case of the transition probabilities $\mathrm{Prob}(\Psi_2,t_2 \,|\, \Psi_1,t_1) = |\langle \Psi_2 \,|\, U(t_2,t_1)\Psi_1\rangle|^2$, as will be discussed in detail in *subsection D.2.4*. The commutators of time-evolved observables can be also calculated without the concrete expression of $U(t_2,t_1)$. For instance, from (D.17) we easily obtain

$$\big[Q_H(t_1,t_0), Q_H(t_2,t_0)\big] = is(t_1,t_2)\mathbf{1}\,,$$

where we have used the relation (D.7) stated in *section D.1.* As expected, the commutator given above is proportional to the identity operator and independent of the choice of the initial time t_0. Note, in contrast with the transition probabilities, that the calculation of transition amplitudes of the type $\langle \Psi_2 \,|\, U(t_2,t_1)\Psi_1\rangle$ does require the explicit knowledge of (the phase of) the evolution operator. This is also the case of the (strong) derivatives of both $U(\cdot,t_0)$ and $U(t,\cdot)$.

The dynamics of the quantum TDHO is governed by an (unbounded) nonautonomous Hamiltonian operator $H(t):\mathscr{H}\to\mathscr{H}$, $t\in I$, satisfying

$$\dot{U}(t,t_0) = -iH(t)U(t,t_0)\,. \tag{D.18}$$

Given the quadratic nature of the classical Hamiltonian (D.13), $H(t)$ must coincide with the operator directly promoted from the classical function modulo a t-dependent real term proportional to the identity $\mathbf{1}$ encoding the election of $U(t,t_0)$. For a concrete representation of the CCR, we will simply take

$$H(t) := \frac{1}{2}\left(P^2 + \kappa(t)Q^2\right). \tag{D.19}$$

This choice fixes $U(t,t_0)$ uniquely. The Hamiltonian (D.19) is a self-adjoint operator with dense domain $\mathscr{D}_{H(t)}$ –equal to $C_0^\infty(\mathbb{R})$ in the standard Schrödinger representation– for each value of the time parameter t. We will prove the following theorem in the next subsections.

Theorem D.2.1. *The action of the unitary TDHO evolution operator $U(t,t_0)$ corresponding to the Hamiltonian (D.19) on any state vector $\psi \in \mathscr{S}(\mathbb{R}) \subset L^2(\mathbb{R},\mathrm{d}q)$ in the traditional Schrödinger representation is given by*

$$\big(U(t,t_0)\psi\big)(q) = \int_{\mathbb{R}} K(q,t;q_0,t_0)\psi(q_0)\,\mathrm{d}q_0\,,$$

where the propagator $K(q,t;q_0,t_0)$ depends on the times t_0 and t through the classical TDHO solutions c and s. Explicitly,

$$K(q,t;q_0,t_0) = \frac{1}{\sqrt{2\pi i}}\, s^{-1/2}(t,t_0)\exp\left(\frac{i}{2s(t,t_0)}\Big(c(t_0,t)q^2 + c(t,t_0)q_0^2 - 2qq_0\Big)\right), \tag{D.20}$$

wherever $s(t,t_0) \neq 0$ *, and*

$$K(q,t;q_0,t_0) = c^{-1/2}(t,t_0)\exp\left(i\frac{\dot{c}(t,t_0)}{2c(t,t_0)}\right)\delta(q_0 - q/c(t,t_0)) \tag{D.21}$$

if $s(t,t_0) = 0$.

Remark D.2.1. Given a solution $u(t)$ to the TDHO equation (D.1) which is positive in some interval $(t_0, t_0+\varepsilon) \subset I$, $\varepsilon > 0$, we define

$$u^\epsilon(t,t_0) := \exp\big(i\epsilon\pi\,\mathfrak{m}(u;t,t_0)\big)|u(t)|^\epsilon\,,\ \ \epsilon \in \mathbb{R}\,,\ \ t \in I\,,$$

where $\mathfrak{m}(u;t,t_0) \in \mathbb{Z}$ is the index function of u, with $\mathfrak{m}(u;t_0,t_0) = 0$, in such a way that $\mathfrak{m}(u;t_2,t_0) - \mathfrak{m}(u;t_1,t_0)$, $t_1 < t_2$, gives the number of zeros of $u(\cdot,t_0)$ in the interval $(t_1,t_2]$. Finally, $\delta(q)$ denotes the Dirac delta distribution.

Remark D.2.2. Let $\vartheta : I \to \mathbb{R}$ be a real-valued continuous function and consider the Hamiltonian

$$H_1(t) := H(t) + \vartheta(t)\mathbf{1}$$

defined in terms of (D.19). The unitary evolution $U_1(t,t_0)$ associated with $H_1(t)$ satisfying (D.16) gives rise to the propagator

$$K_1(q,t;q_0,t_0) = K(q,t:q_0,t_0)\exp\left(-i\int_{t_0}^t \vartheta(\tau)\mathrm{d}\tau\right). \tag{D.22}$$

Note that $U_1^{-1}(t,t_0)\,\mathcal{O}\,U_1(t,t_0) = U^{-1}(t,t_0)\,\mathcal{O}\,U(t,t_0)$ for any quantum observable $\mathcal{O}$.

Remark D.2.3. In the $L^2(\mathbb{R},\mathrm{d}\mu_\alpha)$-representation defined by the unitary transformation $V_\alpha(\beta)$ (see equation (D.15)), the evolution is given by

$$\big(U(t,t_0)\Psi\big)(q) = \int_{\mathbb{R}} K_{\alpha\beta}(q,t;q_0,t_0)\Psi(q_0)\,\mathrm{d}\mu_\alpha(q_0)\,,$$

where

$$K_{\alpha\beta}(q,t;q_0,t_0) := \sqrt{2\pi}|\alpha|\exp\left(\frac{i\beta}{2\alpha}q_0^2 - \frac{i\bar{\beta}}{2\bar{\alpha}}q^2\right)K(q,t;q_0,t_0)\,. \tag{D.23}$$

D.2.2 Constructing the evolution operator

In order to calculate the unitary evolution operator $U(t,t_0)$ we will perform a generalization of the method developed in [6] that will clarify the appearance of the auxiliary Ermakov-Pinney solution (D.10) in this context, and will allow us also to warn the reader about other problematic choices that have appeared before in the related literature. We first introduce on $\mathscr{H}$ the (one-parameter family of) unitary operators

$$D(x) := \exp\left(-\frac{i}{2}xQ^2\right),\ \ x \in \mathbb{R}\,,$$

generating a displacement of the momentum operator, $D(x)PD^{-1}(x) = P + xQ$ (the position operator being unaffected by them), and define the unitary squeeze operators

$$S(y) := \exp\left(\frac{i}{2}y\big(QP + PQ\big)\right), \quad y \in \mathbb{R},$$

scaling both the position and momentum operator respectively as $S(y)QS^{-1}(y) = e^{y}Q$ and $S(y)PS^{-1}(y) = e^{-y}P$. Let $\Psi(t) \in \mathscr{D}_{H(t)}$, $t \in I$, be a solution to the Schrödinger equation, i.e., $i\dot{\Psi}(t) = H(t)\Psi(t)$, and let $x, y \in C^1(I)$. We now introduce the unitary operators

$$T(t) = T(t; x, y) := S(y(t))D(x(t)),$$

where the functions x and y remain arbitrary at this stage. Let us consider the time evolution for the transformed state vector

$$\Phi(t) = \Phi(t; x, y) := T(t; x, y)\Psi(t),$$

given by

$$\begin{aligned} i\dot{\Phi}(t) &= \Big(T(t)H(t)T^{-1}(t) - iT(t)\dot{T}(t)\Big)\Phi(t) \\ &= \frac{1}{2}\Big(e^{-2y(t)}P^2 + (x(t) - \dot{y}(t))(QP + PQ) + e^{2y(t)}(x^2(t) + \kappa(t) + \dot{x}(t))Q^2\Big)\Phi(t). \end{aligned}$$

We note at this point that it is possible to get a notable simplification of the previous expression just by imposing

$$x(t) = \dot{y}(t) \quad \text{and} \quad x^2(t) + \kappa(t) + \dot{x}(t) = \exp(-4y(t)). \tag{D.24}$$

The most natural way to achieve this is to choose

$$y(t) := \log \rho(t) \quad \text{and, hence,} \quad x(t) = \dot{\rho}(t)/\rho(t),$$

with ρ being *any* solution to the auxiliary EP equation (D.9) introduced in *section D.1*. In this way, the state vector $\Phi(t; \dot{\rho}/\rho, \log\rho) =: \Phi_\rho(t)$ satisfies the differential equation

$$i\dot{\Phi}_\rho(t) = \frac{1}{2\rho^2(t)}\big(P^2 + Q^2\big)\Phi_\rho(t).$$

Solving this equation and going back to the original state vector $\Psi(t)$, we finally obtain the unitary evolution operator for the system. We can then enunciate the following theorem.

Theorem D.2.2. *The time evolution operator $U(t, t_0)$ for the quantum TDHO whose dynamics is governed by the Hamiltonian (D.19) is given by a composition of unitary operators*

$$U(t, t_0) = T_\rho^{-1}(t)R_\rho(t, t_0)T_\rho(t_0),$$

where

$$R_\rho(t,t_0) := \exp\left(-\frac{i}{2}\int_{t_0}^{t}\frac{\mathrm{d}\tau}{\rho^2(\tau)}\big(P^2+Q^2\big)\right), \tag{D.25}$$

and $T_\rho(t) = S_\rho(t)D_\rho(t)$, *with*

$$D_\rho(t) := \exp\left(-\frac{i}{2}\frac{\dot\rho(t)}{\rho(t)}Q^2\right) \quad \text{and} \quad S_\rho(t) := \exp\left(\frac{i}{2}\log\rho(t)\big(QP+PQ\big)\right). \tag{D.26}$$

Remark D.2.4. Note that instead of introducing ρ, we could have used other choices for the x and y functions. In these cases, conditions (D.24) may not hold and the expressions of the evolution operator would differ from the one obtained here. For instance, one can select $x(t) = \dot u(t)/u(t)$ and $y(t) = \log u(t)$ as in [6], with $u(t)$ being any solution to the TDHO equation, but this choice is problematic because the set $\{t \in I \,|\, u(t) = 0\}$ may be non-empty and, hence, the resulting formula for the unitary operator is generally not well-defined for all values of the time parameter t. This is the reason why the election of the Ermakov-Pinney solution is especially convenient in this context –recall that ρ is a positive function. It follows from the above argument that the appearance of this solution is nearly unavoidable in this context.

Note that the eigenstates of the $R_\rho(t,t_0)$ operator (D.25) are given by those of the Hamiltonian operator corresponding to a quantum harmonic oscillator with unit frequency $\sqrt{\kappa(t)} = 1$,

$$H_0 := \frac{1}{2}\big(P^2+Q^2\big). \tag{D.27}$$

This fact will be shown particularly useful to calculate the Feynman propagator. It is also important to point out that the procedure employed in this section is implicitly based upon the transformation of the so-called Lewis invariant [7]

$$I_\rho(t) := \frac{1}{2}\left(\frac{Q^2}{\rho^2(t)} + \big(\rho(t)P - \dot\rho(t)Q\big)^2\right), \quad \dot I_{\rho_H} = 0, \tag{D.28}$$

into an explicitly time-independent quantity –although in order to obtain the unitary operator it has not been necessary to use it. In this case, we simply have

$$T_\rho(t)I_\rho(t)T_\rho^{-1}(t) = H_0. \tag{D.29}$$

The Lewis invariant is often used to generate exact solutions to the Schrödinger equation, and turns out to be especially useful to construct semiclassical states for these systems, as will be discussed later.

D.2.3 Propagator formula

We finally proceed to derive the Feynman propagator for the quantum TDHO corresponding to the Hamiltonian (D.19). In the previous subsection, we have written down the evolution operator for this system explicitly in closed form in terms of the position and momentum operators (see *Theorem D.2.2*). It is given by the product of the unitary operators (D.25) and (D.26). We calculate now the action of these factors on test functions $\psi \in \mathscr{S}(\mathbb{R}) \subset L^2(\mathbb{R}, \mathrm{d}q)$ in the standard Schrödinger representation. First, it is straightforward to see that

$$\begin{aligned}\big(T_\rho(t)\psi\big)(q) &= \sqrt{\rho(t)}\exp\left(-\frac{i}{2}\dot\rho(t)\rho(t)q^2\right)\psi(\rho(t)q) = \int_{\mathbb{R}} K_\rho^+(q,t;q_0)\psi(q_0)\,\mathrm{d}q_0\,,\\ \big(T_\rho^{-1}(t)\psi\big)(q) &= \frac{1}{\sqrt{\rho(t)}}\exp\left(\frac{i}{2}\frac{\dot\rho(t)}{\rho(t)}q^2\right)\psi(q/\rho(t)) = \int_{\mathbb{R}} K_\rho^-(q,t;q_0)\psi(q_0)\,\mathrm{d}q_0\,,\end{aligned}$$

where we have introduced the distributions

$$K_\rho^+(q,t;q_0) := \sqrt{\rho(t)}\exp\left(-\frac{i}{2}\dot\rho(t)\rho(t)q^2\right)\delta(q_0-\rho(t)q)\,, \tag{D.30}$$

$$K_\rho^-(q,t;q_0) := \frac{1}{\sqrt{\rho(t)}}\exp\left(\frac{i}{2}\frac{\dot\rho(t)}{\rho(t)}q^2\right)\delta(q_0-q/\rho(t))\,. \tag{D.31}$$

The propagator for $R_\rho(t,t_0)$, satisfying

$$\big(R_\rho(t,t_0)\psi\big)(q) = \int_{\mathbb{R}} K_\rho^0(q,t;q_0,t_0)\psi(q_0)\,\mathrm{d}q_0\,,$$

can be easily derived from the one corresponding to the TIHO with unit frequency. As is well known [8, 9], the Green function K^0 for the Hamiltonian (D.27) is given by the Feynman-Soriau formulae

$$K^0(q,\upsilon;q_0,0) = \frac{1}{\sqrt{2\pi i}}\sin^{-1/2}(\upsilon,0)\exp\left(\frac{i}{2\sin\upsilon}\Big((q^2+q_0^2)\cos\upsilon-2qq_0\Big)\right),$$

whenever $\upsilon \not\equiv 0 \pmod{\pi}$, and

$$K^0(q,\upsilon;q_0,0) = \cos^{-1/2}(\upsilon,0)\exp\left(-\frac{i\sin\upsilon}{2\cos\upsilon}\right)\delta(q_0-q/\cos\upsilon)\,,\quad \upsilon\equiv 0 \pmod{\pi}\,,$$

where the so-called Maslov correction factor [9], which allows the calculation of the propagator beyond the caustics $\{\upsilon \in \mathbb{R} : \sin(\upsilon) = 0\} = \{\pi k : k \in \mathbb{Z}\}$, has been conveniently absorbed into the definition of $\sin^{1/2}(\upsilon,0)$ and $\cos^{1/2}(\upsilon,0)$ given in the formulation of *Theorem D.2.1.* In view of (D.25), we simply get

$$K_\rho^0(q,t;q_0,t_0) = K^0\left(q,\int_{t_0}^t \frac{\mathrm{d}\tau}{\rho^2(\tau)}\,;q_0,0\right). \tag{D.32}$$

Therefore,

$$\big(U(t,t_0)\Psi\big)(q)=\big(T_\rho^{-1}(t)R_\rho(t,t_0)T_\rho(t_0)\Psi\big)(q)=\int_{\mathbb{R}}K(q,t;q_0,t_0)\Psi(q_0)\,\mathrm{d}q_0\,,$$

where

$$K(q,t;q_0,t_0)\;=\;\int_{\mathbb{R}^2}K_\rho^-(q,t;q_2)K_\rho^0(q_2,t;q_1,t_0)K_\rho^+(q_1,t_0;q_0)\,\mathrm{d}q_1\,\mathrm{d}q_2\,. \tag{D.33}$$

By combining (D.30)-(D.33) with (D.11) and (D.12), we find the formula for the propagator (D.20) enunciated in *Theorem D.2.1* expressed in terms of the c and s solutions to the classical TDHO equations (D.1). As expected, the propagator –and hence the evolution operator itself– does not depend on the particular solution ρ to the EP equation (D.9) chosen to factorize $U(t,t_0)$. Taking the appropriate limits one obtains, after straightforward calculations, the propagator evaluated at caustics (D.21). The resulting expressions are in agreement with those obtained by other authors (see, for example, [9, 10, 11, 12], where more complicated path integration techniques are often employed), though in our case they have been achieved within a different scheme, based essentially on the previous obtention of a closed expression for the evolution operator. Finally, a direct calculation shows that the propagator $K(q,t;q_0,t_0)$, viewed as a function of (q,t), formally satisfies the evolution equation

$$i\partial_t K=-\frac{1}{2}\partial_q^2K+\frac{1}{2}q^2\kappa(t)K\,.$$

D.2.4 Transition amplitudes and vacuum instability

The exact expressions for the Green functions (D.20) and (D.21) can be used to *exactly* compute both transition amplitudes and probabilities. Here, we will restrict ourselves to the class of normalized states ϕ_n^ω defined in $L^2(\mathbb{R},\mathrm{d}q)$ as

$$\phi_n^\omega(q):=\frac{\omega^{1/4}}{\sqrt{2^n n!\sqrt{\pi}}}\exp\Big(-\omega q^2/2\Big)H_n(\sqrt{\omega}q)\,,\;\;\omega>0\,,\;\;n\in\mathbb{N}_0\,, \tag{D.34}$$

with $H_n(z)$ denoting the n-th Hermite polynomial in the variable z. For any fixed value ω, the set $(\phi_n^\omega : n\in\mathbb{N}_0)$ defines the usual orthonormal basis of $L^2(\mathbb{R})$ constituted by the eigenvectors of the quantum Hamiltonian (D.19) corresponding to a TIHO of constant frequency $\sqrt{\kappa(t)}=\omega$. Since the ϕ_n^ω states are complete, the corresponding transition amplitudes and probabilities for other states are readily obtainable. By using the generating function for Hermite polynomials,

$$\exp\big(2\sqrt{\omega}qx-x^2\big)=\sum_{n=0}^{\infty}H_n(\sqrt{\omega}q)\frac{x^n}{n!}\,,$$

it is clear that

$$\langle \phi_{n_2}^{\omega_2} \,|\, U(t_2,t_1)\phi_{n_1}^{\omega_1}\rangle = \frac{1}{\pi}\left(\frac{n_1!n_2!\sqrt{\omega_1\omega_2}}{2^{n_1+n_2+1}i}\right)^{1/2} s^{-1/2}(t_2,t_1)\,[x_1^{n_1}x_2^{n_2}]\,I(x_1,x_2;\Lambda(t_1,t_2;\omega_1,\omega_2))\,, \tag{D.35}$$

where $[x_1^{n_1}x_2^{n_2}]f(x_1,x_2)$ denotes the complex coefficient appearing in the $x_1^{n_1}x_2^{n_2}$-term of the Taylor expansion of the function f. Here, for any matrix $\Lambda \in \mathrm{Mat}_{2\times 2}(\mathbb{C})$, we define

$$\begin{aligned} I(x_1,x_2;\Lambda) \;&:=\; \exp\big(-(x_1^2+x_2^2)\big)\int_{\mathbb{R}^2}\exp\left(-\frac{1}{2}\vec{q}^{\,t}\Lambda\,\vec{q}+2\vec{x}^{\,t}\,\mathrm{diag}(\sqrt{\omega_1},\sqrt{\omega_2})\,\vec{q}\right)\mathrm{d}^2\vec{q} \\ &=\; \frac{2\pi}{\sqrt{\det\Lambda}}\exp\left(\vec{x}^{\,t}\Big(2\mathrm{diag}(\sqrt{\omega_1},\sqrt{\omega_2})\Lambda^{-1}\mathrm{diag}(\sqrt{\omega_1},\sqrt{\omega_2})-\mathbb{I}\Big)\vec{x}\right), \end{aligned}$$

whenever $\mathrm{Re}[\Lambda]\geq 0$ and $\det\Lambda\neq 0$. In this formula, $\vec{x}$ denotes the column vector with first and second components given by x_1 and x_2, respectively; we define $\vec{q}$ similarly. In our case,

$$\Lambda(t_1,t_2;\omega_1,\omega_2) := \begin{bmatrix} \omega_1 - i\dfrac{c(t_2,t_1)}{s(t_2,t_1)} & \dfrac{i}{s(t_2,t_1)} \\ \dfrac{i}{s(t_2,t_1)} & \omega_2 - i\dfrac{c(t_1,t_2)}{s(t_2,t_1)} \end{bmatrix},$$

with

$$\det\Lambda(t_1,t_2;\omega_1,\omega_2) = \left(\omega_1\omega_2 - \frac{\dot{c}(t_2,t_1)}{s(t_2,t_1)}\right) - i\left(\frac{\omega_1 c(t_1,t_2)+\omega_2 c(t_2,t_1)}{s(t_2,t_1)}\right).$$

Here, $\mathrm{Re}[\Lambda(t_0,t;\omega_1,\omega_2)]\geq 0$ and $\det\Lambda(t_0,t;\omega_1,\omega_2)\neq 0$ for all $(t_0,t)\in I\times I$ and $\omega_1,\omega_2\in(0,+\infty)$. The Taylor expansion of $I(x_1,x_2;\Lambda)$ can be efficiently computed by applying the following lemma, that trivially follows from the multinomial formula.

Lemma D.2.1. *Let*

$$B = B^t = \begin{bmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{bmatrix} \in \mathrm{Mat}_{2\times 2}(\mathbb{C})\,.$$

Then, using the notation introduced above, we have

$$[x_1^{n_1}x_2^{n_2}]\exp\left(\vec{x}^{\,t}B\vec{x}\right) = b_{11}^{(n_1-n_2)/2}(2b_{12})^{n_2}\sum_{m\in\Delta(n_1,n_2)}\frac{(b_{11}b_{22})^m(4b_{12}^2)^{-m}}{m!(m+(n_1-n_2)/2)!(n_2-2m)!}\,,$$

whenever n_1 and n_2 have the same parity, and vanishes otherwise. Here, $\Delta(n_1,n_2) := \big(m\in\mathbb{N}_0 \,:\, \max\{0,(n_2-n_1)/2\}\leq m\leq\lfloor n_2/2\rfloor\big)$, where $\lfloor x\rfloor$ denotes the largest integer less than or equal to $x\in\mathbb{R}$. In particular, taking $n_1=0$, we get

$$[x_1^0x_2^{n_2}]\exp\left(\vec{x}^{\,t}B\vec{x}\right) = \frac{b_{22}^{n_2/2}}{(n_2/2)!} \quad \text{for} \quad n_2\equiv 0 \pmod 2\,, \tag{D.36}$$

and vanishes if n_2 is an odd number.

Remarks. Note that the TDHO quantum dynamics is invariant under parity inversion $\mathbf{P}$ and states ϕ_n^ω satisfy $\mathbf{P}\phi_n^\omega = (-1)^n\phi_n^\omega$. Hence, $\langle \phi_{n_2}^{\omega_2} \,|\, U(t_2,t_1)\phi_{n_1}^{\omega_1}\rangle = 0$ if n_1 and n_2 have different parity.

As a concrete example, in the case of a TIHO with constant frequency $\omega = \omega_1 = \omega_2$, we identify

$$B = 2\,\mathrm{diag}(\sqrt{\omega},\sqrt{\omega})\,\Lambda^{-1}(t_1,t_2;\omega,\omega)\,\mathrm{diag}(\sqrt{\omega},\sqrt{\omega}) - \mathbb{I} = \exp\big(-i\omega(t_2-t_1)\big)\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

and, hence,

$$I(x_1,x_2;\Lambda(t_1,t_2;\omega,\omega)) = \sum_{n=0}^{\infty}\frac{2^n}{n!}\exp\big(-i\omega n(t_2-t_1)\big)x_1^n x_2^n\,.$$

This is in perfect agreement with

$$\langle \phi_{n_2}^{\omega} \,|\, U(t_2,t_1)\phi_{n_1}^{\omega}\rangle = \exp\big(-i\omega(n_1+1/2)(t_2-t_1)\big)\delta(n_1,n_2)\,,$$

where $\delta(n_1,n_2)$ denotes the Kronecker delta. For arbitrary time-dependent frequencies the formula (D.35), when restricted to the same initial and final frequencies $\omega_1 = \omega_2$, coincides with the one given in [13] written in terms of associated Legendre functions.

We conclude this section with the analysis of the instability of the vacuum state ϕ_0^ω due to the nonautonomous nature of the Hamiltonian (D.19). This can be easily derived from the formulae (D.35) and (D.36).

Theorem D.2.3. *The quantum time evolution of the vacuum state ϕ_0^ω is generally given by a superposition of states $U(t,t_0)\phi_0^\omega = \sum_{n\in\mathbb{N}_0}\langle\phi_{2n}^\omega \,|\, U(t,t_0)\phi_0^\omega\rangle\phi_{2n}^\omega$, where the probability amplitudes $\langle\phi_{2n}^\omega \,|\, U(t,t_0)\phi_0^\omega\rangle$ are given by*

$$\langle\phi_{2n}^\omega \,|\, U(t,t_0)\phi_0^\omega\rangle = \frac{\sqrt{(2n)!}}{2^n n!}\big(2\omega(\Lambda^{-1}(t_0,t;\omega,\omega))_{22}-1\big)^n\langle\phi_0^\omega \,|\, U(t,t_0)\phi_0^\omega\rangle\,,\quad n\in\mathbb{N}\,, \tag{D.37}$$

in terms of the the expectation value

$$\langle\phi_0^\omega \,|\, U(t,t_0)\phi_0^\omega\rangle = \sqrt{\frac{2\omega}{\det\Lambda(t_0,t;\omega,\omega)}}\exp(-i\pi/4)\,s^{-1/2}(t,t_0)\,,$$

with

$$(\Lambda^{-1}(t_0,t;\omega,\omega))_{22} = \frac{\omega s^2(t_2,t_1) - is(t_2,t_1)c(t_2,t_1)}{1+\omega^2 s^2(t_2,t_1) - c(t_2,t_1)c(t_1,t_2) - i\omega s(t_2,t_1)\big(c(t_2,t_1)+c(t_1,t_2)\big)}\,.$$

Remarks. Consider the usual annihilation and creation operators

$$a_\omega := \frac{1}{\sqrt{2}}\big(\sqrt{\omega}Q + iP/\sqrt{\omega}\big)\quad\text{and}\quad a_\omega^* := \frac{1}{\sqrt{2}}\big(\sqrt{\omega}Q - iP/\sqrt{\omega}\big)\,, \tag{D.38}$$

with $[a_\omega, a_\omega^*] = \mathbf{1}$ and $[a_\omega, a_\omega] = 0 = [a_\omega^*, a_\omega^*]$, such that $a_\omega^* \phi_n^\omega = \sqrt{n+1}\phi_{n+1}^\omega$ and $a_\omega \phi_n^\omega = \sqrt{n}\phi_{n-1}^\omega$, $\forall\, n \in \mathbb{N}$, with $a_\omega \phi_0^\omega = 0$. The evolution of these operators in the Heisenberg picture can be obtained directly from (D.16),

$$\begin{aligned} U^{-1}(t,t_0)\, a_\omega\, U(t,t_0) &= A_\omega(t,t_0) a_\omega + B_\omega(t,t_0) a_\omega^* \,, \\ U^{-1}(t,t_0)\, a_\omega^*\, U(t,t_0) &= \bar{B}_\omega(t,t_0) a_\omega + \bar{A}_\omega(t,t_0) a_\omega^* \,, \end{aligned} \tag{D.39}$$

where $A_\omega(t,t_0)$ and $B_\omega(t,t_0)$ are the Bogoliubov coefficients

$$A_\omega(t,t_0) := \frac{1}{2}\Big(c(t,t_0) + \dot{s}(t,t_0) + i\big(\omega^{-1}\dot{c}(t,t_0) - \omega s(t,t_0)\big)\Big)\,, \tag{D.40}$$

$$B_\omega(t,t_0) := \frac{1}{2}\Big(c(t,t_0) - \dot{s}(t,t_0) + i\big(\omega^{-1}\dot{c}(t,t_0) + \omega s(t,t_0)\big)\Big)\,, \tag{D.41}$$

satisfying $A_\omega(t,t_0) = \bar{A}_\omega(t_0,t)$, $B_\omega(t,t_0) = -B_\omega(t_0,t)$, and $|A_\omega(t,t_0)|^2 - |B_\omega(t,t_0)|^2 = 1$, $\forall\,(t,t_0) \in I \times I$. Note, in particular, that $A_\omega(t,t_0)$ never vanishes. For example, for the TIHO of constant frequency $\omega > 0$ we have $B_\omega(t,t_0) = 0$ and $A_\omega(t,t_0) = \exp(-i(t-t_0)\omega)$. A straightforward calculation yields (see also [14])

$$U(t,t_0)\phi_0^\omega = \langle \phi_0^\omega \,|\, U(t,t_0)\phi_0^\omega\rangle \exp\left(-\frac{1}{2}\frac{B_\omega(t_0,t)}{A_\omega(t_0,t)} a_\omega^{*2}\right)\phi_0^\omega\,, \tag{D.42}$$

This formula is in perfect agreement with the transitions (D.37). Indeed, it is straightforward to check that

$$2\omega(\Lambda^{-1}(t_0,t;\omega,\omega))_{22} - 1 = -B_\omega(t_0,t)/A_\omega(t_0,t)\,.$$

Since $\det\Lambda(t_0,t;\omega,\omega) = -2i\omega s^{-1}(t,t_0)A_\omega(t_0,t)$, the expectation value $\langle \phi_0^\omega \,|\, U(t,t_0)\phi_0^\omega\rangle$ can be rewritten as

$$\langle \phi_0^\omega \,|\, U(t,t_0)\phi_0^\omega\rangle = \frac{1}{\sqrt{|A_\omega(t_0,t)|}}\exp(i\sigma(t,t_0))\,, \tag{D.43}$$

where the phase $\sigma(t,t_0) \in C^1(I \times I)$ comes from a careful calculation of the principal argument. For a TIHO with constant frequency $\omega > 0$, we have $\sigma(t,t_0) = (t_0 - t)\omega/2$ for all $t, t_0 \in \mathbb{R}$. Given an arbitrary squared frequency $\kappa(t)$, the phase $\sigma(t,t_0)$ evaluated at times t close to t_0 is simply given by

$$\sigma(t,t_0) = -\frac{1}{2}\arctan\left(\frac{\omega s(t,t_0) - \omega^{-1}\dot{c}(t,t_0)}{c(t,t_0) + \dot{s}(t,t_0)}\right)\,. \tag{D.44}$$

The σ phase can be conveniently canceled through a suitable redefinition of the Hamiltonian (D.19) just in the case when $\dot{\sigma}(t,t_0)$ is independent of t_0. In that situation, by identifying $\vartheta(t) = \dot{\sigma}(t,t_0)$ in equation (D.22), we have that the redefined evolution operator satisfies $\langle \phi_0^\omega \,|\, U_1(t,t_0)\phi_0^\omega\rangle = 1/\sqrt{|A_\omega(t_0,t)|}$. In the TIHO case, we get $\vartheta(t) = -\omega/2$ (this amounts to considering normal order). In general, it is not possible to proceed in this way in all cases when dealing with arbitrary time-dependent frequencies. In any case, the σ phase is irrelevant for the calculation of transition probabilities. In particular, given $\Psi_1, \Psi_2 \in \mathscr{H}$ with $\Psi_1 = F_1(a_\omega, a_\omega^*)\,\phi_0^\omega$, where F_1 is some analytic function, we have

$$\begin{aligned}\mathrm{Prob}(\Psi_2, t_2 \,|\, \Psi_1, t_1) &= |\langle \Psi_2 \,|\, U(t_2, t_1)\Psi_1\rangle|^2 \\ &= \frac{|\langle \Psi_2 \,|\, F_1(a_{\omega H}(t_1,t_2), a^*_{\omega H}(t_1,t_2)) \exp\big(- B_\omega(t_1,t_2)/(2A_\omega(t_1,t_2)) a_\omega^{*2}\big)\phi_0^\omega\rangle|^2}{|A_\omega(t_1,t_2)|}\,,\end{aligned}$$

where the time dependence only appears through the Bogoliubov coefficients (D.40) and (D.41). Finally, it is important to point out that the transformations (D.39) and the evolution of the vacuum state (D.42) fully characterize the quantum time evolution of the TDHO. By using these relations, we can easily compute the action of $U(t,t_0)$ on any basic vector $\phi_n^\omega = (1/\sqrt{n!})\, a_\omega^{*n}\phi_0^\omega$.

D.3 Semiclassical states

In this section, we will look for states that behave semiclassically under the dynamics defined by the quantum Hamiltonian (D.19). We will base our study on the concrete factorization of the evolution operator defined in *Theorem D.2.2*. To achieve this goal, note that the eigenvalue problem for the Lewis invariant (D.28) can be exactly solved. Indeed, let us fix $t_0 \in I$ and let $(\phi_n : n \in \mathbb{N}_0)$ be the eigenstates (D.34) of the auxiliary Hamiltonian H_0 (D.27) corresponding to unit frequency $\omega = 1$. According to relation (D.29), the initial states $\psi_n^\rho(t_0) := T_\rho^{-1}(t_0)\phi_n$,

$$\psi_n^\rho(t_0, q) = \left(\frac{1}{2^n n! \sqrt{\pi}\rho(t_0)}\right)^{1/2} \exp\left(\frac{i}{2}\left(\frac{\dot\rho(t_0)}{\rho(t_0)} + \frac{i}{\rho^2(t_0)}\right) q^2\right) H_n(q/\rho(t_0)) \in L^2(\mathbb{R}, \mathrm{d}q)\,,$$

labeled both by ρ and the integers $n \in \mathbb{N}_0$, are eigenstates of $I_\rho(t_0)$ with eigenvalues equal to $n + 1/2$. Consider now the initial pure state

$$\Phi_\rho^{(z)}(t_0) := T_\rho^{-1}(t_0)\Phi^{(z)} = e^{-|z|^2/2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\psi_n^\rho(t_0)\,, \quad z \in \mathbb{C}\,, \tag{D.45}$$

with $\Phi^{(z)} := e^{-|z|^2/2}\sum_{n=0}^\infty \frac{z^n}{\sqrt{n!}}\phi_n$ being the well-known coherent states for the Hamiltonian H_0 . Let us take the annihilation and creation operators a and a^* for unit frequency $\omega = 1$ defined in (D.38). The superposition (D.45) is a normalized eigenvector of the (time-dependent) annihilation operator

$$a_\rho(t_0) := T_\rho^{-1}(t_0)\, a\, T_\rho(t_0) = \frac{1}{\sqrt{2}}\big(Q/\rho(t_0) + i(\rho(t_0)P - \dot\rho(t_0)Q)\big)\,, \tag{D.46}$$

in the sense that $a_\rho(t_0)\Phi_\rho^{(z)}(t_0) = z\Phi_\rho^{(z)}(t_0)$. This operator, together with the associated creation operator

$$a_\rho^*(t_0) := T_\rho^{-1}(t_0)\, a^*\, T_\rho(t_0) = \frac{1}{\sqrt{2}}\big(Q/\rho(t_0) - i(\rho(t_0)P - \dot{\rho}(t_0)Q)\big)\,,$$

satisfies the Heisenberg algebra, $[a_\rho(t_0), a_\rho^*(t_0)] = \mathbf{1}$, $[a_\rho(t_0), a_\rho(t_0)] = 0 = [a_\rho^*(t_0), a_\rho^*(t_0)]$, for each initial value of the time parameter t_0 . In particular, the Lewis invariant (D.28) may be expressed in terms of these operators as $I_\rho(t_0) = a_\rho^*(t_0)a_\rho(t_0) + (1/2)\mathbf{1}$. Through unitary time evolution, we get

$$\Phi_\rho^{(z)}(t, t_0) := U(t, t_0)\Phi_\rho^{(z)}(t_0) = \exp\left(-\frac{i}{2}\int_{t_0}^{t}\frac{\mathrm{d}\tau}{\rho^2(\tau)}\right)\Phi_\rho^{(z_\rho(t,t_0))}(t)\,, \tag{D.47}$$

where we have denoted

$$z_\rho(t, t_0) := \exp\left(-i\int_{t_0}^{t}\frac{\mathrm{d}\tau}{\rho^2(\tau)}\right) z\,, \quad z \in \mathbb{C}\,.$$

We want to remark that the time-dependent phase appearing in (D.47) is necessary for these states to verify the Schrödinger equation. In our case, they coincide with those defined in equation (4.6) of reference [15]. We conclude that the family of states (D.45) is closed under the dynamics. Moreover, the following theorem can be used to justify that these states can be considered as semiclassical under certain assumptions.

Theorem D.3.1. *Let $z = x + iy \in \mathbb{C}$ and $t_0 \in I$. The position and momentum expectation values in the state $\Phi_\rho^{(z)}(t, t_0) = U(t, t_0)\Phi_\rho^{(z)}(t_0)$ satisfy*

$$\begin{aligned} q_H(t, t_0) &= \big\langle \Phi_\rho^{(z)}(t, t_0) \,\big|\, Q\, \Phi_\rho^{(z)}(t, t_0)\big\rangle = \sqrt{2}\rho(t)\,\mathrm{Re}\big[z_\rho(t, t_0)\big]\,, \\ p_H(t, t_0) &= \big\langle \Phi_\rho^{(z)}(t, t_0) \,\big|\, P\Phi_\rho^{(z)}(t, t_0)\big\rangle = \sqrt{2}\,\mathrm{Re}\big[\big(\dot{\rho}(t) - i/\rho(t)\big)z_\rho(t, t_0)\big]\,, \end{aligned}$$

where (q_H, p_H) is the classical solution (D.14) determined by the Cauchy data $(q, p) = \big(\sqrt{2}\rho(t_0)x, \sqrt{2}(\dot{\rho}(t_0)x + y/\rho(t_0))\big)$ at time t_0 . Moreover, the mean square deviations of the position and momentum operators with respect to the evolved state $\Phi_\rho^{(z)}(t, t_0)$,

$$\Delta_{\Phi_\rho^{(z)}(t,t_0)}Q = \frac{1}{\sqrt{2}}\,\rho(t)\,, \quad \Delta_{\Phi_\rho^{(z)}(t,t_0)}P = \frac{1}{\sqrt{2}}\,\big|\dot{\rho}(t) - i\rho^{-1}(t)\big|\,, \tag{D.48}$$

are independent of both t_0 and the Cauchy data defined by z .

Remark D.3.1. Given any observable $\mathcal{O}$, its uncertainty in the state $\Psi \in \mathscr{D}_{\mathcal{O}}$ is defined as $\Delta_\Psi\mathcal{O} := \big(\langle\Psi \,|\, \mathcal{O}^2\Psi\rangle - \langle\Psi \,|\, \mathcal{O}\Psi\rangle^2\big)^{1/2}$. Note that, in general, the elements of the family of states under consideration are neither standard coherent states nor squeezed states. For instance, for the free particle (D.4) one can choose $\rho(t) = \sqrt{1 + (t - t_0)^2}$ and, hence, $\Delta_{\Phi_\rho^{(z)}(t,t_0)}Q \sim t/\sqrt{2}$ for large values of t ; similar results occur for other elections of ρ . Nevertheless, it is obvious that we will obtain good semiclassical states for a system whenever the solution ρ to the auxiliary EP equation (D.9) has a suitable behavior, for instance, if ρ is periodic in time or is simply a bounded function. We will analyze some clarifying examples in this respect.

Example 1 (Vertically driven pendulum)**.** Consider the vertically driven pendulum [16], i.e., the motion of a physical pendulum whose supporting point oscillates in the vertical direction. In the small angles regime, it is described by the Mathieu equation in its canonical form [17]

$$\ddot{u}(t) + \kappa(t;a,b)u(t) = 0\,, \quad \kappa(t;a,b) := a - 2b\cos(2t)\,, \quad a, b \in \mathbb{R}\,.$$

The general solution to this equation is a real linear combination of the so-called Mathieu cosine and sine functions [18, 19], denoted respectively as $Ce(t;a,b)$ and $Se(t;a,b)$. Given a nonzero b value, it is a well-known fact that the Mathieu cosine and sine functions are periodic in the time parameter t only for certain (countable number of) values of the a parameter, called *characteristic values*. The procedure to calculate these characteristic values for even or odd Mathieu functions with *characteristic exponent*[1] $r \in \mathbb{Z}$ and parameter b can be efficiently implemented in a computer. In this case, solutions to the EP equation (D.9) inherit the periodic behavior from the Mathieu solutions, in such a way that one obtains well-behaved semiclassical states for which the average position and momentum follow the classical trajectories, whereas the corresponding uncertainties vary periodically in time. Note that, for small values of the b parameter, we have $Ce(t;a,b) \sim \cos(\sqrt{a}t)$ and $Se(t;a,b) \sim \sin(\sqrt{a}t)$, and the system closely approximates the TIHO with squared frequency given by the a parameter.

Example 2 ($\mathbb{T}^3$ Gowdy-like oscillator)**.** Consider the TDHO equation

$$\ddot{u}(t) + \kappa(t;\omega)u(t) = 0\,, \quad \kappa(t;\omega) := \omega^2 + \frac{1}{4t^2}\,, \;\; \omega \in \mathbb{R}\,, \;\; t \in (0, +\infty)\,.$$

This equation is satisfied for each mode of the scalar fields encoding the information about the gravitational local degrees of freedom of the $\mathbb{T}^3$ Gowdy models. In terms of the zero Bessel functions of first and second kind [19], denoted J_0 and Y_0 respectively, the c and s solutions introduced in *section D.1* are given by

$$\begin{aligned} c(t,t_0) &= \frac{\pi}{4}\Big(\sqrt{\frac{t}{t_0}}Y_0(\omega t_0) - 2\omega\sqrt{t_0 t}\,Y_1(\omega t_0)\Big)J_0(\omega t) \\ &- \frac{\pi}{4}\Big(\sqrt{\frac{t}{t_0}}J_0(\omega t_0) - 2\omega\sqrt{t_0 t}\,J_1(\omega t_0)\Big)Y_0(\omega t), \end{aligned} \tag{D.49}$$

$$s(t,t_0) = -\frac{\pi}{2}\sqrt{t_0 t}\,Y_0(\omega t_0)J_0(\omega t) + \frac{\pi}{2}\sqrt{t_0 t}\,J_0(\omega t_0)Y_0(\omega t)\,. \tag{D.50}$$

Note that the squared frequency is a sum of a positive constant ω^2 plus a decreasing function of time, so that the system approaches a time-independent oscillator as t tends to infinity. In *figure D.1*, we show states $\Phi_\rho^{(z)}(t,t_0)$ that behave as coherent states for large values of the time parameter. The classical equation of motion has a singularity

[1]All Mathieu functions have the form $\exp(irt)F(t)$, where r is the characteristic exponent and the function $F(t)$ has period 2π.

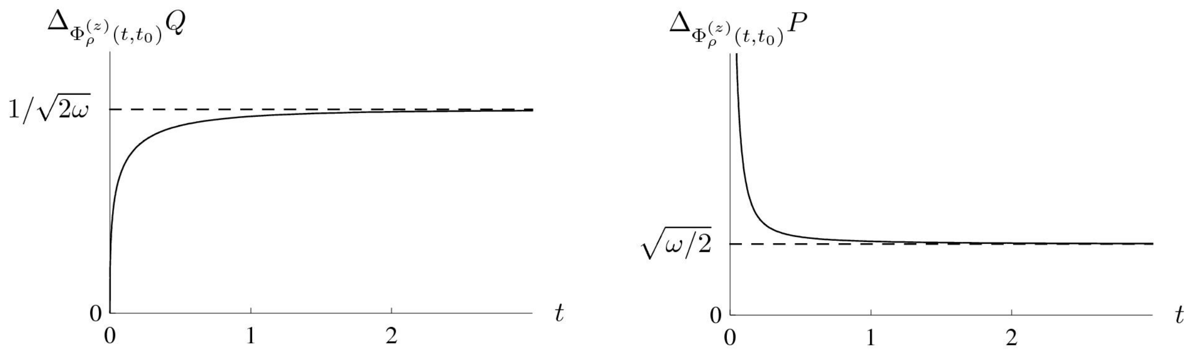

Figure D.1: Variances of the position and momentum operators for the 3-torus Gowdy-type oscillator. Here, $\rho(t) = \sqrt{\pi t\big(J_0^2(\omega t) + Y_0^2(\omega t)\big)/2}$. The $\Phi_\rho^{(z)}(t, t_0)$ are states of minimum uncertainty for times t far from the singularity at $t = 0$.

at $t = 0$ which translates into the vanishing of the uncertainty of the position operator –and, hence, into the divergence of the variance for the conjugate momentum– at that instant of time.

There are other interesting effects due to the classical singularity. Let us consider again the study of transition amplitudes developed in *subsection D.2.4* and take $\omega_1 = \omega_2 = \omega$. We proceed to analyze the behavior of the (unique) state $\Psi(t_2, t_1)$ that evolves to the vacuum state ϕ_0^ω at time t_2 when used as Cauchy data in $t_1 < t_2$, i.e.,

$$U(t_2, t_1)\Psi(t_2, t_1) = \phi_0^\omega \Leftrightarrow \Psi(t_2, t_1) = U(t_1, t_2)\phi_0^\omega \,.$$

The transition amplitudes $\langle \phi_{2n}^\omega \,|\, \Psi(t_2, t_1)\rangle = \langle \phi_{2n}^\omega \,|\, U(t_1, t_2)\phi_0^\omega\rangle$, $n \in \mathbb{N}_0$, can be computed by using (D.37). We recognize two regions of interest in the time domain,

$$T_{0+} := \{(t_1, t_2) \mid 0 < t_1 \ll \omega^{-1} \ll t_2\} \quad \text{and} \quad T_{++} := \{(t_1, t_2) \mid \omega^{-1} \ll t_1 < t_2\} \,.$$

In T_{++}, the asymptotic behavior of the Bessel functions for large values of the time parameter [19] leads the system to behave as a TIHO of constant frequency ω, with $\Psi(t_2, t_1) \sim \phi_0^\omega$. On the other hand, in the region T_{0+}, the proximity of t_1 to the classical singularity manifests itself in the fact that the wave function takes the form $\Psi(t_2, t_1) \sim 0$. Note that this behavior is in conflict with the unitary evolution of the system, which implies $\|\Psi(t_2, t_1)\| = 1$.

Example 3 Let us consider now a harmonic oscillator of the type analyzed in *Chapters 1* and *2* corresponding to the $\mathbb{S}^1 \times \mathbb{S}^2$ and $\mathbb{S}^3$ Gowdy models. Here, the modes satisfy equations of motion of the form

$$\ddot{u}(t) + \kappa(t;\omega)u(t) = 0 \,, \quad \kappa(t;\omega) := \omega^2 + \frac{1}{4}(1 + \csc^2 t) \,, \;\; \omega \in \mathbb{R} \,, \;\; t \in (0, \pi) \,.$$

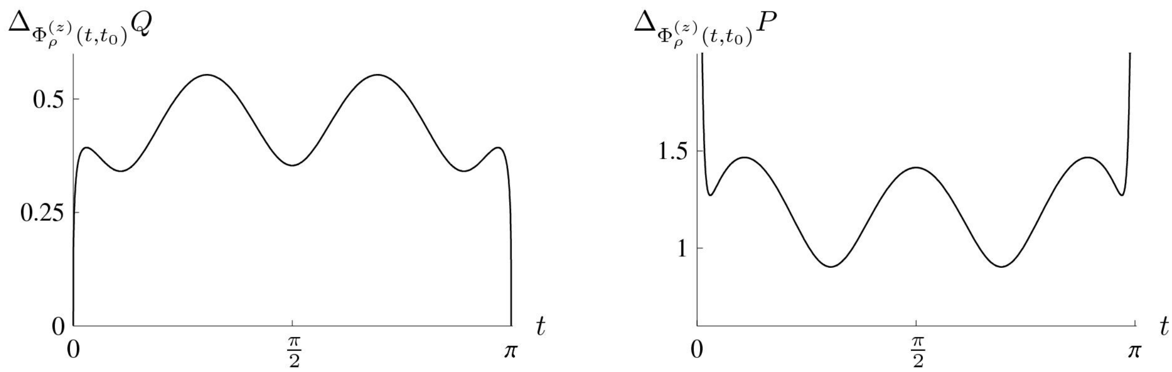

Figure D.2: Variances of the position and momentum operators for the 3-handle and 3-sphere Gowdy-type oscillators. Here, we take the solution $\rho(t) = \sqrt{\sin t}\big(\mathscr{P}^2_{(\omega'-1)/2}(\cos t) + \mathscr{Q}^2_{(\omega'-1)/2}(\cos t)\big)^{1/2}$ to the auxiliar Ermakov-Pinney equation. In particular, graphics correspond to $\omega' = 5$.

In this case, in terms of first and second class Legendre functions [19] $\mathscr{P}_x$ and $\mathscr{Q}_x$, $x \in \mathbb{R}$, we have

$$\begin{aligned} c(t,t_0) &= \frac{1}{2}\sqrt{\sin t/\sin t_0}\,\mathscr{Q}_{\frac{\omega'-1}{2}}(\cos t)\big((1+\omega')\mathscr{P}_{\frac{1+\omega'}{2}}(\cos t_0) - \omega'\mathscr{P}_{\frac{\omega'-1}{2}}(\cos t_0)\big) \\ &\quad -\frac{1}{2}\sqrt{\sin t/\sin t_0}\,\mathscr{P}_{\frac{\omega'-1}{2}}(\cos t)\big((1+\omega')\mathscr{Q}_{\frac{1+\omega'}{2}}(\cos t_0) - \omega'\mathscr{Q}_{\frac{\omega'-1}{2}}(\cos t_0)\big)\,, \\ s(t,t_0) &= \sqrt{\sin t \sin t_0}\big(\mathscr{Q}_{\frac{\omega'-1}{2}}(\cos t_0)\mathscr{P}_{\frac{\omega'-1}{2}}(\cos t) - \mathscr{P}_{\frac{\omega'-1}{2}}(\cos t_0)\mathscr{Q}_{\frac{\omega'-1}{2}}(\cos t)\big)\,, \end{aligned} \tag{D.51}$$

where $\omega' := \sqrt{1+4\omega^2}$. In *figure D.2*, we show the behavior of states $\Phi_\rho^{(z)}(t,t_0)$ for which the uncertainties of the position and momentum operators have an oscillatory behavior far enough from the singularities occurring at $t=0$ and $t=\pi$. Although ρ does not vary periodically, the function remains bounded and, thus, the $\Phi_\rho^{(z)}(t,t_0)$ states can be used to perform a semiclassical study of these models. Finally, one may proceed as in the 3-torus case in order to analyze the way the classical singularities affect the quantum behavior of the systems, obtaining similar results.

References

1 V. P. Ermakov, Univ. Izv. Kiev. **20**,1 (1880); see Appl. Anal. Discrete Math. **2**, 123-145 (2008) for an English translation of Ermakov's original paper.

2 E. Pinney, Proc. Amer. Math. Soc. **1**, 681 (1950).

3 P. G. L. Leach and K. Andriopoulos, Appl. Anal. Discrete Math. **2**, 146-157 (2008).

4 H. R. Lewis, Jr., J. Math. Phys. **9**, 1976 (1968).

5 M. Lutzky, Phys. Lett. A **68**, 3 (1978).

6 M. Fernández Guasti and H. Moya-Cessa, J. Phys. A: Math. Gen. **36**, 2069-2076 (2003).

7 H. R. Lewis, Jr., Phys. Rev. Lett. **18**, 510, 636 (1967).

8 B. Felsager, *Geometry, Particles and Fields*, Odense University Press, (1981).

9 J. Rezende, J. Math. Phys. **25**, 3264-3269 (1984).

10 D. C. Khandekar and S. V. Lawande, J. Math. Phys. **16**, 384-388 (1973).

11 A. K. Dhara and S. V. Lawande, Phys. Rev. A **30**, 560-567 (1984).

12 B. K. Cheng and F. T. Chan, J. Phys. A: Math. Gen. **20**, 3771-3775 (1987).

13 L. F. Landovitz, A.M. Levine, and W.M. Schreiber, J. Math. Phys. **21**, 2159-2163 (1980).

14 K. Pilch and N. Warner, Class. Quant. Grav. **4**, 1183 (1987).

15 J. G. Hartley and J. R. Ray, Phys. Rev. D **25**, 382-386 (1982).

16 J. V. José and E. J. Saletan, *Classical Dynamics: A Contemporary Approach*, Cambridge University Press, (1998).

17 E. Mathieu, Journal of Mathematiques Pures et Appliquees **13**, 137203 (1868).

18 N. W. McLachlan, *Theory and Application of Mathieu Functions*, Dover, (1965).

19 M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, Dover, (1964).

Appendix E
Fock Spaces

Consider a quantum mechanical system consisting of (possibly a variable number of) identical particles. Their indistinguishability at the atomic level is reflected by the so-called *symmetrization principle*, according to which the pure states of the system under consideration must be either completely symmetric or antisymmetric under the exchange of any two particles. Starting from such a general assumption, it is then possible to prove in the context of the quantum theory of local fields the so-called *spin-statistics theorem*, which divides particles into two groups: The pure states of a system of identical particles are symmetric (antisymmetric) if they have integer (half-integer) spin. Particles which exhibit symmetric states (bosons) satisfy the Bose-Einstein statistics, whereas particles with antisymmetric states (fermions) obey the Fermi-Dirac statistics. In this appendix, we construct the bosonic/fermionic Fock spaces used for the description of these systems, as well as the representation of the corresponding canonical commutation/anticommutation relations.

E.1 Symmetric and antisymmetric Fock spaces

Let $\mathscr{H}$ be a (separable) one-particle Hilbert space. Denote by $\mathscr{H}^{\otimes n}$, $n \in \mathbb{N}$, the n-fold Hilbert tensor product of $\mathscr{H}$, i.e., the Cauchy completion of the pre-Hilbert space of finite linear combinations of elements of the form $x_1 \otimes \cdots \otimes x_n$, $x_1, \ldots, x_n \in \mathscr{H}$, with respect to the inner product

$$\langle x_1 \otimes \cdots \otimes x_n \,|\, y_1 \otimes \cdots \otimes y_n \rangle_{\mathscr{H}^{\otimes n}} := \langle x_1 \,|\, y_1 \rangle_{\mathscr{H}} \cdots \langle x_n \,|\, y_n \rangle_{\mathscr{H}} \,, \quad x_1, \ldots, y_n \in \mathscr{H} \,.$$

If $\{\varphi_k \,:\, k \in \mathbb{N}\}$ is an orthonormal basis in $\mathscr{H}$, then $\{\varphi_{k_1} \otimes \varphi_{k_2} \otimes \cdots \otimes \varphi_{k_n} \,:\, k_i \in \mathbb{N}\}$ is an orthonormal basis in $\mathscr{H}^{\otimes n}$. We define the *Fock space* over $\mathscr{H}$ by the direct sum

$$\mathscr{F}(\mathscr{H}) := \bigoplus_{n=0}^{\infty} \mathscr{H}^{\otimes n} = \mathbb{C} \oplus \mathscr{H} \oplus \mathscr{H}^{\otimes 2} \oplus \cdots \,,$$

where we have set $\mathscr{H}^{\otimes 0} := \mathbb{C}$. This is the state space for an indeterminate number of particles of the same species. It is separable if $\mathscr{H}$ is. Note that each element $\psi \in$

$\mathscr{F}(\mathscr{H})$ can be identified with a sequence of vectors $\psi = \{\psi^{(n)}\}_{n\geq 0}$, with $\psi^{(0)} \in \mathbb{C}$ and $\psi^{(n)} \in \mathscr{H}^{\otimes n}$, $n \geq 1$. The inner product of any two vectors $\varphi, \psi \in \mathscr{F}(\mathscr{H})$ is then given by

$$\langle \varphi \,|\, \psi \rangle_{\mathscr{F}(\mathscr{H})} = \bar{\varphi}^{(0)}\psi^{(0)} + \sum_{n=1}^{\infty} \langle \varphi^{(n)} \,|\, \psi^{(n)} \rangle_{\mathscr{H}^{\otimes n}} .$$

Obviously, it is not $\mathscr{F}(\mathscr{H})$ itself but the closed subspaces of symmetric/antisymmetric tensor products which are frequently used in quantum field theory. Denote by Π_n the permutation group of n elements. For each $\sigma \in \Pi_n$, we define the operator T_σ on basis elements of $\mathscr{H}^{\otimes n}$ by

$$T_\sigma \left(\varphi_{k_1} \otimes \cdots \otimes \varphi_{k_n} \right) := \varphi_{k_{\sigma(1)}} \otimes \cdots \otimes \varphi_{k_{\sigma(n)}} .$$

T_σ extends by linearity to a unitary operator on $\mathscr{H}^{\otimes n}$. The map $\sigma \in \Pi_n \mapsto T_\sigma \in \mathscr{B}(\mathscr{H}^{\otimes n})$ then defines a unitary representation of Π_n on $\mathscr{H}^{\otimes n}$, with $T_{\sigma_1\sigma_2} = T_{\sigma_1}T_{\sigma_2}$ and $T_\sigma^\dagger = T_\sigma^{-1} = T_{\sigma^{-1}}$. A tensor $u \in \mathscr{H}^{\otimes n}$ is called *symmetric* if $T_\sigma u = u$, $\forall\, \sigma \in \Pi_n$, and *antisymmetric* if $T_\sigma u = \mathrm{sgn}(\sigma) u$, $\forall\, \sigma \in \Pi_n$, where $\mathrm{sgn} : \Pi_n \to \{-1, 1\}$ takes the values $+1$ or -1 depending on whether σ is an even or odd permutation, respectively. It is easy to show that the operators

$$\begin{aligned} \mathscr{P}_+^{(n)} &:= \frac{1}{n!} \sum_{\sigma \in \Pi_n} T_\sigma , \\ \mathscr{P}_-^{(n)} &:= \frac{1}{n!} \sum_{\sigma \in \Pi_n} \mathrm{sgn}(\sigma) T_\sigma , \end{aligned}$$

are orthogonal projections on $\mathscr{H}^{\otimes n}$. The range of $\mathscr{P}_+^{(n)}$ (resp. $\mathscr{P}_-^{(n)}$) is called the n-fold symmetric (resp. antisymmetric) tensor product of $\mathscr{H}$. We now define the *bosonic* or *symmetric Fock space* over $\mathscr{H}$ by

$$\mathscr{F}_+(\mathscr{H}) = \mathscr{P}_+\mathscr{F}(\mathscr{H}) := \bigoplus_{n=0}^{\infty} \mathscr{P}_+^{(n)} \left(\mathscr{H}^{\otimes n} \right) ,$$

and, similarly, the *fermionic* or *antisymmetric Fock space* over $\mathscr{H}$ as

$$\mathscr{F}_-(\mathscr{H}) = \mathscr{P}_-\mathscr{F}(\mathscr{H}) := \bigoplus_{n=0}^{\infty} \mathscr{P}_-^{(n)} \left(\mathscr{H}^{\otimes n} \right) ,$$

with $\mathscr{P}_\pm : \mathscr{F}(\mathscr{H}) \to \mathscr{F}_\pm(\mathscr{H})$ being called the *symmetrization* (the + sign) and *antisymmetrization* (the − sign) *projections*. Finally, we introduce the so-called *vacuum state*,

$$\Psi_0 := (1, 0, 0, \ldots) ,$$

which represents the state of the system with no particles. Note that the state so defined is normalized.

Let $\{\varphi_k\}$ be an orthonormal basis of $\mathscr{H}$. With the aim of constructing an orthonormal basis for the Fock spaces $\mathscr{F}_\pm(\mathscr{H})$, it suffices to consider the states

$$|n_1, n_2, \ldots\rangle_\pm := \Theta_\pm \mathscr{P}_\pm(\varphi_1^{\otimes n_1} \otimes \varphi_2^{\otimes n_2} \otimes \ldots)\,, \quad \sum_k n_k = N < +\infty\,,$$
$$\Theta_+ = \left(\frac{(\sum_k n_k)!}{\prod_k (n_k!)}\right)^{1/2}\,, \quad \Theta_- = \left(\frac{1}{\prod_k (n_k!)}\right)^{1/2}\,,$$

for finite nonzero sequences $\{n_k \in \mathbb{N}_0\}$. The $|n_1, n_2, \ldots\rangle_\pm$ vector describes an assembly of N identical bosonic (the $+$ sign) or fermionic (the $-$ sign) particles, in which the state φ_k is occupied by n_k particles. The integers n_k, $k \in \mathbb{N}$, are called the *occupation numbers* of these states. Note that $\mathscr{P}_-(\varphi_1^{\otimes 2} \otimes \cdots) = 0$ in the antisymmetric case, so that two identical fermions cannot occupy the same quantum state at the same time. This last result is referred to as the *Pauli exclusion principle*, according to which $n_k \in \{0, 1\}$, $\forall\, k$, for fermionic systems. This is precisely the main qualitative difference between fermion and boson particles; the absence of the Pauli principle for the latter particles implies that there is no bound on the number of bosons that can occupy a state.

E.2 Creation and annihilation operators

Let N be the self-adjoint *number operator* on $\mathscr{F}(\mathscr{H})$,

$$N\psi = \{n\psi^{(n)}\}_{n\geq 0}\,, \quad \psi \in \mathscr{D}_N\,,$$

with dense domain $\mathscr{D}_N = \{\psi = \{\psi^{(n)}\}_{n\geq 0} \mid \sum_{n\geq 0} n^2 \|\psi^{(n)}\|^2 < +\infty\}$. For each vector $f \in \mathscr{H}$ we define the *creation* and *annihilation operators* on $\mathscr{F}(\mathscr{H})$, respectively $C(f)$ and $A(f)$, by initially setting $A(f)\psi^{(0)} = 0$, $C(f)\psi^{(0)} = f$, $f \in \mathscr{H}$, and

$$\begin{aligned} C(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n) &= (n+1)^{1/2} f \otimes f_1 \otimes \cdots \otimes f_n\,, \\ A(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n) &= n^{1/2} \langle f \mid f_1\rangle_{\mathscr{H}} f_2 \otimes \cdots \otimes f_n\,. \end{aligned}$$

Extension by linearity leads to densely defined operators. Given $\psi^{(n)} \in \mathscr{H}^{\otimes n}$, it is straightforward to check that

$$\|C(f)\psi^{(n)}\| \leq (n+1)^{1/2}\|f\|\|\psi^{(n)}\| \quad \text{and} \quad \|A(f)\psi^{(n)}\| \leq n^{1/2}\|f\|\|\psi^{(n)}\|\,, \tag{E.1}$$

so that $C(f)$ and $A(f)$ have well-defined extensions to the domain of the $N^{1/2}$ operator, satisfying

$$\|C(f)\psi\|, \|A(f)\psi\| \leq \|f\|\|(N+1)^{1/2}\psi\|\,, \quad \psi \in \mathscr{D}_{N^{1/2}}\,. \tag{E.2}$$

The adjoint relation

$$\langle C(f)\varphi \mid \psi\rangle_{\mathscr{F}(\mathscr{H})} = \langle \varphi \mid A(f)\psi\rangle_{\mathscr{F}(\mathscr{H})} \tag{E.3}$$

holds for all $\varphi, \psi \in \mathscr{D}_{N^{1/2}}$. We then define the creation and annihilation operators on the symmetric/antisymmetric Fock spaces $\mathscr{F}_\pm(\mathscr{H})$ by

$$C_\pm(f) = \mathscr{P}_\pm C(f) \mathscr{P}_\pm\,, \quad A_\pm(f) = \mathscr{P}_\pm A(f) \mathscr{P}_\pm\,,$$

verifying, by virtue of relations (E.2) and (E.3),

$$\langle C_\pm(f)\varphi \,|\, \psi\rangle_{\mathscr{F}(\mathscr{H})} = \langle \varphi \,|\, A_\pm(f)\psi\rangle_{\mathscr{F}(\mathscr{H})}\,, \quad \|C_\pm(f)\psi\| \le \|f\| \|(N+1)^{1/2}\psi\|\,,$$

for all $\varphi, \psi \in \mathscr{D}_{N^{1/2}}$. Moreover, since $A(f)$ leaves the subspaces $\mathscr{F}_\pm(\mathscr{H}) \prec \mathscr{F}(\mathscr{H})$ invariant, i.e., $[A(f), \mathscr{P}_\pm] = 0$, $f \in \mathscr{H}$, we get

$$C_\pm(f) = \mathscr{P}_\pm C(f)\,, \quad A_\pm(f) = A(f)\mathscr{P}_\pm\,.$$

Note that the maps $f \mapsto C_\pm(f)$ and $f \mapsto A_\pm(f)$, $f \in \mathscr{H}$, are linear and antilinear, respectively. Finally, it is straightforward to calculate the *canonical commutation relations*

$$[A_+(f), A_+(g)] = 0 = [C_+(f), C_+(g)]\,, \quad [A_+(f), C_+(g)] = \langle f \,|\, g\rangle_{\mathscr{H}} \mathbb{I}\,, \quad f, g \in \mathscr{H}\,, \tag{E.4}$$

as well as the *canonical anticommutation relations*

$$\{A_-(f), A_-(g)\} = 0 = \{C_-(f), C_-(g)\}\,, \quad \{A_-(f), C_-(g)\} = \langle f \,|\, g\rangle_{\mathscr{H}} \mathbb{I}\,, \quad f, g \in \mathscr{H}\,, \tag{E.5}$$

where we have used the notation $\{A, B\} := AB + BA$. The fact that the occupation numbers can vary over all $\mathbb{N}$ for bosonic particles is reflected by the unboundedness of the creation and annihilation operators. On the contrary, these operators have bounded extensions in the antisymmetric case as a consequence of Pauli principle.

References

1 O. Bratteli and D. W. Robinson, *Operator Algebras and Quantum Statistical Mechanics II. Equilibrium States. Models in Quantum Statistical Mechanics*, 2ª ed., Springer (1997).

2 M. Reed and B. Simon, *Methods of Modern Mathematical Physics I: Functional Analysis; II: Fourier Analysis. Self-Adjointness*, Academic Press, New York (1975).