CENTRO DE INVESTIGACIÓN Y DE ESTUDIOS AVANZADOS
DEL INSTITUTO POLITÉCNICO NACIONAL

UNIDAD ZACATENCO
DEPARTAMENTO DE FÍSICA

"Aspectos cuánticos de la materia y el espacio-tiempo"

Tesis que presenta

Omar Gallegos Santiago

para obtener el Grado de

Doctor en Ciencias

en la Especialidad de

Física

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Ciudad de México Diciembre, 2023

CENTER FOR RESEARCH AND ADVANCED STUDIES OF THE NATIONAL POLYTECHNIC INSTITUTE

UNIT ZACATENCO
PHYSICS DEPARTMENT

"Quantum aspects of matter and space-time"

by

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In order to obtain the

Doctor of Science

degree, speciality in

Physics

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Mexico City December, 2023

ABSTRACT

Quantum nature of matter has been extensively studied since the beginning of the twentieth century, having successful results. However, a quantum description of space-time is an open fundamental problem in modern physics without a final answer, and there are only tentative proposals. In this work, some aspects on quantization of matter and spacetime are discussed.

As for matter, a hydrodynamic approach is adopted for non-relativistic and relativistic systems, which is extended to fermions described by the Dirac equation in curved spacetime. The Madelung transformation is implemented to obtain the hydrodynamic description in this case. In addition, using conservative forces and taking into account the Bernoulli principle, it is possible to find an energy balance equation.

Regarding quantum aspects of spacetime, it is now known that some problems in standard cosmology can be solved taking into account the discreteness of spacetime. For example, it is possible to replace the classical big bang singularity by a quantum bounce. In this work, we use the formalism of loop quantum cosmology (LQC), which is a reduced-symmetric model of loop quantum gravity (LQG). This is a non-perturbative and background-independent approach. We first focus on an isotropic and homogeneous flat universe, in order to implement unitary evolution. The self-adjoint character of the scalar constraint is considered, which contains a weight parameter between the Euclidean and Lorentzian terms. Additionally, different shapes of classical and effective universes including both Lorentzian and Euclidean terms are compared, where an emergent cosmological constant is obtained, while preserving the replacement of the big bang singularity by quantum bounce.

New results are contained in Sections 5.4, 6.2, 6.4 and 6.5, included in references [1–3].

RESUMEN

La naturaleza cuántica de la materia ha sido ampliamente estudiada desde inicios del siglo veinte teniendo resultados exitosos. Sin embargo, una descripción cuántica del espacio-tiempo es un problema abierto en la física moderna sin una respuesta definitiva, sólo propuestas tentativas. En este trabajo se discuten algunos aspectos sobre la cuantización de la materia y el espacio-tiempo.

Para la materia, una representación hidrodinámica es adoptada para sistemas relativistas y no-relativistas, la cual se extiende a fermiones descrita por la ecuación de Dirac en espacio-tiempos curvos. La transformación de Madelung es implementada para obtener la representación hidrodinámica. Además, haciendo uso de la conservación de las fuerzas y la ecuación de Bernoulli es posible encontrar una ecuación de balance de la energía.

Con respecto a los aspectos cuánticos del espacio-tiempo, es ahora conocido que algunos problemas que existen en la cosmología estándar pueden ser resueltos si se toma en cuanta una descripción discreta del espacio-tiempo. Por ejemplo, es posible reemplazar la sigularidad clásica del big bang por un rebote. En este trabajo utilizamos el formalismo de la cosmología cuántica por lazos o bucles (LQC), el cual es un modelo simétrico reducido de la gravedad cuántica por lazos (LQG), la cual es una propuesta no perturbativa e independiente del fondo. Nos enfocamos en un universo plano isótropo y homogéneo al inicio, con el fin de implementar la evolución unitaria. El carácter auto-adjunto de una constricción escalar es considera la cual contiene un parámetro de peso entre el término Euclideano y Lorentziano. Adicionalmente, se comparan las diferentes formas de universos clásicos y efectivos incluyendo los términos Euclideano y Lorentzian, donde se puede obtener una constante cosmológica emergente, mientras se preserva el reemplazo del rebote cuántico por la singularidad del big bang.

Los nuevos resultados están contenidos en las secciones 5.4, 6.2, 6.4 y 6.5, e incluidos en las referencias [1–3].

CONTENTS

ACKNOWLEDGES

Quisiera plasmar mis agradecimientos en español, a pesar que esta tesis no estará escrita en este idioma.

A mis padres y mi familia que siempre me ha apoyado en todos los aspectos de la vida, es algo que jamás podré compensar.

A mis asesores, Dr. Tonatiuh Matos quien desde la maestría me ha guiado a investigar algo que en verdad me apasione, al Dr. Hugo A. Morales quien me ha instruido a comprender de la mejor manera conceptos complicados y quien siempre ha tenido las mejores palabras para corregir mis errores. A ambos por todo su apoyo e inspirarme en ir más lejos y conocer cada vez más.

Al Dr. Alejandro Corichi, Dr. Hugo García-Compeán, Dr. Omar Miranda, y Dr. José David Vergara por sus invaluables comentarios y sugerencias a esta tesis.

A las secretarias Malu y Mariana quienes a pesar de las complicaciones burocráticas, su trabajo siempre fue impecable, eficiente y hacían más ligero todos los trámites.

A mis amigos, compañeros y profesores dentro y fuera del Cinvestav y la UAM, particularmente a Abraham, Angelica, Benjamin, Erick, Fernando, Gonzalo, Horacio, Jesus, Joel, Marcela, Mario, Pedro, Saul. Un agradecimiento especial a Leonardo Rubio por sus correciones con el inglés, a Leonardo Sánchez por ayudarme con las gráficas, así como a Juan Carlos por sus sugerencias y correcciones. Gracias por su apoyo y consejos en diferentes aspectos no sólo académicos.

A Tomasz Pawłowski por su hospitalidad durante mi estancia en Polonia, y por las discusiones sobre LQC, en específico sobre las extensiones autoadjuntas.

A Dra. Ana Avilés por sus sugerencias en el avance de tesis, a Pierre-Henri Chavanis por su colaboración en la escritura del paper sobre la representación hidrodinámica de los fermiones.

A CONACYT y ahora CONAHCYT por el apoyo financiero durante mis estudios de doctorado.

CHAPTER

ONE

INTRODUCTION

At the beginning of the twentieth century there was a revolution in the understanding of the behavior that our universe presents because some observations and experimental results were inconsistent with the theory that existed in those days. Historically, the solution of the ultraviolet catastrophe problem opened the door to quantum revolution because the classical theory could not give an explanation of this problem, which was solved by Max Planck proposing that matter is composed by minimum pieces of it or quanta. Because of the idea that matter cannot be infinitely divided because there exists a minimum subdivision, the Greeks called this minimum an atom. However, in physics, an atom is formed by other more fundamental particles such as electrons, protons, and neutrons, where these last two in turn contain particles that are even yet more fundamental such as quarks. In addition, particles such as electrons, muons, taus, and their respective neutrinos are called leptons. All of these particles come from a more fundamental description, which is named the quantum field.

The description of the structure of an atom was an important problem in classical physics because at that time physicists thought that there could be an analogy between the planetary system and an atom. Nevertheless, in the classical perspective, a model with these characteristics should be unstable because electrons would radiate and then lose energy as they orbit around a nucleus, which is formed by protons and neutrons. Finally, electrons would collapse into the nucleus, which would lead to the nonexistence of atoms; therefore, neither living beings nor stars, galaxies or anything we observe should exist. With the development and a better understanding of the quantum nature of matter, this theoretical inconsistency was solved by using the Pauli exclusion principle.

Quantum mechanics (QM) is a mathematical tool that helps us to give a better understanding of tiny particles, and also an explanation and solution to some problems that physicists had when using classical theory. Nevertheless, the mathematical formalism of this theory and the contraintuitive ideas with respect to Newtonian theory arrive at different interpretations, the most popular and extensively studied by scientists is the Copenhagen interpretation, which was promoted by Niels Bohr and collaborators in Denmark [4]. This interpretation of quantum theory leaves some paradoxes, which were highlighted by Albert Einstein, Erwing

Schrödinger, Boris Podolsky, Nathan Rosen [5], and many more criticisms of quantum theory in those years.

The observed paradoxes were derived from the interpretation of the wave function, its collapse, and the violation of the locality principle. Coupled to those problems in this interpretation, the quantum description of nature has a probabilistic behavior instead of a deterministic one as in the classical theory. This leads us into a discussion about the completeness of the theory, where some proposals included hidden variables to solve the probabilistic interpretation of quantum mechanics. However, to distinguish between the different interpretations of quantum mechanics John Stewart Bell presented some inequalities, which today bear his name [6]. In this work, the de Broglie-Bohm and Copenhagen interpretations will be used, the first one being utilized to build the hydrodynamic representation of quantum particles using the Madelung transformation [7]. This interpretation of quantum mechanics is an example of hidden variables that try to solve the problem of the collapse of the wave function and some paradoxes. Furthermore, the de Broglie-Bohm interpretation has a deterministic description [8–11]. On the other hand, the Copenhagen interpretation is the most widely studied by physicists worldwide.

Relativistic QM starts with the Klein-Gordon (KG) equation and then the Dirac equation. However, the KG equation presents a negative probability problem, which the Dirac equation solves. The KG equation describes boson particles and the Dirac equation defines the behavior of fermion particles; the fundamental difference between both kinds of particles is the symmetry and antisymmetry of the wave function, respectively. Furthermore, the spin number for bosons is an integer and that for fermions is a half-odd integer. In fact, the spin property is a consequence of a relativistic quantum effect, which appears naturally in the construction of the Dirac equation due to the gamma matrices being related with the Pauli matrices, which follow the same algebra of spin. The extension to curved spacetimes can be applied with a minimum coupling principle, which is explained in more detail in the following sections. In this context, the background is fixed and the matter field is quantized; in quantum gravity, the gravitational field or spacetime is quantized.

The hydrodynamic representation of classical particles is described by the Navier-Stokes equation; this equation does not have an analytical solution; in fact, it is one of the problems of the millennium. However, it is possible to introduce a hydrodynamic representation of QM using the Madelung transformation, that is, to rewrite the wave function in a polar way. With this different form to see QM, and using the de Borglie-Bohm interpretation, it is possible to transform the Scrödinger equation to the quantum Navier-Stokes equation. These ideas can be extended to the relativistic case using the Klein-Gordon (KG) equation in curved spacetimes, as is shown by Ana Avilez, Tula Bernal, Pierre-Henri Chavanis, and Tonatiuh Matos [12, 13], where it is possible to rewrite the KG equation as a quantum Navier-Stokes equation in curved spacetimes; this representation is useful to describe the hydrodynamics of a scalar field, as some candidates of dark matter propose. In this thesis, we seek to complete the hydrodynamic description for the fermion case, where a generalized Madelung transformation is proposed for spinors. Although we can find a quantum Bernoulli equation, that is, the first integral of the Naviers-Stokes equation, a fundamental difference from previous cases, in which it is possible to separate into real and imaginary parts, is that in our approach, the complex structure due to the gamma matrices remains. This difficulty is reflected in the fact that we cannot provide an adequate physical interpretation; we think that a better description will be available to solve specific symmetric cases because the work in [1] is quite general. However, that work is not yet developed.

During the development and foundations of quantum theory, the other pillar of modern physics was proposed by Albert Einstein starting in 1905 with the special relativity theory, which changed our understanding of space-time. Opposed to the past belief in Newtonian theory, in special relativity there is not an absolute frame of reference. In this first work, the gravitational interaction was not included, but it was not until 1915 when Einstein presented his general relativity theory, which is our best way of understanding the behavior of gravity to this day.
General relativity (GR) teaches us that gravity is a manifestation of the geometry of spacetime by an elegant formalism. From a Newtonian perspective, gravity is the force between two objects with mass. However, in this new vision, gravity is more fundamental than a force, which is a consequence of the curvature of spacetime. Furthermore, using GR, gravity can interact with massless particles because they follow a given geodesic (the minimum path between two points in an arbitrary geometry is not necessarily a straight line) along the curvature of spacetime. As we shall see in the review of general relativity in this work, gravity obeys the Einstein equation, which is an equality between geometry and matter.

General relativity theory began its success when its predictions came true. The first one was the measurement of the deviation of light that passed between the Sun and Earth coming from distant stars during a solar eclipse. Moreover, GR explained the precession of the orbit of Mercury, which is affected by the intense gravitational field of the Sun. Other predictions such as gravitational waves and black holes have recently been verified. In fact, GR helps to have more precise GPS because the satellites that orbit Earth are undergoing a small time dilation due to them being affected by the gravitational field of the Earth. This time delay is reflected in the poor precision of the GPS coordinates on the ground. Although GR is not necessary in order to send a satellite into orbit, the error produced by relativistic effects could probably be solved by using curve adjustments. GR gives the right fit of this delay, but most importantly, it not only solves this problem, it gives the correct explanation to this physical phenomenon. Therefore, thanks to GR, we can use Google Maps to get where we want and we can also ask for Uber or any service at home. Although there are certain GR applications that are useful in everyday life, the motivation to better understand the behavior of the universe and the technological applications was a consequence of this more fundamental description of gravity. Thus, the objective of basic or fundamental physics is to understand in a better way the description of some phenomena, instead of producing an immediate technological application.

Many of the predictions made by GR have been verified with great precision,

but there are others, such as the existence of wormholes, that are not yet to be proven. Furthermore, the theory has an important problem, that is, singularities. In these regions of spacetime, the theory predicts that the gravitational field is so intense such that some quantities have an infinite value. Examples of these regions are the singularities located in black holes and the big bang.
In this work, we focus on the big bang region, which is described by cosmology, that is, the description of the Universe as a whole, derived from observations. We know that the Universe is expanding in an accelerated manner and that galaxies are becoming more and more separated from each other; this accelerated expansion is caused by dark energy; then, it is concluded that the Universe had a start. The Universe satisfies the cosmological principle which describes an isotropic and homogeneous universe at large scales; that is, there is no privileged direction and, wherever one looks, it seems to be the same. However, GR and standard cosmology predict that in the beginning all matter was concentrated at a point, which implies that quantities such as density and curvature are infinity. This is a theoretical problem, which could be solved by taking into account quantum effects of spacetime, which can be analogous to when Newtonian problems were solved applying quantum theory.

A quantum description of gravity is the most fundamental problem in modern physics because it is about unifying the most important theories of physics into a single one. QM describes the physical phenomena of tiny particles. On the other hand, GR describes the dynamics of cosmic structures. However, each theory seems to be fundamentally incompatible. We could find a better description of gravity using a classical theory, which could solve the singularity problem. A proposal of this approach is the $f(R)$ and MOND theories, which are a modification of classical theories, but they do not comply with many of the measurements already made and verified by GR. Another point in favor of quantization is the fact that three of the four fundamental interactions are of a quantum nature. What makes us think that gravity could not have a quantum description?

In recent decades, there have been various candidate theories for the theory of quantum gravity, such as string theory, lattice quantum gravity, casual set theory, causal dynamics, loop quantum gravity, and more candidates. In this fundamental description, we expect that spacetime emerges for some more fundamental objects such as strings, triangulations, loops, etc., just like Newtonian force and general relativity. In this work, we focus on the loop quantum gravity (LQG) formalism [14–16], whose foundations have been laid since the 1980s by Abhay Ashtekar, Carlo Rovelli, Lee Smolin, Thomas Thiemann, Rodolfo Gambini, Jerzy Lewandoski, and other physicists. LQG is a non-perturbative and background-independent approach, which is based on general relativity. Compared to the most popular candidate, that is, string theory, which is described by higher dimensions, the LQG formalism uses the same number of dimensions as in GR. Furthermore, LQG is not as ambitious as string theory, which tries to unify all fundamental interactions, LQG only tries to give a quantum description of gravity by a canonical or Hamiltonian formalism of GR. This description has been criticized because the theory is not manifestly covariant, but due to it being based on GR, LQG obeys Lorentz transformations. However, in LQG there exists a covariant formulation that is called spin foams. This fact about covariance is analogous to using the description of the electric and magnetic fields separately instead of the covariant form using the Faraday tensor. Nevertheless, both descriptions satisfy Lorentz transformations.

The full theory, LQG, contains complicated and sophisticated details because the gravitational field has a discrete description. However, for just over two decades LQG tools have been applied to reduced-symmetric models such as cosmological or black hole models to find phenomenological results in models easier to understand than in the full theory. This simplified reduction has had successful consequences, such as replacing the classical singularity with a quantum bounce due to the fact that there exists a minimum nonzero value of the area, which is at Planck scales. This description applied to reduced-symmetric models was proposed by Martin Bojowald [17–22], which consists in expressing the classical Ashtekar-Barbero variables with the corresponding symmetry and then quantizing the symmetric model using LQG methods. Thus, it is possible to obtain different results, such as a quantum description, dynamics, effective models, etc. The cosmological case using analogous techniques developed by LQG, is called loop quantum cosmology (LQC).

The LQC strategy to obtain a quantum description of a cosmological model used by Abhay Ashtekar, Martin Bojowald, Alejandro Corichi, Wojciech Kamiński, Jerzy Lewandoski, Tomasz Pawłowski, Parampreet Singh, Kevin Vandersloot, and more authors is to build the classical reduced-symmetric Ashtekar-Barbero variables which describe an isotropic and homogeneous universe [23–26]. The constraints that make up the total Hamiltonian constraint may then be expressed as fundamental variables, which are Poisson brackets of the holonomies and fluxes. These classical variables are promoted to quantum operators by Dirac quatization in this description, the Hilbert space is built so that the flux and holonomy algebra is fulfilled. In LQC models, the only constraint that is not trivially solved is the Hamiltonian constraint, which is formed by two terms, Euclidean and Lorentzian.

In the first LQC papers, it was noted that both classical terms are proportional in this symmetric flat model; for this reason, the LQC models only quantize one term. However, then it was noted by Jinsong Yang, You Ding and Yongge Ma [27] that using the Thiemann regularization [14], such as in the full theory, where both terms are quantized independently, an emergent or effective cosmological constant can be obtained. However, the theoretical and observational values of the cosmological constant differ by 120 orders of magnitude, as noted by Medhi Assonioussi, Andrea Dapor, Klaus Liegerner, and Tomasz Pawłowski [28, 29]. In response to this discrepancy, Xiangdong Zhang, Gaoping Long, and Yongge Ma [30] introduced a weight parameter between the Euclidean and Lorentzian terms to match the theoretical and observational values, which is considered as fine tuning. However, in this thesis, we use the weight parameter to characterize the unitary evolution of the geometrical operator as a generalized model, which contains a massless scalar field that is interpreted as an evolution parameter. This problem has physical interest because an observable in QM may be self-adjoint, we emphasize on the definition of an operator that is the hermitian, self-adjoint, symmetric, adjoint. In this work, we give some important definitions and their applications on LQC models in which the authors are A. Ashtekar, A. Assonioussi, A. Dapor, W. Kamiński, J. Lewandowski, K. Liegerner, T. Pawłowski. More results have been developed [26, 28, 29, 31, 32], as they note that the quantum Hamiltonian constraint only contains the Euclidean term, which is essentially self-adjoint, but when the Lorentzian term or an explicit cosmological constant is introduced in the quantum constraint, self-adjointness is lost. However, it is possible to apply the deficiency index method to find possible self-adjoint extensions. Here, we discuss this method and the characterization of a generalized flat LQC model, in addition to the advantages and disadvantages of writing the geometric operator in different representations. As we shall see, it is convenient to use b-representation because the operator takes a differential form instead of v-representation, which is a difference form. Contrary to difference equations, the theory and methods for solving differential equations have been studied extensively.

Curvature in LQC models has been another important aspect that different authors have considered [33–39]. In this thesis, we consider Lorentzian models with curvature, which use the Thiemann regularization as in the full theory, which was implemented by Y. Ma and collaborators. It is possible to build a quantum description of cosmological models with hyperbolic, flat, and spherical geometries and to get their corresponding effective models where the comparison with the classical models is direct; we use a pictorial comparison by graphs that are used in standard cosmology for different shapes of the universe. In these figures, it is possible to see that the description at large scales is the same, but at small scales the big bang singularity is replaced by the quantum bounce, and effective dynamics converges quickly to classical evolution, as we would expect. Thus, in this work, as happens in standard cosmology, it is possible to generalize the cosmological models with curvature in the LQC context.

Effective models for loop-quantized spacetimes have been obtained by different ways, the easiest and less formal consists in only removing the hat symbol above the operator and transform it into effective variables; then an effective Hamiltonian constraint is found, and it is possible to build effective equations of motion such as the modified or effective Friedmann equation. The second form to obtain an effective Hamiltonian is to use the expectation value method, which consists in calculating the expectation value of the Hamiltonian operator using quantum states. The cases that are shown in this thesis consider Gaussian states, where it is possible to obtain corrections up to different orders. Finally, another method implemented to find effective models in LQC is to use the path-integral formalism, where all possible paths are considered, and with this method it is possible to obtain higher-order corrections. These three methods lead to consistent results in the lowest order of approximation. The modified Friedmann equation in some limit recovers the classical description in standard cosmology.

Even though that with this LQC formalism, successful and interesting results have been obtained, this is not the true LQC, which should be a symmetric reduction of loop quantum gravity. However, finding a symmetric or cosmological sector of LQG is an open problem of the theory. The difficulties of this problem lie in the complexity that LQG presents, which is not complete yet. If we had a true cosmological sector of LQG, we would have a true quantum description of a cosmological model, which would probably be a modified and completed description of the LQC models presented in this thesis. However, this work is not as ambitious as to attempt to find this symmetric sector of LQG. This remains a work in the future.

This thesis is organized as follows. A brief review on the Hamiltonian formulation of general relativity is presented in Chapter 2, where the ADM formalism is applied to the Holst action, that is, the tetrad formulation of the Einstein-Hilbert action to introduce the Ashtekar-Barbero formulation. Chapter 3 contains some important concepts of standard cosmology including its ADM formulation and the Ashtekar-Barbero variables for the cosmological case, which are relevant to the quantum cosmology formulation. In Chapter 4, a brief standard formulation of quantum mechanics is shown; this chapter emphasizes the self-adjoint character of a bounded operator, the path-integral formulation, and the quantum relativistic description. In addition, an alternative formulation using polymeric quantum mechanics is presented in Subsection 4.6, which is a formulation analogous to that used in LQG. Chapter 5 introduces a different representation of quantum mechanics, which is studied by a hydrodynamic description. The main hydrodynamic equation for classical and quantum particles is studied, where an extension to the description for bosons to fermions in curved spacetimes is proposed. Furthermore, Chapter 6 describes in detail some important steps to build the loop quantization for an isotropic and homogeneous universe, where the unitary evolution by the self-adjoint property of the gravitational operator and its possible extensions is studied taking into account a generalized flat universe, which includes a weight parameter between the Euclidean and Lorentzian terms in the Hamiltonian constraint. In addition, a generalized model with curvature is obtained, where it is possible to compare effective and classical models. Finally, conclusions and possible perspectives for future work are discussed.

CHAPTER

TWO

GRAVITY

Gravity is one of the four fundamental interactions of nature along with electromagnetism, strong and weak interactions, these have a quantum description unlike gravity, that obeys a classical field theory.
Since Newton's theory of gravitation, we have had better knowledge of gravitational phenomena such as the orbits of planets, kinematics, and dynamics of bodies in Earth. However, through the formulation of special relativity in 1905 we learned a new vision of space-time as a unified object. Relativity effects can be appreciable when we study objects with a speed near that of light, in this region Newtonian mechanics fail.
Nevertheless, in 1915 General Relativity (GR) was presented by Albert Einstein, this theory is a generalization of special relativity that includes a description of gravity. Until today, GR encodes our best knowledge of gravity as a classical theory. Since GR tells us that gravity is only a manifestation of the geometry of space-time, and not a force as had been thought until then, it changed our understanding and comprehension of gravity.
In this section, a brief review of the GR formalism based on the Lagrangian and Hamiltonian formulation of GR is presented. The Hamiltonian description and $3+1$ decomposition of GR were implemented in a first instance to be able to take a step in the direction of quantum gravity. These ideas motivated the creation of the Ashtekar-Barbero variables, which are fundamental pieces of loop quantum gravity (LQG), on which the work studied in this thesis will be based.

2.1 Einstein- Hilbert action

From general relativity, we know that gravity is a manifestation due to space-time curvature, which is described by the Einstein field equations, namely [40–42]

$$G_{ab} + \Lambda g_{ab} = R_{ab} - \frac{1}{2} R g_{ab} + \Lambda g_{ab} = \frac{8\pi G}{c^4} T_{ab}, \tag{2.1}$$

where Λ is the so-called cosmological constant, and G_{ab} is the Einstein tensor defined by

$$G_{ab} = R_{ab} - \frac{1}{2} R g_{ab}. \tag{2.2}$$

Here, R is the curvature scalar, that is, the contraction of the Ricci tensor R_{ab}, that is, $R = R^a{}_a = R^a_{bad} g^{bd}$. Furthermore, R_{abcd} is the Riemann tensor, and g_{ab} is the metric tensor. In addition, G is Newton's gravitational constant and c is the speed of light. For convenience, natural units will be used, where $c = G = 1$.
The first part of equation (2.1) describes the geometric part of gravity. In contrast, the last part gives the behavior of its matter counterpart, which follows the dynamics of the energy-momentum tensor T_{ab}.
Note that equation (2.1) vanishes when we take the covariant derivative on both sides of the equation. Thus, we obtain the continuity equation.
Equation (2.1) can be obtained from an action through the Lagrangian formalism. The Einstein-Hilbert action S_{EH} for the vacuum Einstein equations is given by

$$S_{EH}\left[g^{ab}\right] = \int L_G \mathbf{e} = \frac{c^4}{16\pi G}\int_M \mathrm{d}^4x\sqrt{-g}(R - 2\Lambda), \tag{2.3}$$

where g is the determinant of the metric tensor, $L_G = \frac{c^4}{16\pi G}\sqrt{-g}(R - 2\Lambda)$ is the Lagrangian density of the geometrical part, $\mathbf{e}$ is the volume element and M is the space-time manifold. We obtain the Einstein field equations if we perform an infinitesimal variation with respect to g^{ab}. Furthermore, we can take the metric tensor g^{ab} and the derivative operator ∇_a as independent variables. Therefore, it is possible to define the Palatini action as follows,

$$S_G[g^{ab}, \nabla_a] = \int L_G[g^{ab}, \nabla_a]\mathbf{e} = \frac{c^4}{16\pi G}\int \sqrt{-g}(R_{ab} - 2\Lambda g_{ab})g^{ab}. \tag{2.4}$$

Computing the variation with respect to g^{ab}, we recover the vacuum Einstein equations. Varying next the action with respect to ∇_a, we obtain the metric compatibility condition, that is $\nabla_c g^{ab} = 0$. However, for simplicity, we assume $\Lambda = 0$ until something different is explicitly written.

2.2 Hamiltonian formulation

The Hamiltonian formulation of GR was developed by Arnowitt, Deser, and Misner [43], this formalism is known as the ADM formalism. The objective of this formulation was to approach to a quantum theory of gravity, due to quantum mechanics being given by a Hamiltonian formulation, which can be obtained from a Lagrangian formulation of a theory.
To develop this Hamiltonian formulation [14–16, 40, 43] we need to choose a time function t and a time flux vector field t^a in the manifold M, which satisfies $t^a\nabla_a t = 1$. Given a metric g_{ab} it is convenient to do a decomposition of t^a into normal and tangent components with respect to the surface Σ_t of constant t.
We define the lapse function N as

$$N = -g_{ab}t^a n^b = (n^a\nabla_a t)^{-1}, \tag{2.5}$$

and the shift vector N^a is defined as

$$N^a = q^a{}_b t^b, \tag{2.6}$$

where n^a is an unitary normal vector to Σ_t. In addition, h_{ab} is the induced spatial metric in Σ_t, which can be written as

$$q_{ab} = g_{ab} + n_a n_b. \tag{2.7}$$

The lapse function (2.5) measures the ratio between the flux of the proper time τ and the time coordinate while it moves normally to Σ_t. On the other hand, the shift vector (2.6) measures the ratio in the tangential part of Σ_t. It is possible to write n^a in terms of N, N^a, and t^a, i.e.,

$$n^a = \frac{1}{N}(t^a - N^a). \tag{2.8}$$

Therefore, we can write the inverse of the spatial metric as

$$g^{ab} = q^{ab} - N^{-2}(t^a - N^a)(t^b - N^b). \tag{2.9}$$

It fulfills $q^{ac}q_{cb} = \delta^a{}_b$ in the tangent space Σ_t and $q^{ab}\nabla_b t = 0$. We fix a volume element e_{abcd} in the space-time that obeys $\mathcal{L}_t e_{abcd} = 0$, where $\mathcal{L}_t$ is the Lie derivative and we define ${}^{(3)}e_{abc} = e_{abcd}t^d$ in Σ_t. Furthermore, we have ${}^{(3)}\epsilon_{abc} = \sqrt{q}e_{abc}$, q being the determinant of the spatial metric (2.7). Therefore,

$$\sqrt{-g} = N\sqrt{q}. \tag{2.10}$$

To do the ADM decomposition of action (2.4), we can express the scalar curvature R from the Einstein tensor (2.2) as

$$R = 2(G_{ab}n^a n^b - R_{ab}n^a n^b). \tag{2.11}$$

Moreover, we have the following,

$$G_{ab}n^a n^b = \frac{1}{2}\left[{}^{(3)}R - K_{ab}K^{ab} + K^2\right], \tag{2.12}$$

where K_{ab} is the extrinsic curvature of Σ_t, $K = K^a{}_a$ is its trace, and ${}^{(3)}R$ is the scalar curvature in three dimensions. Additionally, the definition of a Riemann tensor is given by

$$R_{ab}n^a n^b = K^2 - K_{ac}K^{ac} - \nabla_a(n^a\nabla_c n^c) + \nabla_c(n^a\nabla_a n^c). \tag{2.13}$$

We can express the Lagrangian density (2.3) with this decomposition using equations (2.10), (2.11), (2.12) and (2.13), such that

$$L_G = N\sqrt{h}\left[{}^{(3)}R - K_{ab}K^{ab} - K^2\right]. \tag{2.14}$$

Here, we see that the extrinsic curvature is related to the time derivative of h_{ab}, $\dot{q}_{ab} = q_a{}^c q_b{}^d \mathcal{L}_t h_{cd}$ as follows

$$K_{ab} = \frac{1}{2N}\left[\dot{q}_{ab} - D_a N_b - D_b N_a\right], \tag{2.15}$$

where D_a is the derivative operator in Σ_t associated to q_{ab}. Furthermore, it satisfies $D_a q_{bc} = 0$. Replacing (2.15) in (2.14), we can obtain the same Lagrangian density

found by Arnowitt, Deser and Misner [43].
The conjugated canonical momentum π^{ab} to q_{ab} is

$$\pi^{ab} = \frac{\partial L_G}{\partial \dot{q}_{ab}} = \sqrt{q}\left(K^{ab} - K h^{ab}\right). \tag{2.16}$$

Note that L_G does not depend on the time derivative of N, nor of N_a. Therefore, the conjugated canonical momenta are equal to zero. Thus, these variables are associated with constraints.
We can redefine the configuration space that consists of the Riemannian metric h_{ab} in Σ_t. Hence, we define the Hamiltonian density $\mathcal{H}_G$ as

$$\begin{aligned}
\mathcal{H}_G &= \pi^{ab}\dot{q}_{ab} - L_G \\
&= \sqrt{q}N^{(3)}R + Nq^{-1/2}\left[\pi^{ab}\pi_{ab} - \frac{1}{2}\pi^2\right] + 2\pi^{ab}D_{(a}N_{b)} \\
&= \sqrt{q}\left[N\left(-^{(3)}R + q^{-1}\pi^{ab}\pi_{ab} - \frac{1}{2}q^{-1}\pi^2\right) - 2N_b D_a\left(q^{-1/2}\pi^{ab}\right)\right] \\
&+ \sqrt{q}\left[2D_a\left(q^{-1/2}N_b\pi^{ab}\right)\right],
\end{aligned} \tag{2.17}$$

where $\pi = \pi^a{}_a$. The last term does not contribute to the boundary conditions. The variation of $\mathcal{H}_G$ with respect to N and N_a gives the following equations

$$C = -^{(3)}R + q^{-1}\pi^{ab}\pi_{ab} - \frac{1}{2}q^{-1}\pi^2 = 0, \tag{2.18}$$

$$C^b = D_a\left(q^{-1/2}\pi^{ab}\right) = 0, \tag{2.19}$$

these expressions are the constraints related to N and N_a, respectively.
The dynamical behavior of the configuration and momentum variables follow from the Hamilton equations. They are called the ADM equations and are given by

$$\dot{q}_{ab} = \frac{\delta H_G}{\delta \pi^{ab}} = q^{-1/2}N\left(\pi_{ab} - \frac{1}{2}q_{ab}\pi\right) + 2D_{(a}N_{b)}, \tag{2.20}$$

$$\begin{aligned}
\dot{\pi}^{ab} &= -\frac{\delta H_G}{\delta \pi^{ab}} = -Nq^{-1/2}\left({}^{(3)}R^{ab} - \frac{1}{2}{}^{(3)}R h^{ab}\right) \\
&+ \frac{1}{2}Nh^{-1/2}q^{ab}\left(\pi_{cd}\pi^{cd} - \frac{1}{2}\pi^2\right) - 2Nq^{-1/2}\left(\pi^{ac}\pi_c{}^b - \frac{1}{2}\pi\pi^{ab}\right) \\
&+ q^{-1/2}\left(D^a D^b N - q^{ab}D^c D_c N\right) + q^{-1/2}D_c\left(q^{-1/2}N^c\pi^{ab}\right) - 2\pi^{c(a}D_c N^{b)},
\end{aligned} \tag{2.21}$$

where (2.18), (2.19), (2.20) and (2.21) are equivalent to the Einstein equations in the vacuum, $G_{ab} = 0$.
Due to the constraints (2.19), there exists gauge arbitrariness in the configuration space q_{ab}. If ψ is any diffeomorphism of Σ_t, then q_{ab} and $\psi^* q_{ab}$ have the same physical configuration. Therefore, we must take the configuration space of GR as the set of equivalence classes of the Riemannian metric $\tilde{q}_{ab}$ in Σ_t. Here, we consider two metrics equivalent if they can be obtained through a diffeomorphism. This configuration space is known as the superspace.
However, the constraint (2.18) remains even if we redefine the configuration space as the superspace. The interpretation of this constraint is due to the arbitrariness

of the gauge in choosing the space-time slices.
The choice of the configuration space for GR is such that it is not possible to isolate the true dynamics of the degrees of freedom. This constraint cannot be eliminated from the Hamiltonian formulation of GR. This is a reason why we do not have a quantum gravity formulation through a canonical approach.

2.3 Holst action

We can use the tetrad formalism [1, 44–48], which allows us to write the metric tensor as

$$g_{ab}(x) = e^I_a(x) e^J_b(x) \eta_{IJ}, \tag{2.22}$$

where e^I_ν are the tetrad components. We can also define the vector basis of the tangent space to M as $e_a = e^I_a \partial_I$, additionally $e^a = e^a_I dx^I$ is one-form basis of the cotangent space of the manifold. Thus, e^a_I and e^I_a are the inverse of each other. We can introduce a new symmetry in comparison with the geometrical interpretation of gravity in metric terms. Note that (2.22) is invariant under Lorentz transformations, which are given by

$$\tilde{e}^I_a(x) = \Lambda^I_J e^J_a(x), \tag{2.23}$$

here, the indices I, J are internal indices of the Lorentz group representation. Thus, we introduce the connection ω^{IJ}_a, which is a 1-form. This is analogous to the definition of the Levi-Civita connection $\nabla_a = \partial_a + \Gamma_a$, where Γ_a is the spin connection. Analogous to the Levi-Civita connection being compatible with the metric, that is, $\nabla_c g_{ab} = 0$, we have similirly that $D_a e^I_b = 0$. Explicitly,

$$D_a e^I_b = \partial_a e^I_b + \omega^I_{aJ} e^J_b - \Gamma^c_{ba} e^I_c. \tag{2.24}$$

We can obtain an expression which relates both connections, such as the following

$$\omega^I_{aJ} = e^I_b \nabla_a e^b_J. \tag{2.25}$$

Indeed, the spin connection obeys the following relation

$$d_\omega e^I = de^I + \omega^I_J \wedge e^J. \tag{2.26}$$

Equation (2.26) is the Cartan first structure equation. We define d_ω as the exterior covariant derivative, d is the exterior derivative, and $\wedge$ is the wedge product.
Given the connection, we can define its curvature F^{IJ} as

$$F^{IJ} = d\omega^{IJ} + \omega^I_k \wedge \omega^{kJ}. \tag{2.27}$$

Furthermore, we can obtain an expression for its components, as follows

$$F^{IJ}{}_{ab} = \partial_a \omega^{IJ}_b - \partial_b \omega^{IJ}_a + \omega^I_{ka} \omega^{kJ}_b - \omega^I_{kb} \omega^{kJ}_a. \tag{2.28}$$

We can define

$$F^{IJ}_{ab}(\omega(e)) = e^{Ic} e^{Jd} R_{abcd}(e). \tag{2.29}$$

Expression (2.29) is known as the Cartan second structure equation. Here, $R_{\mu\nu\rho\sigma}$ is the Riemann tensor. Another main equation is the relationship between the determinant of metric g and the determinant of tetrad e, that is,

$$g = -e^2. \tag{2.30}$$

Using these equations we can transform the Einstein-Hilbert action (2.3) in terms of tetrads. Therefore,

$$S_{EH}(g_{\mu\nu}(e)) = \frac{1}{2}\epsilon_{IJKL} \int e^I \wedge e^J \wedge F^{KL}(\omega(e)). \tag{2.31}$$

Analogously as in the Palatini action in GR, we consider the connection ω_μ^{IJ} and the tedrads e_μ^I as independent variables. Thus, we can write the action in the following form

$$S_G[e_\mu^I, \omega_\mu^{IJ}] = \frac{1}{2}\epsilon_{IJKL} \int e^I \wedge e^J \wedge F^{KL}(\omega). \tag{2.32}$$

Doing the infinitesimal variation with respect to the tetrad and connection, it is possible to obtain the equations of motion

$$\frac{1}{2}\epsilon_{IJKL} e^J \wedge F^{KL}(\omega) = 0, \tag{2.33}$$

$$\frac{1}{2}\epsilon_{IJKL} e^I \wedge d_\omega e^J = 0. \tag{2.34}$$

Equation (2.33) is obtained when varying with respect to the tetrad and it gives the Einstein equations in tetrad terms. In addition, doing the variation with respect to the connection and assuming that the tetrad has an inverse then $d_\omega e^J = 0$, which is the compatibility condition.
Since the connection is an independent variable, an extra term can be added to the Lagrangian density, which is compatible with all the symmetries used

$$\delta_{IJKL} e^I \wedge e^J \wedge F^{KL}(\omega) = \epsilon^{\mu\nu\rho\sigma} R_{\mu\nu\rho\sigma}, \tag{2.35}$$

where $\delta_{IJKL} = \delta_{I[K}\delta_{L]J}$. This added term is the first Bianchi identity, multiplying it by a constant $1/\gamma$, we obtain the Holst action, which is

$$S_H[e, \omega] = \left(\frac{1}{2}\epsilon_{IJKL} + \frac{1}{\gamma}\delta_{IJKL}\right) \int e^I \wedge e^J \wedge F^{KL}(\omega). \tag{2.36}$$

If we again compute the infinitesimal variation with respect to the tetrad and connection, we can obtain the equations of motion plus additional terms, which are proportional to the Barbero-Immirzi parameter γ. Therefore,

$$\left(\frac{1}{2}\epsilon_{IJKL} + \frac{1}{\gamma}\delta_{IJKL}\right) F^{KL}(\omega) = 0, \tag{2.37}$$

$$\left(\frac{1}{2}\epsilon_{IJKL} + \frac{1}{\gamma}\delta_{IJKL}\right) e^I \wedge d_\omega e^J = 0. \tag{2.38}$$

Note that if the Barbero-Immirzi parameter goes to infinity, we return to the Einstein equations, as in GR.

2.4 Ashtekar-Barbero variables

Analogously, as was done with the ADM formulation of GR, we can obtain the Ashtekar-Barbero variables [49, 50] performing a Hamiltonian formulation of the Holst action (2.36). These variables are fundamental to build the quantization in the loop quantum gravity scheme, this is because of it consists of an innovative perspective to see gravity and also because the quantization with these variables permits one to remove the singularity, which is a classical problem. Thus, we can write in component terms the Holst action in the following manner,

$$S[e,\omega] = \frac{1}{16\pi G}\int d^4x|e|e^a_I e^b_J P^{IJ}{}_{KL}F^{KL}_{ab}(\omega), \tag{2.39}$$

where

$$P^{IJ}{}_{KL} = \delta^{[I}_K\delta^{J]}_L - \frac{1}{2\gamma}\epsilon^{IJ}{}_{KL}. \tag{2.40}$$

In the same way as in the canonical spatial metric (2.7), which was considered in the ADM formalism, we introduce a spatial tensor field ε^a_I given by

$$\varepsilon^a_I = e^a_I + n^a n_I, \tag{2.41}$$

where n^a is the unitary normal to the spatial slice, which satisfies $\varepsilon^a_I n_a = \varepsilon^a_I n^I = 0$. Moreover, $n_I = e^a_I n_a$. We fix the boost part of the internal Lorentz transformations, which we require to obey $e^a_0 = n^I e^a_I = n^a$, to be the unitary normal to the foliation. We take $n^I = \delta^I_0$ as a time-like internal vector field. The unitary normal vector is given by eq.(2.8). Therefore, (2.41) is written as

$$e^a_I = \varepsilon^a_I + N^{-1}(t^a - N^a)n_I. \tag{2.42}$$

Furthermore, $|e| = N\sqrt{\text{det}q}$, note also that $P^{IJ}{}_{KL}$ is an antisymmetric tensor. If we take into account that

$$P^a_i = \frac{\sqrt{\text{det}q}}{8\pi\gamma G}\varepsilon^a_i, \tag{2.43}$$

when doing the decomposition in metric (2.39), we can get

$$\begin{aligned} S = \int d^4x t^a\gamma\left(\omega^{0j}_a\left(\partial_b P^b_j + \omega_{bj}{}^k P^b_k - \frac{1}{\gamma}\epsilon^k_{jl}\omega_{b0}{}^l P^b_k\right)\right) \\ + \frac{t^a}{2}\epsilon^j_{kl}\omega_a{}^{kl}\left(\partial_b P^b_j - \frac{1}{2}\epsilon^{nm}_j\epsilon_{nqp}\omega^{pq}_b P^b_m + \gamma\epsilon_{nj}{}^m\omega^{0n}_b P^b_m\right). \end{aligned} \tag{2.44}$$

The conjugated variable to P^a_j is given by

$$A^i_a = \gamma\omega^{0i}{}_a + \frac{1}{2}\epsilon^i_{kl}\omega_a{}^{kl}. \tag{2.45}$$

We can interpret $\Gamma^i_a = \frac{1}{2}\epsilon^i_{kl}\omega^{kl}{}_a$ as the spin connection. Furthermore, the first term is associated with $K^i_a = \omega^{0i}{}_a$. Therefore,

$$A^i_a = \gamma K^i_a + \Gamma^i_a, \tag{2.46}$$

which is called the Ashtekar-Barbero connection.

At the limit when $\gamma \longrightarrow \infty$ in the Holst action (2.36), we can return to the

Palatini action (2.32) in tetrad and connection terms. Canonical variables (A^i_a, P^b_j) cannot reach this limit directly. However, it is well defined for $(\gamma^{-1}A^i_a, \gamma P^b_j)$. For $\gamma \longrightarrow \infty$ one gets $(K^i_a, (8\pi G)^{-1}E^a_j)$, where the densitized triad is defined by $E^a_i = \sqrt{\det(q)}\varepsilon^a_i$ and the extrinsic curvature tensor is given by $K^j_b = \varepsilon^{aj}K_{ab}$. The action (2.45) can be written as

$$S = \int d^4x \left(\Lambda^j \mathcal{D}^{(A)}_b P^b_j + (1+\gamma^2)\epsilon_{jm}{}^n \omega_t{}^{0j}\omega_b{}^{0m}P^b_n\right), \tag{2.47}$$

where $\mathcal{D}^{(A)}_b$ is the covariant derivative using the Ashtekar-Barbero connection. We have defined additionally $\Lambda^j = \frac{1}{2}\epsilon^j_{kl}\omega^{kl}_t + \gamma\omega^{0j}_t$.
The components of Λ^j and $\omega_t{}^{0i}$ do not appear with their time derivative in the action. Their momenta are constraints, and these are promoted to Lagrange multipliers of secondary constraints. The Gaussian constraint is given by

$$G_j = \mathcal{D}^{(A)}_b P^b_j = 0. \tag{2.48}$$

The constraint associated to $\omega_t{}^{0i}$ is

$$S_j = \epsilon_{jm}{}^n \omega_b{}^{0m} P^b_n = \epsilon_{jm}{}^n K^m_b P^b_n = 0, \tag{2.49}$$

where $K_{ab} = K^i_a \varepsilon_{bi}$ satisfies

$$0 = K_{ab}\epsilon^{ijk}\varepsilon^a_i P^b_j = \frac{1}{8\pi\gamma G}K_{ab}\epsilon^{abc}\varepsilon^k_c. \tag{2.50}$$

Thus, $D_b P^b_j = 0$ using the spin connection. On the other hand, the diffeomorphism and Hamiltonian constraints are given by terms in the action which are proportional to N^a and N, respectively. These constraints are obtained in component terms of the purely spatial curvature F^l_{ab}, that is,

$$F^l_{ab} = \frac{1}{2}\epsilon^l_{ij}F^{ij}_{ab} = 2\partial_{[a}\Gamma^l_{b]} - \epsilon^l_{jk}\Gamma^j_{[a}\Gamma^k_{b]}. \tag{2.51}$$

The canonical connection is the Ashtekar-Barbero connection, and not the spin connection. Thus, the curvature used for A^i_a is given by

$$\mathcal{F}^l_{ab} = F^l_{ab} + 2\gamma D_{[a}K^l_{b]} + \gamma^2\epsilon^l_{jk}K^j_a K^k_b. \tag{2.52}$$

The contribution of the diffeomorphism constraint is given by

$$\begin{aligned} N^a C^{grav}_a &= -\gamma n_I N^a P^b_j P^{IJ}{}_{KL}F_{ab}{}^{KL} \\ &= N^a P^b_j \left(\mathcal{F}^j_{ab} + (1+\gamma^2)\epsilon^j_{kl}K^k_a K^l_b\right), \end{aligned} \tag{2.53}$$

while that of the Hamiltonian constraint by

$$\begin{aligned} C_{grav} &= -4\pi G\gamma^2 \frac{P^a_i P^b_j}{\sqrt{\det q}} P^{ij}{}_{KL}F_{ab}{}^{KL}, \\ &= -4\pi G\gamma^2 \frac{P^a_i P^b_j}{\sqrt{\det q}}\epsilon^{ij}{}_k \left[\mathcal{F}^k_{ab} + (1+\gamma^2)\epsilon^k_{mn}K^m_a K^n_b - 2\frac{1+\gamma^2}{\gamma}\epsilon^{ij}_k\varepsilon^a_i P^b_j D_{[a}K^k_{b]}\right]. \end{aligned} \tag{2.54}$$

Therefore, we can write the Hamiltonian as a sum of the past constraints as follows

$$H_{grav}[A^i_a, P^b_j] \int d^3x \left(-\Lambda^i G_i - (1+\gamma^2)\omega^{0j}_t S_j + NC_{grav} + N^a C^{grav}_a \right). \tag{2.55}$$

Note that we have an extra constraint compared to the ADM formulation; this new constraint is the Gaussian constraint; this is due to the Lorentz symmetry of the tetrad formalism in the Holst action. In the same way as the ADM formalism, the shift vector and lapse function are Lagrange multipliers and we refer to C and C_a as the Hamiltonian and diffeomorphism constraints, respectively.
The algebra generated by the Gauss constraint is

$$\{G(\Lambda_1), G(\Lambda_2)\} = \frac{\gamma}{2} G([\Lambda_1, \Lambda_2]), \tag{2.56}$$

where

$$G(\Lambda) = \int d^3x G_i(x) \Lambda^i(x). \tag{2.57}$$

Equation (2.57) is the smeared Gauss constraint, furthermore Λ^i is the t component of A^i_a and $G_i = \partial_a E^a_i + \epsilon_{jik} A^j_a E^{ak}$.
Moreover, the Poisson bracket with the Ashtekar-Barbero canonical variables are given by

$$\{G(\Lambda), E^a_i(y)\} = \gamma \epsilon_{ijn} \Lambda^j(y) E^{an}(y). \tag{2.58}$$

Note that this Poisson bracket is an infinitesimal rotation, such as a vector definition, where Λ^j is the angle, further this is invariant under spatial rotations. Additionally, it is possible to get the Poisson bracket between the Gauss constraint and the Ashtekar-Barbero connection as follows

$$\{G(\Lambda), A^i_a(y)\} = \gamma \partial_a \Lambda^i(y) + \gamma \epsilon_{mji} \Lambda^j(y) A^m_a(y), \tag{2.59}$$

where we have as a result that Λ^j transforms as a covariant derivative. We note that the Poisson bracket with the Gauss constraint and the densitized triad (2.58) transforms as a vector. On the other hand, equation (2.59) transforms as a connection; this is the reason why we refer to A_a as the Ashtekar-Barbero connection. In addition, we have the Poisson brackets relation of the conjugated canonical variables, which are the Ashtekar-Barbero variables, namely,

$$\{A^i_a(x), E^b_j(y)\} = 8\pi G \gamma \delta^i_j \delta^a_b \delta(x, y). \tag{2.60}$$

Furthermore, for the densitized triad is written as

$$E_i(s) = \int_S n_a E^a_i d^2\sigma, \tag{2.61}$$

where $n_a = \epsilon_{abc} \dfrac{\partial x^b}{\partial \sigma_1} \dfrac{\partial x^c}{\partial \sigma_2}$ is the normal to the surface. The quantity $E_i(S)$ is the flux of E through S.
On the other hand, A is a 1-form, thus the smering is through the use a 1-dimensional path. In what follows we denote an arbitrary path by β and a parametrization as a map $x^a(s) : [0,1] \longrightarrow \Sigma$ such that $s \longrightarrow x^\mu(s)$. Given the connection A^i_a, we can associate it with an element of $su(2)$, we have thus that

$A_a = A_a^i \tau_i$ where τ_i is the generator of the $SU(2)$ group.
In addition, integrating A_a along the path β yields

$$A_a^i \longrightarrow \int_\beta A = \int_0^1 ds A_a^i(x(s))\dot{\beta}^a(s)\tau_i, \tag{2.62}$$

where $\dot{\beta}^a(s) = \dfrac{dx^\mu(s)}{ds}$ is the tangent to the curve. We define the holonomy of A along the path β as

$$h_\beta[A] = \mathcal{P}\exp\left(\int_\beta A\right), \tag{2.63}$$

where $\mathcal{P}$ is the path-ordered product. That is,

$$h_\beta[A] = \sum_{n=0}^{\infty} \int ... \int_{1>s_n>...>s_1>0} A(\beta(s_1))...A(\beta(s_n))ds_1...ds_n, \tag{2.64}$$

where the line is parametrized by $s \in [0,1]$.
More precisely, the holonomy is the solution to the differential equation of parallel transport

$$\frac{d}{dt}h_\beta[A](t) - h_\beta[A](t)A(\beta(t)) = 0, \tag{2.65}$$

where $h_\beta[A](0) = \mathbb{I}$, and $h_\beta[A] = h_\beta[A](1)$. Thus, integrating and iterating, we obtain

$$\begin{aligned} h_\beta[A](t) &= \mathbb{I} + \int_0^t h_\beta[A](s)A(\beta(s))ds \\ &= \mathbb{I} + \int_0^t h_\beta[A](s_1)A(\beta(s_1))ds_1 + \int_0^t \int_{s_1}^1 A(\beta(s_1))A(\beta(s_2))h_\beta[A](s_2)ds_1 ds_2 \\ &= ... \\ &= \sum_{n=0}^{\infty} \int ... \int_{1>s_n>...>s_1>0} A(\beta(s_1))...A(\beta(s_n))ds_1...ds_n. \end{aligned} \tag{2.66}$$

In GR the physical quantities, such as lengths and areas, are nonlocal; in this way, they depend on finite but extended regions, such as lines and surfaces. Furthermore, the holonomy $h_\beta[A]$ of the gravitational connection ω (or its self-dual A) along a curve β is another nonlocal quantity, which is relevant in quantum theory.

CHAPTER

THREE

COSMOLOGY

The study of the Universe as an entire object has been an open question for millennia, cosmology, [40, 41, 47, 51–55]. This simplification to see it as a single object may seem risky, because we leave out each individual structure as planets, stars, or galaxies. However with this reduction we can get a description of the history of our universe from which observable quantities can be obtained and compared with the astronomical data. A reasonable proposition is the cosmological principle: a homogeneous and isotropic Universe on a suitable scale in the early universe. Now, in the early universe there seems to be an inflation period where the fluctuations of inhomogeneities of space-time grow and they can be seen in the cosmological microwave background (CMB) [56–58].
Another important aspects in cosmology are the shape of Universe, curvature, matter contents, cosmological constant. In this work we do not include fluctuation and restrict ourselves to the simplest models, namely hyperbolic, flat, or spherical Universe. Another important ingredient is the cosmological constant that encodes the contribution of dark energy, which is responsible for the accelerated expansion of our Universe.
Standard classical cosmology presents some problems, like for instance the nature of dark energy, dark matter, and the the big bang singularity. Dark matter has been infered through the analysis of the rotation curves in the galaxies [59–67][68, 69]. On the other hand, the Big Bang singularity is a theoretical problem. Some quantities diverge, which is not theoretically consistent, for example the scalar curvature and energy density. Quantum gravity is expected to provide a better description of such a stage. In this chapter we provide the standard arena required to describe FLRW quantum cosmology later. First in GR, then in canonical form and finally in the framework of Ashterkar-Barbero.

3.1 Standard Classical Cosmology

In line with the cosmological principle we consider a universe accordingly. A space-time is spatially homogeneous if there is a group of isometries which acts freely on M, whose surfaces of transitivity are space-like three-surface Σ_t that slice space-time, that is any point on one of these surfaces is equivalent to any other point on the same surface. Note that universe is not exactly spatially homogeneous, there are local irregularities. However, it is a reasonable assumption that the universe

is spatially homogeneous on large scales.
On the other hand, a space-time is spatially isotropic if there is not a privileged direction, that is at each point exists a congruence of time-like curves, i.e. observers, with tangents u^a filling the space-time. Given any point p and given any two unitary spatial tangential vectors s_1^a and s_2^a, vectors at p orthogonal to u^a, there exists an isometry of g_{ab} which leaves p and u^a at fixed but rotates s_1^a into s_2^a. Thus, in an isotropic universe, it is not possible to geometrically build a preferential orthogonal tangential vector to u^a in Σ_t. Moreover, due to homogeneity, there exist isometries of q_{ab}, which go to any $p \in \Sigma_t$ in any $q \in \Sigma_t$.
Let us consider the three dimensional Riemann tensor ${}^{(3)}R_{abc}{}^{d}$ associated with the metric q_{ab} on Σ_t, that is,

$$ {}^{(3)}R_{ab}{}^{cd} = k\delta^{c}{}_{[a}\delta^{d}{}_{b]}, \tag{3.1} $$

or lowing the indices

$$ {}^{(3)}R_{abcd} = kq_{c[a}q_{b]d}. \tag{3.2} $$

Due to homogeneity k is constant, that is, it cannot vary from point to point in Σ_t. Also isotropy requires k constant. This can be shown using eq.(3.2) in the Bianchi identity. For a space with constant curvature, we can analyze three different options, where k is positive, zero, or negative. The first case, when $k > 0$. We have space is given by 3-spheres, which are defined as surfaces in a four-dimensional Euclidean space. In cartesian coordinates we have

$$ x^2 + y^2 + z^2 + w^2 = R^2. \tag{3.3} $$

Transforming to spherical coordinates, the 3-sphere unitary metric is given by

$$ \mathrm{d}\Omega_1^2 = \mathrm{d}\psi^2 + \sin^2\psi(\mathrm{d}\theta^2 + \sin^2\theta \mathrm{d}\varphi^2). \tag{3.4} $$

For $k = 0$ we have a 3-D flat space, which can be described in cartesian coordinates by

$$ \mathrm{d}\Omega_2^2 = \mathrm{d}x^2 + \mathrm{d}y^2 + \mathrm{d}z^2. \tag{3.5} $$

For $k < 0$ we have 3-D hyperboloids defined as surfaces in a flat space-time with Lorentz signature in 4-D, whose inertial global coordinates satisfy

$$ t^2 - x^2 - y^2 - z^2 = R^2. \tag{3.6} $$

In this case the metric, in hyperboloid coordinates, is given by

$$ \mathrm{d}\Omega_3^2 = \mathrm{d}\psi^2 + \sinh^2\psi(\mathrm{d}\theta^2 + \sin^2\theta \mathrm{d}\varphi^2). \tag{3.7} $$

Since isotropic observers are orthogonal to homogeneous surfaces we can express the space-time metric g_{ab} as

$$ g_{ab} = -u_a u_b + q_{ab}(t), \tag{3.8} $$

where $q_{ab}(t)$ is the spatial metric which describes some of the geometries that we have mentioned above and u^a stands for a orthogonal vector of any two vectors s_1^a and s_2^a at p. Furthermore, the hyperbolic and flat universe are called open geometries, instead of spherical universe is called closed.
If we label each hypersurface by a proper time τ for each isotropic observer, then

the observers shall be ad hoc with the difference between two hypersurfaces. Thus, the proper time τ and spatial coordinates label each event of the Universe. Each possible geometry described previously is related to curvature, which can be expressed, in cosmology, the element of line for an isotropic and homogeneous universe; it is also called the Friedmann-Lemaître-Robertson-Walker metric (FLRW) such as

$$\mathrm{d}s^2 = -c^2 N^2(t)\mathrm{d}t^2 + a(t)^2 \left[\frac{\mathrm{d}r^2}{1-kr^2} + r^2 \mathrm{d}\Omega_j^2 \right], \tag{3.9}$$

where a is the scale factor of Universe, Ω_j with $j = 1, 2, 3$ define each geometry of Universe and N is the lapse function, which gives a time reparametrization by $N(t) = \frac{\mathrm{d}\tau}{\mathrm{d}t}$. For $N = 1$ one obtains the Friedmann equation of standard cosmology using the Einstein equations

$$H^2 = \left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3}\rho - \frac{k}{a^2} + \frac{\Lambda}{3}, \tag{3.10}$$

where ρ is the energy density, Λ is the cosmological constant, the curvature that determines the shape of universe is given by $k = -1, 0, 1$, and H is the standard Hubble parameter, where the matter content of the universe describes by the stress-energy tensor T_{ab} in the Einstein equation, the most general form of T_{ab} consistent with homogeneity and isotropy is the general perfect fluid

$$T_{ab} = \rho u_a u_b + P(g_{ab} + u_a u_b), \tag{3.11}$$

where P is the pressure of matter considered. The factor a is a dimensionless factor, called the cosmic scale factor or the Robertson-Walker scale factor, which measures the relative expansion of the universe. Thus, the Hubble parameter encodes how fast the universe is expanding. This parameter is one of the most important observable quantities in standard cosmology.
Furthermore, the Raychaudhuri equation or the acceleration equation is given by

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho + 3P). \tag{3.12}$$

Note that the universe cannot be static if $0 \leq P$ and $0 < \rho$ because of $\ddot{a}$. In fact, the universe is always expanding ($\dot{a} > 0$) or contracting ($\dot{a} < 0$). The distance scale between all isotropic observers changes with time, but there is not preferred direction of expansion or contraction. The Ricci scalar R for these models read

$$R = 6\left(\left(\frac{\dot{a}}{a}\right)^2 + \frac{\ddot{a}}{a} + \frac{k}{a^2}\right). \tag{3.13}$$

For kinetic energy dominated by a scalar field $P = \rho$, then substituting in (3.13) we have $R = -16\pi G\rho$. An illustrative way to see what is the contribution of radiation, matter, cosmological constant and curvature in the shape of universe. We focus on the Hubble parameter (3.10) which measures the entire history of our Universe, we can take its value today, H_0. Thus, dividing the eq.(3.10) by H_0^2 where we can get

$$H_0(t - t_0) = \int_0^a \frac{da}{[\Omega_{r,0}/a^2 + \Omega_{m,0}/a + \Omega_{\Lambda,0}a^2 + (1-\Omega_0)]^{1/2}}, \tag{3.14}$$

where $\Omega_{r,0} = \rho_{r,0}/\rho_{c,0}$, with $\rho_{r,0}$ is the radiation energy density, $\Omega_{m,0} = \rho_{m,0}/\rho_{c,0}$, with $\rho_{m,0}$ is the matter energy density, $\Omega_{\Lambda,0} = \rho_{\Lambda,0}/\rho_{c,0}$, with $\rho_{\Lambda,0}$ indicates the contribution of cosmological constant energy density, and the full relative energy density is given by $\Omega_0 = \Omega_{r,0} + \Omega_{m,0} + \Omega_{\Lambda,0}$. Taking into account only the contribution of matter and curvature, that is $\Omega_{m,0} = \Omega_0$. It is possible to calculate the critical energy density today $\rho_{c,0}$ using (3.14)

$$\rho_{c,0} = \frac{3H_0^2}{8\pi G}. \tag{3.15}$$

For our analysis, only the matter part is considered. Thus, the scale factor at the time of maximum expansion is given by

$$a_{\max} = \frac{\Omega_0}{1-\Omega_0} \tag{3.16}$$

which occurs when $H = 0$. Moreover, the curvature k implies that Ω_0 takes different values, which determines the shape of the universe. For all cases, the classical universe begins with the Big Bang at $a = 0$. The relative energy density $\Omega_0 = 1$ for $k = 0$ ends with a big chill, and the scale factor in this region takes a behavior of $a \propto t^{2/3}$. The hyperbolic universe takes values $\Omega_0 < 1$, in this case the end is also in an icy Big Chill and $a \propto t$. On the other hand, for a closed universe ($k = 1$) takes values $\Omega > 1$ and the ultimate fate is a fiery Big Crunch. Therefore, for a matter-dominated universe the end is a Big Chill if the critical density is greater than or equal to the density energy, and the end is a Big Crunch when the critical density is less than the energy density.
The values taken in Figure 3.1.1 and Figure 3.1.2 are $\Omega_0 = 1$ for a flat universe, $\Omega_0 = 1.1$ for a spherical universe, and $\Omega_0 = 0.9$ for a hyperbolic universe. Note that Figure 3.1.1 describes the behavior at large scale comparing the $H_0(t-t_0)$ respects to a, this plot illustrates open and closed universes since Big Bang singularity at $H_0 = 0$ to ultimate fates, either Big Chill or Big Crunch. Nevertheless, Figure 3.1.2 focuses on small scales, that is, close to the Big Bang, the universes have a similar description, and it is not easy to distinguish the shape of universe. Therefore, it is not possible to predict how the destiny is; this depends on density and curvature, which will be a universe that will always expand or will recollapse.

3.2 ADM formulation

To proceed to the quantum formulation in later chapter it is useful to recast GR in canonical form. Let us consider the Einstein-Hilbert action given by Eq.(2.3) with cosmological constant Λ as

$$S_{EH} = \frac{c^4}{16\pi G}\int_M \mathrm{d}^4x\sqrt{-g}(R-2\Lambda) - \frac{c^4}{8\pi G}\int_{\partial M}\mathrm{d}^3x\sqrt{q}K, \tag{3.17}$$

where M is the spacetime manifold and ∂M is the boundary of M [40, 43, 54]. The extrinsic curvature K_{ab} from eq.(2.15) for a cosmological model is given by

$$K_{ab} = \frac{1}{2N}\frac{\partial q_{ab}}{\partial t} = \frac{\dot{a}}{Na}q_{ab}, \tag{3.18}$$

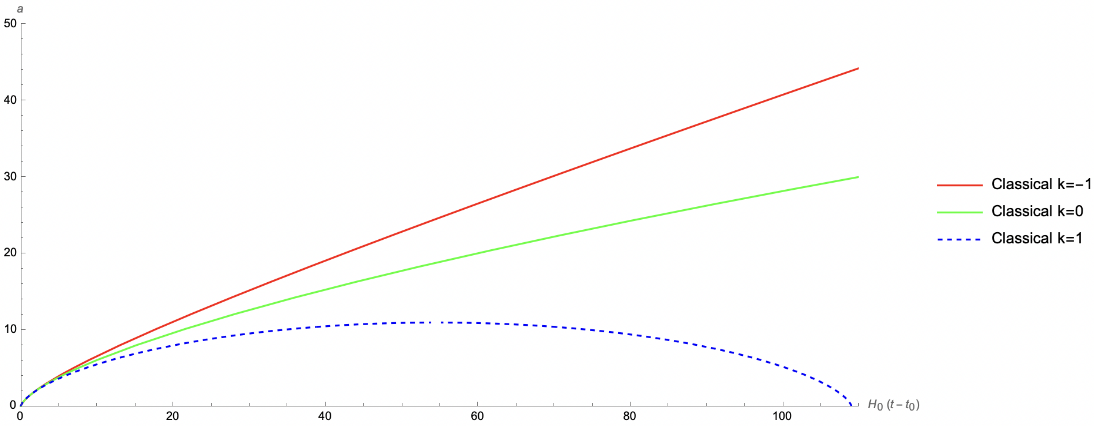

Figure 3.1.1: Scale factor as a function of cosmic time in units of H_0^{-1}. At long times all three shape possibilities differ

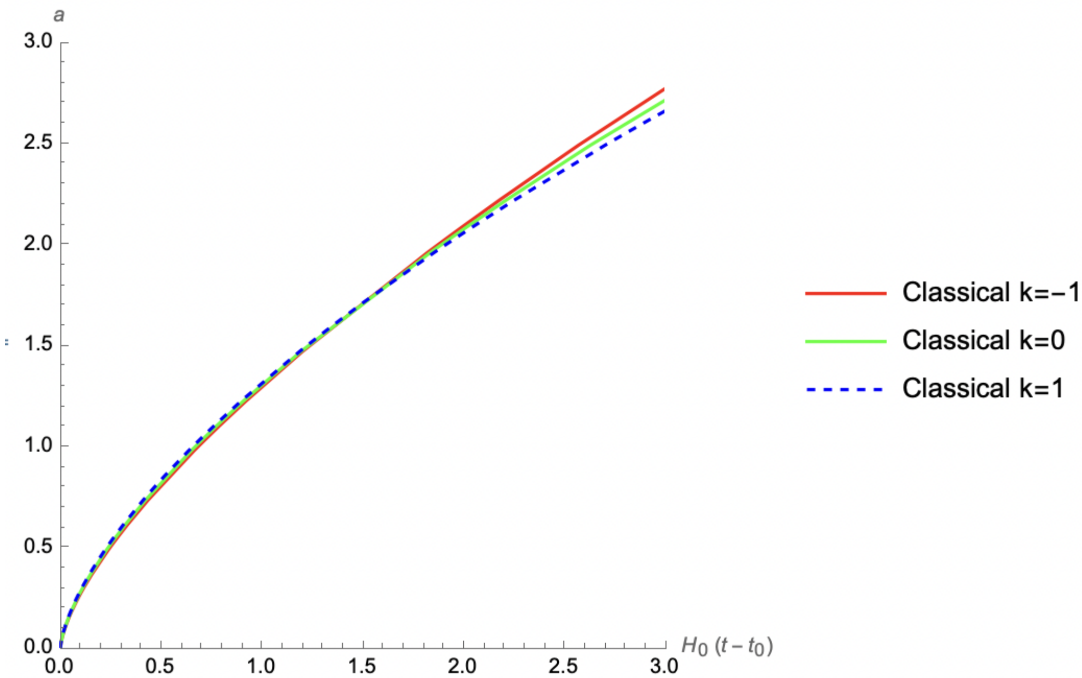

Figure 3.1.2: Scale factor as a function of cosmic time in units of H_0^{-1}. At early times, e.g. near the Big Bang different shapes of the Universe are almost indistinguishable.

further, its trace K reads

$$K = K_{ab}q^{ab} = \frac{\dot{a}}{Na}q_{ab}q^{ab} = \frac{3\dot{a}}{Na}. \tag{3.19}$$

We can see this quantity is proportional to Hubble parameter $\dot{a}/a$. The volume element for each spatial metric (2.10) is $\sqrt{q}\mathrm{d}^3x = a^3\mathrm{d}^3\Omega_j$, where $\mathrm{d}^3\Omega_j$. Furthermore, the scalar curvature in the ADM formalism (2.11) for cosmology case is written

$$R = \frac{6}{N}\left(-\frac{\dot{N}\dot{a}}{N^2a} + \frac{\ddot{a}}{aN} + \frac{1}{N}\left(\frac{\dot{a}}{a}\right)^2 + \frac{N}{a^2}\right). \tag{3.20}$$

Writing these expressions on the Einstein-Hilbert action (3.17), we can get the following action

$$\begin{aligned} S_{EH} =& \frac{c^4}{16\pi G}\int_M \mathrm{d}\Omega\mathrm{d}tNa^3\left[\frac{6}{N}\left(-\frac{\dot{N}\dot{a}}{N^2a} + \frac{\ddot{a}}{Na} + \frac{1}{N}\left(\frac{\dot{a}}{a}\right)^2 + \frac{N}{a^2}\right) - 2\Lambda\right] \\ &- \frac{c^4}{8\pi G}\int_{\partial M}\mathrm{d}^3\Omega a^3\left(\frac{3\dot{a}}{Na}\right). \end{aligned} \tag{3.21}$$

Thus, if we rearrange the terms of this equation and using the fact that $(\partial/\partial t)(\dot{a}a^2/N) = \ddot{a}a^2/N + 2a\dot{a}^2/N - \dot{N}\dot{a}a^2/N^2$ we get

$$S_{EH} = \frac{3c^4}{8\pi G}\int_M \mathrm{d}^3\Omega\mathrm{d}t\left[-\frac{a\dot{a}^2}{N} + Na - \frac{N\Lambda a^3}{3}\right], \tag{3.22}$$

which upon integrating over a finite spatial region V_0 and taking units such that $2G/3\pi = 1$ leads to

$$S_g = \frac{1}{2}\int \mathrm{d}tNV_0\left(-\frac{a\dot{a}^2}{N^2} + a - \frac{\Lambda a^3}{3}\right). \tag{3.23}$$

S_g is the gravitational action for the cosmic model. Furthermore, to add the part of matter to the action, it is convenient to rescale the homogeneous scalar field from ϕ to $\phi/\sqrt{2\pi}$ and use units $\hbar = 1$. The action for matter S_m is

$$S_m = \frac{1}{2}\int \mathrm{d}tNV_0a^3\left(\frac{\dot{\phi}^2}{N^2} - m^2\phi^2\right). \tag{3.24}$$

The Hamiltonian formulation is obtained next. The canonical momentum p_N to N yields

$$p_N = \frac{\partial L}{\partial \dot{N}} = 0. \tag{3.25}$$

Note that the Lagrangian does not depend explicitly on $\dot{N}$, then N is a constant of motion. In addition, the momenta p_a and p_ϕ, which are related to a and ϕ, respectively, read

$$p_a = \frac{\partial L}{\partial \dot{a}} = -\frac{a\dot{a}}{N}, \tag{3.26}$$

$$p_\phi = \frac{\partial L}{\partial \dot{\phi}} = \frac{a^3\dot{\phi}}{N}. \tag{3.27}$$

Using the momenta (3.25), (3.26) and (3.27) we can build the Hamiltonian H as follows

$$\begin{aligned} H =& p_N \dot{N} + p_a \dot{a} + p_\phi \dot{\phi} - L, \\ =& \frac{N}{2}\left(-\frac{p_a^2}{a} + \frac{p_\phi^2}{a^3} - a + \frac{\Lambda a^3}{3} + m^2 a^3 \phi^2\right) \end{aligned} \tag{3.28}$$

On the other hand, in the canonical formalism due to (3.25) the primary constraint $\{p_N, H\} = 0$ implies the Hamiltonian constraint $H \simeq 0$, that is, the Hamiltonian H is weakly zero.
In the Lagrangian formalism, corresponds to the Friedman equation when $N = 1$, which is

$$\dot{a}^2 = -1 + a^2\left(\dot{\phi} + \frac{\Lambda}{3} + m^2\phi^2\right). \tag{3.29}$$

Doing an infinitesimal variation over the action (3.28) respect to the scalar field ϕ, we get the following

$$\ddot{\phi} + \frac{3\dot{a}}{a}\dot{\phi} + m^2\phi = 0. \tag{3.30}$$

It is possible to solve analytically for $m = 0$, where we get $p_\phi = a^3\dot{\phi} = cte = \mathcal{K}$. Thus, for $\Lambda = 0$ we obtain

$$\phi(a) = \pm\frac{1}{2}\text{arccosh}\left(\frac{\mathcal{K}}{a^2}\right). \tag{3.31}$$

For $m \neq 0$ we have a solution in the configuration space starting with $\phi = 0$ getting closer to the a axis and starting to oscillate around this axis. This model is used in chaotic inflation. Since this trajectory approximating $\phi = 0$ corresponds to an inflationary expansion with respect to the temporal coordinate t. For a close Friedman universe, the trajectory peaks to a maximum and collapses. In this section was applied the ADM formalism to cosmology, where we can find the equations of motions start from the Einstein-Hilbert action.

3.3 Ashtekar-Barbero variables

The first step in introducing the quantum description in loop quantization a cosmological model is the use of the appropriate Ashtekar-Barbero variables. This was first considered by Martin Bojowald [17–22]. The Ashtekar-Barbero variables are given by

$$A_a^i = cV_0^{-1/3}\ {}^o\omega_a^i, \qquad E_i^a = pV_0^{-2/3}\sqrt{{}^oq}\ {}^oe_i^a, \tag{3.32}$$

where E_i^a is the densitized triad, which is related with the spatial metric q_{ab}, A_a^i is the Ashtekar-Barbero connection, that is the conjugated momentum of the triad, where $A_a^i = \gamma K_a^i$ for a flat FRLW ($\Gamma_a^i = 0$). In addition, the canonical pair is related to scale factor by $c = \gamma\dot{a}$ and $p = a^2$. For open models a fidutial volume V_0 is introduced, where all integrations are restricted to V_0, that is, the volume of the elementary cell $\mathcal{V}$ in this geometry has finite integrals. In classical geometry, p describes the physical volume of the elementary cell via $V = |p|^{3/2}$- The pair (c, p)

are the fundamental variables that make up the gravitational phase space, where these variables obey the nonvanishing Poisson bracket

$$\{c, p\} = \frac{8\pi G\gamma}{3}, \tag{3.33}$$

where G is the Newtonian constant and the Barbero-Immirzi parameter is written as γ. Expression (3.33) is obtained substituting the reduced Ashtekar-Barbero variables (3.32) into (2.60), then integrating over a fidutial volume. Furthermore, the pair $({}^o\omega_a^i, {}^oe_i^a)$ is the set of orthonormal co-triads and triads, respectively, which are compatible with the fidutial spatial metric ${}^oq_{ab}$ and its determinant is denoted by ${}^oq$, $\det({}^oq_{ab})$, or $\det({}^oq)$. Furthermore, in terms of p, the physical triad and cotriad read

$$\begin{aligned} e_i^a &= \mathrm{sgn}(p)|p|^{-1/2}V_0^{1/3}\ {}^oe_i^a, \\ e_a^i &= \mathrm{sgn}(p)|p|^{1/2}V_0^{-1/3}\ {}^o\omega_a^i. \end{aligned} \tag{3.34}$$

Note that the Gauss and diffeomorphism constraint in (2.55) is trivially fulfilled due to the symmetry of the FLRW model. Thus, we work only with the Hamiltonian constraint H_g is written as

$$\begin{aligned} H_g &= \frac{1}{16\pi G}\int_{\mathcal{V}} d^3x \frac{E^{aj}E^{bk}}{\sqrt{\det(q)}}\left[\epsilon_{ijk}F_{ab}^i - 2\left(1+\gamma^2\right)K_{[a}^jK_{b]}^k\right], \\ &= H^E(1) - 2\left(1+\gamma^2\right)H^L(1), \end{aligned} \tag{3.35}$$

where the Hamiltonian constraint is divided in two terms, which are the Euclidean term $H^E(N)$ and the Lorentzian term $H^L(N)$. Here we take the lapse function $N = 1$. In terms of these Ashtekar-Barbero variables for a flat cosmological model it is possible to express the Hamiltonian constraint (2.55) as

$$H^E(1) = \frac{1}{16\pi G}\int_{\mathcal{V}} d^3x \frac{E^{aj}E^{bk}}{\sqrt{\det(q)}}\epsilon_{ijk}F_{ab}^i = \frac{3}{8\pi G}c^2\sqrt{|p|}, \tag{3.36}$$

$$H^L(1) = \frac{1}{16\pi G}\int_{\mathcal{V}} d^3x \frac{E^{aj}E^{bk}}{\sqrt{\det(q)}}K_{[a}^jK_{b]}^k = \frac{3}{16\pi G\gamma^2}c^2\sqrt{|p|}. \tag{3.37}$$

We use the notation for $k = 0$, $H_{k=0}^E(1) = H_0^E$, and $H_{k=0}^L(1) = H_0^L$. Therefore,

$$H_g = H_0^E(1) - 2\left(1+\gamma^2\right)H_0^L(1) = -\frac{3}{8\pi G\gamma^2}c^2\sqrt{|p|}. \tag{3.38}$$

Note that, classically, both terms (3.36) and (3.37) are proportional. For this reason, the first models proposed in LQC only took into account the Euclidean term for quantization [23–26, 31–37, 39]. However, there can be significant differences if one keeps the strategy of full LQG of the quantum level [14, 27–30, 38], where both terms are independently quantized. It is possible to get different effects, such as an effective or emergent cosmological constant effect.

CHAPTER

FOUR

QUANTUM MECHANICS

Quantum mechanics (QM) allows us to describe typically tiny scale systems like elementary particles, atoms, molecules, and also macroscopic systems as Bose-Einstein condensates, white dwarfs, neutron stars, and possibly the very early stages of the universe. Just as QM provides a stable model instead of the classical description of the atom, we might expect that it copes with the classical divergences associated to curvature singularities of classical cosmology, i.e., Big Bang. QM and GR are fundamental pillars of modern physics. In this Section we recall come concepts of QM, its extension to curved space-time, and a brief review of polymeric QM.

4.1 Canonical Quantization

Standard quantization is originally due to Dirac. In this formalism, a canonical Hamiltonian formulation is needed to describe the system [70–72], where the classical phase space is described by configuration variables x^a and their conjugated momentum p_a, for $a = 1, ..., n$, where n is the number of degrees of freedom. The Hamiltonian equations of motion for the canonical coordinates $x^a(t)$ and $p_a(t)$ are given by the Poisson brackets

$$\dot{x}^a = \{x^a, H\}\,, \quad \dot{p}_a = \{p_a, H\}\,, \tag{4.1}$$

where $\dot{x}^a = dx^a/dt = \partial_t x^a$ and $H = H(x,p)$ is the Hamiltonian of the system. The evolution parameter, or time t, plays an important role in this description [15, 73–75]. The canonical Poisson bracket of two arbitrary functions f and g on the phase space is defined by

$$\{f, g\} = \frac{\partial f}{\partial x^a}\frac{\partial g}{\partial p_a} - \frac{\partial f}{\partial p_a}\frac{\partial g}{\partial x^a}, \tag{4.2}$$

and we have in particular $\{x^a, p_b\} = \delta^a_b$.

QM is based on the following postulates [76–81]

(i) The physical system at any instant of time is determined by a vector $|\psi\rangle$ in the Hilbert space $\mathcal{H}$, that admits a dense and numerable subset, then a numerable orthonormal basis. This space contains the square integral functions in a interval (a, b), denoted by $L^2(a, b)$. The scalar product of two vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ is

denoted by $\langle\psi_1|\psi_2\rangle$. This vector $|\psi\rangle$ contains the information required to describe the system. Any superposition of state vectors is also a state vector.
(*ii*) Each observable A of the physical system is expressed as a self-adjoint linear operator $\hat{A}$ acting in Hilbert space. The eigenvalues are real.
(*iii*) The possible measurement of a physical quantity A is one of the eigenvalues of the operator $\hat{A}$. If the spectrum of this operator is discrete and $\hat{A}|\phi_n\rangle = a_n|\phi_n\rangle$, the eigenvalues of $\hat{A}$ are the set of real values $\{a_n\}$, and its eigenvectors are the set $\{|\phi_n\rangle\}$. A state is determined by $|\psi\rangle = c_n|\phi_n\rangle$, $c_n \in \mathbb{C}$, where the probability of obtaining the eigenvalue a_n is given by

$$P(a_n) = ||\langle\phi_n|\psi\rangle||^2 = ||c_n||. \tag{4.3}$$

With scalar product we can define the norm $||\psi|| = \sqrt{\langle\psi|\psi\rangle}$.
(*iv*) The dynamics of the quantum system is given by the Schrödinger equation

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle, \tag{4.4}$$

where $\hbar$ is the reduced Planck constant and $\hat{H}$ is the Hamiltonian operator of the system. For a particle in a potential $V(\mathbf{r},t)$ using position representation we have

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right]\psi(\mathbf{r},t). \tag{4.5}$$

4.2 Self-adjointness

An important property of an operator in the dynamical description of a system in QM is self-adjointness because a self-adjoint operator is an observable, which preserves the probability and the scalar product. We include here some important properties and definitions on self-adjoint extensions [81–85]. Let $\mathcal{H}$ be a Hilbert space and A be a linear operator defined on it. The domain of operator A denoted by Dom(A) or $D(A)$, is defined as

$$D(A) = \{f \in \mathcal{H} : Af \in \mathcal{H}\}. \tag{4.6}$$

To simplify notation we temporally write A instead of $\hat{A}$, usual in QM.
The range of A, denoted as ran(A), and the kernel of A written as ker(A), are defined by

$$\text{ran}(A) = \{Af : f \in D(A)\}, \tag{4.7}$$
$$\ker(A) = \{f \in D(A) : Af = 0\}, \tag{4.8}$$

which turn out to be linear sets. An operator A is closed if and only if for all sequences $\{x_n\}_{n\in\mathbb{N}} \subset D(A)$, $(x_n, Ax_n) \to (x,y)$, where $x \in D(A)$ and $y = Ax$. A closed operator is denoted as $A = \bar{A}$ and if $x = 0$, note that the kernel of A is closed, where $\bar{A}$ is the closure of A, which is the smallest closed extension of A in the sense that if $A \subset B$ and B is closed, then $\bar{A} \subset B$.
By definition, an operator A is called a bounded operator if there exists $c > 0$ such that $\|Af\| \leq c\|f\|$ for all $f \in D(A)$. An operator is bounded if and only if the operator is continuous. Furthermore, the norm of this operator is given by

$$\|A\| = \sup_{f\in D(A)} \frac{\|Af\|}{\|f\|} \tag{4.9}$$

for $f \neq 0$. An operator is densely defined if its domain is dense[1], for a densely defined operator A, its adjoint is denoted as $A^{\dagger}$, which is defined as $A^{\dagger}|\phi\rangle = |\varphi\rangle$, for all $|\phi\rangle \in \mathcal{H}$, such that

$$\langle \phi \mid A\psi \rangle = \langle \varphi \mid \psi \rangle = \left\langle A^{\dagger}\phi \mid \psi \right\rangle, \quad \forall |\psi\rangle \in D(A). \tag{4.10}$$

Note that in this case the adjoint operator $A^{\dagger}$ is closed.
Furthermore, an operator A is symmetric or hermitian if it is fulfilled that

$$\langle A\phi \mid \psi \rangle = \langle \phi \mid A\psi \rangle, \quad \forall |\psi\rangle, |\phi\rangle \in D(A), \tag{4.11}$$

that is, $D(\mathrm{A}) \subseteq D\left(A^{\dagger}\right)$. For two operators A and B a usual notation is $A \subseteq B$, where B is the operator with a grater domain, and B is called an extension of A. Moreover, a characteristic of symmetric operators is that they have a real spectrum.
Therefore, an operator A is self-adjoint if $A = A^{\dagger}$ and $D(A) = D(A^{\dagger})$. Moreover, if the operator obeys $\bar{A} = A^{\dagger}$, A is called essentially self-adjoint. The self-adjoint operators defined in $\mathcal{H}$ have all its real eigenvalues, such that with its eigenvector one can build a complete orthonormal basis of $\mathcal{H}$.
Note that the main difference between a symmetric operator and a self-adjoint one is the definition of the domain. A symmetric operator fulfills $D(A) \subseteq D\left(A^{\dagger}\right)$, but a self-adjoint operator also requires $D(A^{\dagger}) \subseteq D(A)$. Thus, all self-adjoint operators are hermitian, but not all hermitian operators are self-adjoint.
The domain of A may satisfy additional conditions. Generally these conditions are related to the boundary conditions, say $\phi \in D(A^{\dagger})$ obey (4.11), that is,

$$\begin{aligned} D(A) &= \{\psi \mid \psi \in \mathcal{H}, \quad A\psi \in \mathcal{H}, \quad BC(\psi)\}, \\ D\left(A^{\dagger}\right) &= \left\{\phi \mid \phi \in \mathcal{H}, \quad A^{\dagger}\phi \in \mathcal{H}\right\}, \end{aligned} \tag{4.12}$$

where $BC(\psi)$ denotes the additional boundary condition that ψ satisfies to belong to $D(A)$, domain of a hermitian operator. In these cases, it is possible to establish a new boundary condition that extends the domain to be equal. Thus, a hermitian operator can become self-adjoint if the domain is extended.
To build self-adjoint extensions of operators one can use the von Neumann method or deficiency index described in [81–85]. In this method, one focuses on the solution of the complex eigenvalue problem

$$A\psi^{\pm} = \pm i\eta\psi^{\pm}, \tag{4.13}$$

where η is a real and positive constant, for simplicity is taken $\eta = 1$; the introduction of η is due to physical dimensions.
The set of solutions for each eigenvalue defines a subset on $\mathcal{H}$. Let $\mathcal{K}^{\pm}$ be the subset of solutions, which are called the subset of deficiency

$$\begin{aligned} \mathcal{K}^{+} &= \left\{\psi^{+} \mid \psi^{+} \in D\left(A^{\dagger}\right), \quad A^{\dagger}\phi^{+} = i\eta\phi^{+}\right\}, \\ \mathcal{K}^{-} &= \left\{\psi^{-} \mid \psi^{-} \in D\left(A^{\dagger}\right), \quad A^{\dagger}\psi^{-} = -i\eta\psi^{-}\right\}, \end{aligned} \tag{4.14}$$

[1]A domain is dense if a $\delta > 0$ given and $\psi \in \mathcal{H}$, then there always exists $\varphi \in D(A)$ such that in $\|\psi - \varphi\| < \delta$.

where the dimensions of the deficiency subsets $\mathcal{K}^{\pm}$ are denoted by $n_+ = \dim(\mathcal{K}^+)$ and $n_- = \dim(\mathcal{K}^-)$, they are also called deficiency indices. Furthermore, the domain of the operator and its adjoint are defined as

$$\begin{aligned} D(A) &= \{\psi \mid \psi \in \mathcal{H}, \quad A\psi \in \mathcal{H}, \quad BC(\psi)\}, \\ D\left(A^{\dagger}\right) &= \left\{\phi \mid \phi \in \mathcal{H}, \quad A^{\dagger}\phi \in \mathcal{H}\right\} \cup \mathcal{K}^+ \cup \mathcal{K}^-. \end{aligned} \tag{4.15}$$

From the von Neumann theorem, it is possible to get three different solutions in the analysis of deficiency indices
(i) If $n_- = n_+ = 0$, the operator is essentially self-adjoint and there exists a unique extension.
(ii) If $n_- = n_+ \geq 1$, the operator admits a family of self-adjoint extensions, which are parameterized for a unitary matrix $n \times n$, which has n^2 real parameters.
(iii) If $n_- \neq n_+$, the operator does not have self-adjoint extensions.
Note that at the first point, $D\left(A^{\dagger}\right) = D(A)$, which implies that the domain of the operator does not need additional boundary conditions. In the second point, we have $D\left(A^{\dagger}\right) \supset D(A)$, but it is possible to build an extension of the domain $D(A)$, and then a restriction of the domain $D(A^{\dagger})$. For the third, we need to obtain $D\left(A\right) \supset D(A^{\dagger})$ and it is not possible to obtain an extension whose domains are equal.
For case (ii) let $\left\{\psi_1^+, \ldots, \psi_n^+\right\}$ and $\left\{\psi_1^-, \ldots, \psi_n^-\right\}$ be the set of solutions generated by the subspaces of deficiency $\mathcal{K}^{\pm}$. A unitary map U between both subspaces is defined by a unitary matrix $n \times n$, which is $U : \mathcal{K}^- \to \mathcal{K}^+$,

$$\psi_i^+ = \sum_{j=1}^{n} u_{ij}\psi_j^-, \tag{4.16}$$

where u_{ij} are the elements of the matrix U. On the other hand, a new domain for the adjoint operator has the following form

$$D\left(A^{\dagger}\right) = \left\{\psi + \psi^+ + U\psi^+ \mid \psi \in D(A), \quad \psi^+ \in \mathcal{K}^+\right\}. \tag{4.17}$$

The action of A and $A^{\dagger}$ is the same for all functions in the new domain. Assume that there exist χ such as

$$A\chi = i\chi, \tag{4.18}$$

then, as the action of A and $A^{\dagger}$ are the same, that is

$$A^{\dagger}\chi = i\chi. \tag{4.19}$$

Therefore, we have the following

$$i\langle\chi \mid \chi\rangle = \langle\chi \mid i\chi\rangle = \left\langle\chi \mid A^{\dagger}\chi\right\rangle = \langle A\chi \mid \chi\rangle = \langle i\chi \mid \chi\rangle = -i\langle\chi \mid \chi\rangle, \tag{4.20}$$

note that this only is valid if $\chi = 0$, that is, there are not square integrable solutions with imaginary eigenvalue, then the deficiency indexes are zero, the operator A is essentially self-adjoint.
Now, let φ be a function belonging to $D(A)$, the operator is hermitian if it satisfies

$$\left\langle\psi + \psi^+ + U\psi^+ \mid A\varphi\right\rangle = \left\langle A\left(\psi + \psi^+ + U\psi^+\right) \mid \varphi\right\rangle, \tag{4.21}$$

separating the expression, we have

$$\langle \psi \mid A\varphi \rangle + \left\langle \psi^+ + U\psi^+ \mid A\varphi \right\rangle = \langle A\psi \mid \varphi \rangle + \left\langle A\left(\psi^+ + U\psi^+\right) \mid \varphi \right\rangle, \tag{4.22}$$

with $\varphi, \psi \in D(A)$, a domain where A is hermitian, we have

$$\langle \psi \mid A\varphi \rangle = \langle A\psi \mid \varphi \rangle. \tag{4.23}$$

Therefore,

$$\left\langle \psi^+ + U\psi^+ \mid A\varphi \right\rangle = \left\langle A\left(\psi^+ + U\psi^+\right) \mid \varphi \right\rangle. \tag{4.24}$$

Explicitly, we have

$$\left\langle \psi_i^+ + \sum_{j=1}^{n} u_{ij}\psi_j^- \mid A\varphi \right\rangle = \left\langle A\left(\psi_i^+ + \sum_{j=1}^{n} u_{ij}\psi_j^-\right) \mid \varphi \right\rangle. \tag{4.25}$$

Since the functions ψ^+ and ψ^- are known, to enforce the previous expression, this goes to new boundary conditions for the function φ, which determine the domain of the self-adjoint operator, that is,

$$D(A) = \{\psi \mid \psi \in \mathcal{H}, \quad A\psi \in \mathcal{H}, \quad NBC\left(\psi; a_n\right)\} = D\left(A^\dagger\right), \tag{4.26}$$

where NBC indicated the new boundary conditions that ψ satisfies and that depends on n^2 real parameters a_n, which are the elements of the unitary matrix U.

4.2.1 Example: Bounded momentum operator

In QM there exist verious examples in which the operators are hermitian but not self-adjoint, but it is possible to apply the deficiency index method to get the self-adjoint extensions for a hermitian operator. In this section, we study one of the most typical examples, that is, the linear momentum operator $\hat{p}$ bounded in a region $[0, L]$, where the momentum operator has the usual x-representation as $\hat{p} = -i\hbar\frac{d}{dx}$. Thus, let $\psi \in D(\hat{p})$ and $\phi, \hat{p}\psi \in \mathcal{H}$, where we have

$$\begin{aligned} \langle \phi \mid \hat{p}\psi \rangle &= -i\hbar \int_0^L \phi^* \frac{d\psi}{dx} dx, \\ &= -i\hbar \left[\phi^*\psi|_0^L - \int_0^L \frac{d\phi^*}{dx}\psi dx \right], \\ &= \int_0^L \left(-i\hbar\frac{d\phi}{dx}\right)^* \psi dx - i\hbar\phi^*\psi|_0^L, \\ &= \langle \hat{p}\phi \mid \psi \rangle - i\hbar\left[\phi^*(L)\psi(L) - \phi^*(0)\psi(0)\right], \end{aligned} \tag{4.27}$$

note that the last line of the eq.(4.27) suggests the adjoint operator of momentum as

$$\left\langle \hat{p}^\dagger \phi \mid \psi \right\rangle = \langle \hat{p}\phi \mid \psi \rangle - i\hbar\left[\phi^*(L)\psi(L) - \phi^*(0)\psi(0)\right], \tag{4.28}$$

so that $\hat{p}$ is a hermitian operator, the functions $\psi \in D(\hat{p})$ must satisfy the boundary conditions which the last two terms vanishing in (4.28). The operator is not self-adjoint in the interval $[0, L]$ without additional conditions. However, it is possible to find a domain where self-adjointness is fulfilled. The von Neumann theorem will be applied. Let

$$\begin{aligned} \hat{p}\Phi_{\pm} &= \pm i\eta\Phi_{\pm}, \\ \Longrightarrow \frac{d\Phi_{\pm}}{dx} &= \mp\lambda\Phi_{\pm}, \end{aligned} \tag{4.29}$$

where η is real and positive scalar, and $\lambda = \frac{\eta}{\hbar}$. Therefore,

$$\Phi_{\pm} = A_{\pm}e^{\mp\lambda x}, \tag{4.30}$$

where $A_{\pm}$ are normalization constants and

$$\int_0^L |\Phi_{\pm}|^2\, dx = A_{\pm}^2 \int_0^L e^{\mp 2\lambda x} dx = \mp\frac{A_{\pm}^2}{2\lambda}e^{\mp 2\lambda x}\Big|_0^L = \mp\frac{A_{\pm}^2}{2\lambda}\left(e^{\mp 2\lambda L} - 1\right) < \infty. \tag{4.31}$$

The normalizable constants $A_{\pm}$ can be calculated from eq.(4.31) where

$$\begin{aligned} A_{+}^2 &= \frac{2\lambda}{(1 - e^{-2\lambda L})}, \\ A_{-}^2 &= \frac{2\lambda}{(e^{2\lambda L} - 1)}. \end{aligned} \tag{4.32}$$

For later convenience, we rewrite them in the following form

$$\begin{aligned} A_{+} &= e^{\frac{\lambda L}{2}}\left(\frac{\lambda}{\sinh\lambda L}\right)^{\frac{1}{2}}, \\ A_{-} &= e^{-\frac{\lambda L}{2}}\left(\frac{\lambda}{\sinh\lambda L}\right)^{\frac{1}{2}}. \end{aligned} \tag{4.33}$$

From eq.(4.30) note that there is only a solution of the eigenvalue problem, then the deficiency indices, that is, the dimension of the solutions is given by $n_{+} = n_{-} = 1$. Therefore, the operator $\hat{p}$ admits a family of self-adjoint extensions, which are characterized by unitary matrix with only one real parameter, namely a phase.
To extend the domain, we need to find new boundary conditions that determine the self-adjoint extensions. For this, we use the expression (4.25) with the following function.

$$\phi = \Phi_{+} + \alpha\Phi_{-}, \tag{4.34}$$

where $\alpha = e^{i\beta}$ is a phase. We must demand

$$\langle \phi \mid \hat{p}\psi \rangle = \langle \hat{p}\phi \mid \psi \rangle. \tag{4.35}$$

If the previous expression is true, the function ψ belongs to the domain of self-adjoint operator, as we see in the eq.(4.28) this equality is true if

$$\phi^*(L)\psi(L) - \phi^*(0)\psi(0) = 0, \tag{4.36}$$

or explicitly

$$\left[\Phi_{+}^*(L) + \alpha^*\Phi_{-}^*(L)\right]\psi(L) - \left[\Phi_{+}^*(0) + \alpha^*\Phi_{-}^*(0)\right]\psi(0) = 0. \tag{4.37}$$

Using the solutions (4.30)

$$\left(A_+e^{-\lambda L} + \alpha^* A_- e^{\lambda L}\right)\psi(L) - \left(A_+ + \alpha^* A_-\right)\psi(0) = 0, \tag{4.38}$$

this implies

$$\frac{\psi(L)}{\psi(0)} = \frac{e^{\frac{\lambda L}{2}} + \alpha^* e^{-\frac{\lambda L}{2}}}{e^{-\frac{\lambda L}{2}} + \alpha^* e^{\frac{\lambda L}{2}}}, \tag{4.39}$$

the squared norm of this ratio reads

$$\begin{aligned}\left|\frac{\psi(L)}{\psi(0)}\right|^2 &= \frac{e^{\frac{\lambda L}{2}} + \alpha^* e^{-\frac{\lambda L}{2}}}{e^{-\frac{\lambda L}{2}} + \alpha^* e^{\frac{\lambda L}{2}}} \cdot \frac{e^{\frac{\lambda L}{2}} + \alpha e^{-\frac{\lambda L}{2}}}{e^{-\frac{\lambda L}{2}} + \alpha e^{\frac{\lambda L}{2}}} \\ &= \frac{e^{\lambda L} + \alpha + \alpha^* + \alpha^*\alpha e^{-\lambda L}}{e^{-\lambda L} + \alpha + \alpha^* + \alpha^*\alpha e^{\lambda L}} = 1,\end{aligned} \tag{4.40}$$

where $\alpha\alpha^* = 1$ because α is a unitary parameter. Therefore,

$$\psi(L) = e^{i\theta}\psi(0). \tag{4.41}$$

These are the new boundary conditions (NBC) in which the operator $\hat{p}$ is self-adjointness. The function is related by a phase in the extremes; this phase θ characterizes the family of self-adjoint extensions for each value of θ. Therefore, we have different physics for different boundary conditions or values of the phase where $\theta \in [0, 2\pi]$, this family of extensions has infinity values.
On the other hand, the domain where the bounded momentum operator $\hat{p}$ is self-adjoint is given by

$$D(\hat{p}) = \left\{\psi \mid \psi \in \mathcal{H}, \quad \hat{p}\psi \in \mathcal{H}, \quad \psi(L) = e^{i\theta}\psi(0)\right\}, \tag{4.42}$$

note that for $\theta = 0$ we regain the periodic boundary condition, where $\psi(L) = \psi(0)$. See the references [81–85] where more examples and more formalism are shown.

4.3 Path Integral

In 1942 Richard Feynman in his Ph.D. thesis proposed [86] this formulation that connects the classical action of the system with quantum amplitude in QM. This formulation introduces the idea that all paths are allowed to go from the configuration q_i to q_f. In this section, a brief review is given to build a path-integral formulation prescription for the transition amplitude. Such quantity to go from a configuration point (q_i, t_i) to (q_f, t_f) is calculated as

$$U\left(q_f, t_f \mid q_i, t_i\right) = \left\langle q_f, t_f \mid q_i, t_i\right\rangle. \tag{4.43}$$

The transition amplitude $U\left(q_f, t_f \mid q_i, t_i\right)$ is the matrix element of the evolution operator

$$U\left(q_f, t_f \mid q_i, t_i\right) = \left\langle q_f \left| e^{\frac{i\hat{H}\left(t_i - t_f\right)}{\hbar}} \right| q_i \right\rangle, \tag{4.44}$$

for simplicity and without loss generality, we take $|q_i, t_i\rangle = |0, 0\rangle$ and $|q_f, t_f\rangle = |q, t\rangle$. From the definition of the matrix element, we find the following

$$\lim_{t\to 0} U\left(q, t | 0, 0\right) = \langle q \mid 0\rangle = \delta(q). \tag{4.45}$$

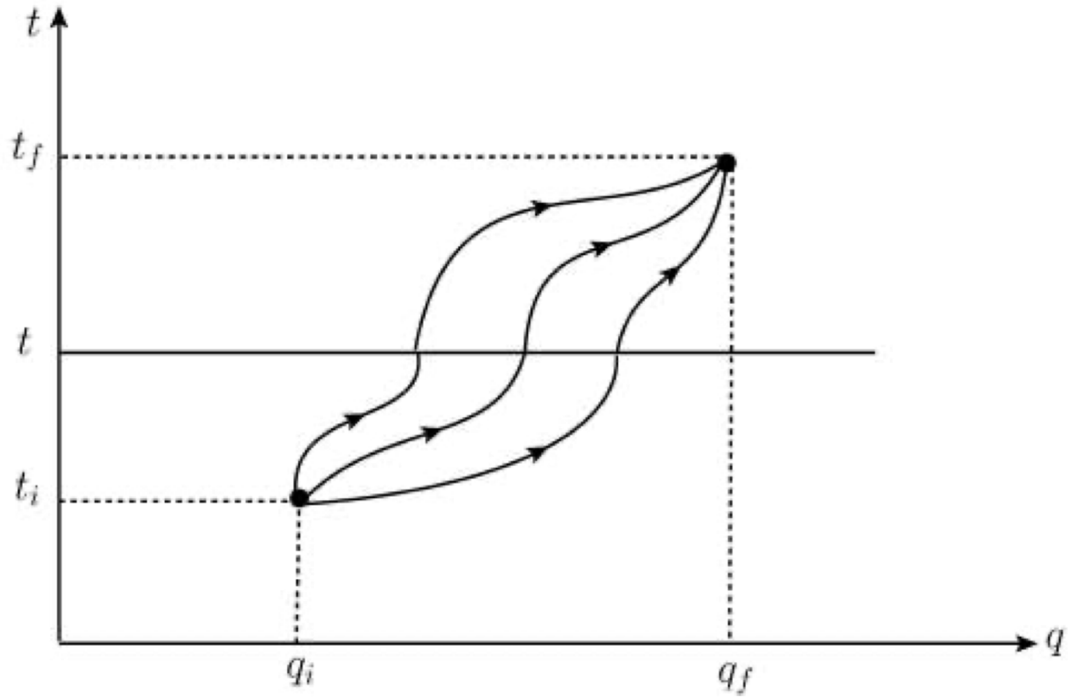

Figure 4.3.1: This plot represents the transition of state (q_i, t_i) to (q_f, t_f) through all trajectories crossing intermediate times like t

Furthermore, the Schrödinger equation plays a role as follows

$$\begin{aligned} i\hbar\frac{\partial U}{\partial t} &= i\hbar\frac{\partial}{\partial t}\langle q, t \mid 0, 0\rangle = i\hbar\frac{\partial}{\partial t}\left\langle q \left| e^{-\frac{iHt}{\hbar}} \right| 0\right\rangle, \\ &= \left\langle q \left| \hat{H} e^{-\frac{i\hat{H}t}{\hbar}} \right| 0\right\rangle, \\ &= \int dq' \left\langle q|\hat{H}|q'\right\rangle \left\langle q' \left| e^{-\frac{i\hat{H}t}{\hbar}} \right| 0\right\rangle, \end{aligned} \tag{4.46}$$

here, the completeness relation is used

$$\mathbb{I} = \int dq' \, |q'\rangle \langle q'| \,, \tag{4.47}$$

as well as states normalized to the Dirac delta

$$\langle q \mid q' \rangle = \delta\left(q - q'\right). \tag{4.48}$$

Therefore,

$$i\hbar\frac{\partial}{\partial t}U(q, t \mid 0, 0) = \int dq' \left\langle q|\hat{H}|q'\right\rangle U\left(q', t \mid 0, 0\right) = \hat{H}U(q, t \mid 0, 0), \tag{4.49}$$

where $U(q, t \mid 0, 0)$ is the solution if the Schrödinger equation that satisfies the initial condition (4.45). For this reason, $U(q, t \mid 0, 0)$ is called the Schrödinger propagator.

Now we use the descomposition property of the propagator

$$U\left(q_f, t_f \mid q_i, t_i\right) = \int dq' \left\langle q_f, t_f \mid q', t'\right\rangle \left\langle q', t' \mid q_i, t_i\right\rangle. \tag{4.50}$$

A partition of the time interval $|t_i, t_f|$ is defined with N subintervals of size Δt, that is $t_f - t_i = N\Delta t$. Let $\{t_j\}$ with $j = 0, ..., N+1$ be the set of points in the interval $[t_i, t_f]$, which is

$$t_i = t_0 \leq t_1 \leq ... \leq t_N \leq t_{N+1} = t_f, \tag{4.51}$$

where $t_k = t_0 + k\Delta t$ for $k = 1, ..., N+1$. Following this process, we obtain

$$\begin{aligned} U(q_f, t_f \mid q_i, t_i) = \int dq_1 \ldots dq_N \langle q_f, t_f \mid q_N, t_N\rangle \langle q_N, t_N \mid q_{N-1}, t_{N-1}\rangle \cdots \\ \langle q_j, t_j \mid q_{j-1}, t_{j-1}\rangle \cdots \langle q_1, t_1 \mid q_i, t_i\rangle, \end{aligned} \tag{4.52}$$

the factor $\langle q_j, t_j \mid q_{j-1}, t_{j-1}\rangle$ has the following form

$$\langle q_j, t_i \mid q_{j-1}, t_{j-1}\rangle = \left\langle q_j \left| e^{-i\hat{H}(t_j - t_{j-1})/\hbar} \right| q_{j-1} \right\rangle = \left\langle q_j \left| e^{-\frac{i\hat{H}\Delta t}{t}} \right| q_{j-1} \right\rangle, \tag{4.53}$$

in the continuous limit $N \to \infty$ with $(t_f - t_i)$ fixed and finite, the interval Δt is infinitesimally small and $\Delta t \to 0$. Thus, as $N \to \infty$ we can approximate the expansion for $\langle q_j, t_j \mid q_{j-1}, t_{j-1}\rangle$ as follows

$$\begin{aligned} \langle q_j, t_j \mid q_{j-1}, t_{j-1}\rangle &= \langle q_j| e^{-\frac{i\hat{H}\Delta t}{\hbar}} |q_{j-1}\rangle \\ &= \left\langle q_j \left| \mathbb{I} - \frac{i\Delta t}{\hbar}\hat{H} + O\left((\Delta t)^2\right) \right| q_{j-1} \right\rangle \\ &= \delta(q_j - q_{j-1}) - \frac{i\Delta t}{\hbar}\left\langle q_j|\hat{H}|q_{j-1}\right\rangle + O\left((\Delta t)^2\right). \end{aligned} \tag{4.54}$$

It is convenient to introduce at each intermediate time t_j a complete set of eigenstates of momentum $\{|p\rangle\}$ using the completeness relation

$$\mathbb{I} = \int_{-\infty}^{\infty} dp|p\rangle\langle p|, \tag{4.55}$$

where we have that

$$\langle q \mid p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipq/\hbar}. \tag{4.56}$$

For a typical Hamiltonian, of the following form

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(q), \tag{4.57}$$

the matrix element is given by

$$\left\langle q_j|\hat{H}|q_{j-1}\right\rangle = \int_{-\infty}^{\infty} \frac{dp_j}{2\pi\hbar} e^{ip_j(q_j - q_{j-1})/\hbar} \left[\frac{p_j^2}{2m} + V(q_j)\right]. \tag{4.58}$$

Also, we have

$$\langle q_j, t_j \mid q_{j-1}, t_{j-1}\rangle \approx \int \frac{dp_j}{2\pi\hbar} \exp\left[i\left(\frac{p_j}{\hbar}(q_j - q_{j-1}) - \Delta t H\left(p_j, \frac{q_j + q_{j-1}}{2}\right)\right], \tag{4.59}$$

thus yielding the amplitude

$$\langle q_f, t_f \mid q_i, t_i \rangle = \lim_{N\to\infty} \int \prod_{j=1}^{N} dq_j \int_{-\infty}^{\infty} \prod_{j=1}^{N+1} \frac{dp_j}{2\pi\hbar}$$
$$\exp\left\{ \frac{i}{\hbar} \sum_{j=1}^{N+1} \left[p_j \left(q_j - q_{j-1}\right) - \Delta t H\left(p_j, \frac{q_j + q_{j-1}}{2}\right)\right]\right\}. \tag{4.60}$$

Therefore, for the limit $N \to \infty$ and taking $(t_i - t_f)$ fixed, the amplitude is expressed as

$$\langle q_f, t_f \mid q_i, t_i \rangle = \int \mathcal{D}p\mathcal{D}q e^{\frac{i}{\hbar}\int_{t_i}^{t_1} dt[p\dot{q} - H(p,q)]}, \tag{4.61}$$

where it is used the notation for the functional measure over the space of the trajectories as

$$\mathcal{D}p\mathcal{D}q = \lim_{N\to\infty} \prod_{j=1}^{N} \prod_{i=1}^{N+1} \frac{dp_i dq_j}{2\pi\hbar}, \tag{4.62}$$

note that as in the classical mechanics, we have for the usual Lagrangian form

$$L = p\dot{q} - H(p, q). \tag{4.63}$$

Therefore,

$$\langle q_f, t_f \mid q_i, t_i \rangle = \int \mathcal{D}q\mathcal{D}p e^{\frac{i}{\hbar}S(p,q)}, \tag{4.64}$$

where $S(p, q)$ is the classical action.

4.4 Relativistic quantum mechanics

The simplest relativistic quantum mechanical equation is the Klein-Gordon´s (KG). It represents a scalar particle without spin. To derive it one considers the classical relativistic energy momentum relation

$$E^2 = p^2c^2 + (mc^2)^2, \tag{4.65}$$

where E is the energy, m is the invariant mass and p denotes the magnitude of the momentum $\boldsymbol{p}$. This expression is promoted to quantum operators, where

$$E \to i\frac{\partial}{\partial t}, \tag{4.66}$$
$$\boldsymbol{p} \to -i\nabla, \tag{4.67}$$

to find

$$-\hbar^2 \frac{\partial^2}{\partial t^2}\phi = -\hbar^2 c^2 \nabla^2 \phi + m^2 c^4 \phi, \tag{4.68}$$

∇^2 denoting the Laplace operator and ϕ is the relativistic wave function. This equation can be written in covariant notation as

$$\left(\tilde{\Box} + \mu^2\right)\phi = 0, \tag{4.69}$$

where the wave operator for a flat space-time with the signature metric $\eta_{\mu\nu} = \mathrm{diag}(-1, +1, +1, +1)$ is

$$\tilde{\Box} = -\eta^{\mu\nu}\partial_\mu\partial_\nu = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2, \tag{4.70}$$

and

$$\mu = \frac{mc}{\hbar}. \tag{4.71}$$

Unless otherwise started we will use natural unities with $c = \hbar = 1$. As classical field, ϕ can be real or complex. KG equation can be generalized to

$$\tilde{\Box}\phi + \frac{\partial V}{\partial \phi^*} = 0, \tag{4.72}$$

with an arbitrary potential V containing the mass of the scalar field and a self-interaction

$$V(\phi, \phi^*) = \frac{1}{2}\mu^2\phi\phi^* + \lambda(\phi\phi^*)^2. \tag{4.73}$$

This equation can be obtained from an action S for a complex scalar field of the form

$$S = \int d^4x \left(\partial^\mu\phi\partial_\mu\phi^* - V(\phi, \phi^*)\right). \tag{4.74}$$

The KG equation (4.72) for a complex scalar field ϕ admits a $U(1)$ symmetry, which obeys the following transformations

$$\begin{aligned} \phi(x) &\mapsto e^{i\theta}\phi(x), \\ \phi^*(x) &\mapsto e^{-i\theta}\phi^*(x). \end{aligned} \tag{4.75}$$

By the Noether theorem [87] for fields, which corresponds to the symmetry described, there exists a current $J^\mu(x)$ for $\lambda = 0$, which is defined as

$$J^\mu(x) = \frac{e}{2m}\left(\phi^*(x)\partial^\mu\phi(x) - \phi(x)\partial^\mu\phi^*(x)\right), \tag{4.76}$$

and the current is conserved, namely $\partial_\mu J^\mu = 0$. The $U(1)$ symmetry is a global symmetry, but a local or gauge symmetry can also be considered. It can be noticed the proposed density $\rho = J^0 = \frac{e}{2m}(\phi^*\partial^0\phi - \phi\partial^0\phi^*)$ is not positive density because of the second order character of KG equation. Dirac proposed to look for a relativistic equation first order in time derivatives, $i\hbar\partial_t\psi = H\psi$. Say

$$H = c\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + \beta mc^2, \tag{4.77}$$

using this proposal to regain KG equation one takes the squared linear operator

$$\left(-i\hbar\partial_t + c\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + \beta mc^2\right)\left(i\hbar\partial_t + c\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + \beta mc^2\right)\psi = 0. \tag{4.78}$$

This leads to the following conditions

$$\alpha_j^2 = \beta^2 = 1, \tag{4.79}$$

$$\alpha_i\alpha_j + \alpha_j\alpha_i = 0, \tag{4.80}$$

$$\alpha_j\beta + \beta\alpha_j = 0. \tag{4.81}$$

α_i and β cannot numbers, but satisfy

$$\{\alpha_\mu, \alpha_\nu\} = 2\delta_{\mu\nu}\mathbb{I}. \tag{4.82}$$

Since the operator $\hat{H}$ is hermitian, the matrices α_i and β should be matrices. Matrices α_i can be expressed using Pauli matrices σ_i

$$\alpha_j = \begin{pmatrix} O & \sigma_j \\ \sigma_j & O \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{I} & O \\ O & -\mathbb{I} \end{pmatrix}. \tag{4.83}$$

It turns out to be convenient to define the gamma matrices $\tilde{\gamma}^j$

$$\tilde{\gamma}^j = \beta\alpha_j, \quad \tilde{\gamma}^0 = \beta, \tag{4.84}$$

Therefore, it is possible to rewrite the Dirac equation as

$$(i\hbar\tilde{\gamma}^\mu\partial_\mu - mc)\,\Psi = 0, \tag{4.85}$$

where $\mu = 0, 1, 2, 3$. One representation of the gamma matrices is

$$\tilde{\gamma}^0 = \begin{pmatrix} \mathbb{I} & O \\ O & -\mathbb{I} \end{pmatrix}, \quad \tilde{\gamma}^j = \begin{pmatrix} 0 & \sigma_j \\ -\sigma_j & 0 \end{pmatrix}. \tag{4.86}$$

Another convenient representation of the gamma matrices is given by the Weyl representation

$$\tilde{\gamma}^0 = \begin{pmatrix} O & \mathbb{I} \\ \mathbb{I} & O \end{pmatrix}, \quad \tilde{\gamma}^j = \begin{pmatrix} 0 & \sigma_j \\ -\sigma_j & 0 \end{pmatrix}. \tag{4.87}$$

From the expression (4.82) it follows that the gamma matrices fulfil the anti-commutation relation as

$$\{\tilde{\gamma}^\mu, \tilde{\gamma}^\nu\} = \tilde{\gamma}^\mu\tilde{\gamma}^\nu + \tilde{\gamma}^\nu\tilde{\gamma}^\mu = 2\eta^{\mu\nu}\mathbb{I}_{4\times4}. \tag{4.88}$$

Additionally, the four-vector current of probability j^μ reads

$$j^\mu = \psi^\dagger\gamma^0\gamma^\mu\psi = \bar{\psi}\psi, \tag{4.89}$$

where ψ is the spinor and $\bar{\psi} = \psi^\dagger\tilde{\gamma}^0$ is the Dirac adjoint spinor. Here, the current probability obeys the continuity equation

$$\partial_\mu j^\mu = 0. \tag{4.90}$$

The Dirac equation historically introduced to solve the problem of negative probability, yields a fundamental quantity in quantum mechanics: spin. Thus theoretically, spin comes from a combination of special relativity and quantum mechanics.

4.5 Quantum Mechanics in curved space-time

We can generalize the KG equation (4.69) for an arbitrary curved space-time, by alluding to the minimum coupling principle [42, 88, 89]. Partial derivatives ∂_μ are replaced by covariant derivatives ∇_μ and the Minkowski tensor metric $\eta_{\mu\nu}$ by the tensor metric $g_{\mu\nu}$. It takes the form

$$\frac{-1}{\sqrt{-g}}\partial_\mu\left(g^{\mu\nu}\sqrt{-g}\partial_\nu\phi\right)+\mu^2\phi=0, \tag{4.91}$$

where the g is the determinant of the metric tensor and $\Gamma^\sigma{}_{\mu\nu}$ are the Christoffel symbol. Therefore, the KG equation is written as follows.

$$\Box\phi-\mu^2\phi=0, \tag{4.92}$$

where the D'Alambertian operator for an arbitrary curved space-time is give by $\Box=g^{\mu\nu}\nabla_\mu\nabla_\nu=\nabla^\mu\nabla_\mu$. Thus, the action for a complex scalar field in curved space-time is read as follows

$$S=\int_M d^4x\sqrt{-g}\left(-g^{\mu\nu}\nabla_\mu\phi\nabla_\nu\phi^*-m^2\phi\phi^*\right). \tag{4.93}$$

On the other hand, to study the Dirac equation in a curved space-time coupled it is convenient to introduce tetrads for the space-time geometry [1, 41, 43–45, 48, 90]. Using the coordinate t as the parameter of evolution as in Section 3.3 the 3+1 metric tetrad vector fields

$$\mathrm{d}s^2=N^2c^2\mathrm{d}t^2-h_{ij}\left(\mathrm{d}x^i+N^ic\,\mathrm{d}t\right)\left(\mathrm{d}x^j+N^jc\,\mathrm{d}t\right), \tag{4.94}$$

with inverse

$$\begin{aligned} e_0 &= \frac{1}{N}\left(\frac{\partial}{c\,\partial t}-N^j\frac{\partial}{\partial x^j}\right),\\ e_k &= \hat{e}_k^{\ j}\frac{\partial}{\partial x^j}, \end{aligned} \tag{4.95}$$

where $\hat{e}^k=\hat{e}^k_i\mathrm{d}x^i$ are the one-form basis for a three-dimensional slice of the such that $h_{ij}=\delta_{kl}\hat{e}^k_i\hat{e}^l{}_j$. The set of vectors based on the tangent spacetime is defined as $e_a=e_a^{\ \mu}\partial_\mu$, such that $e^ae_b=\delta^a_b$ [1, 40, 41, 44, 45, 48, 91].
The Lagrangian density [92–94] we consider here is

$$\mathcal{L}=\sqrt{-g}\frac{i\hbar c}{2}\left[\psi^\dagger B\gamma^\mu\left(D_\mu\psi\right)-\left(D_\mu\psi\right)^\dagger B\gamma^\mu\psi+\frac{2imc}{\hbar}\psi^\dagger B\psi\right], \tag{4.96}$$

where $D_\mu=\nabla_\mu+\dfrac{iq}{\hbar c}A_\mu$ is the total covariant derivative with electromagnetic coupling. The covariant derivative of a spinor ψ is given by $\nabla_\mu\psi=\partial_\mu\psi+\Gamma_\mu\psi$, where Γ_μ is the spin connection[1, 45].The corresponding Dirac equation is given by

$$\left[i\hbar\gamma^\mu(\nabla_\mu+iqA_\mu)-mc\right]\psi=0, \tag{4.97}$$

where q,m are the charge and mass of the fermion particle and ψ is its spinor. γ^μ can be written as $\gamma^\mu=e^\mu_{\ a}\tilde{\gamma}^a$, where $\tilde{\gamma}^a$ are the gamma matrices in flat space-time [95–97]. To simplify the notation, natural units are used ($c=\hbar=1$). Therefore,

$$\begin{aligned} \gamma^0 &= N\tilde{\gamma}^0,\\ \gamma^k &= \hat{e}^k{}_j(\tilde{\gamma}^j+N^j\tilde{\gamma}^0). \end{aligned} \tag{4.98}$$

In general, these matrices fulfill the following anticommutation relation[45, 88]

$$\{\gamma^\mu, \gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}\mathbb{I}, \tag{4.99}$$

where $g_{\mu\nu}$ represents the metric that describes the space-time geometry. The gamma matrices obey the following relation [92–94]

$$(\gamma^\mu)^\dagger = B\gamma^\mu B^{-1}, \tag{4.100}$$

where B is a hermitian matrix, i.e. $B^\dagger = B$, that is uniquely determined by the gamma matrices γ^μ. As usual, $B^\dagger$ denotes the conjugate transpose (or Hermitian) of B. Using eq.(4.100) it is straightforward to see $\psi\bar{\psi}$ as a scalar and $\psi\gamma^\mu\bar{\psi}$ as a four vector, where for curved spacetimes $\bar{\psi} = \psi^\dagger B$ is the adjoint spinor (see [45, 88, 91, 95]).

The equation for the transpose-conjugated spinor is

$$i\left(\nabla_\mu\bar{\psi}\right)\gamma^\mu - i\psi^\dagger\nabla_\mu\left(B\gamma^\mu\right) + i\bar{\psi}\nabla_\mu\gamma^\mu + \bar{\psi}A_\mu\gamma^\mu + m\bar{\psi} = 0, \tag{4.101}$$

where $(\nabla_\mu\psi)^\dagger = \nabla_\mu\psi^\dagger$ and denote the adjoint spinor as $\bar{\psi} = \psi^\dagger B$. The conserved charge is obtained from the Noether theorem [87] yielding

$$J^\mu = \bar{\psi}\gamma^\mu\psi = \psi^\dagger B\gamma^\mu\psi. \tag{4.102}$$

Thus, we obtain the continuity equation where the covariant derivative acts on the current density J^μ

$$\nabla_\mu J^\mu = 0. \tag{4.103}$$

This gives

$$\nabla_\mu J^\mu = (\nabla_\mu\bar{\psi})\gamma^\mu\psi + \bar{\psi}\left(\nabla_\mu\gamma^\mu\right)\psi + \bar{\psi}\gamma^\mu\nabla_\mu\psi. \tag{4.104}$$

From which it follows that

$$\nabla_\mu J^\mu = \psi^\dagger\nabla_\mu\left(B\gamma^\mu\right)\psi, \tag{4.105}$$

the continuity equation (4.103) holds whenever $\nabla_\mu\left(B\gamma^\mu\right) = 0$, or equivalently

$$(\nabla_\mu B)\gamma^\mu = -B\nabla_\mu\gamma^\mu. \tag{4.106}$$

To find the conserved quantity resulting from the continuity equation, we take an arbitrary surface $\mathcal{S}$ that encloses the volume $\mathcal{V}$ that contains the whole system. Let k^j be an orthonormal vector to $\mathcal{S}$ such that

$$\int_{\mathcal{V}}\nabla_\mu J^\mu dV = \int_{\mathcal{V}}\nabla_0 J^0 dV + \int_{\mathcal{S}}k_j J^j\sqrt{h}d^3x = 0. \tag{4.107}$$

where h is the determinant of the slice metric h_{ij}. We assume that far away from the source spinor ψ goes to zero, which means that in this region J^μ is negligible. Then, the surface integral in Eq. (4.107) vanishes and is obtained

$$\frac{dQ}{dt} = \int_{\mathcal{V}}\nabla_0 J^0 dV = 0, \tag{4.108}$$

where $Q = \int_{\mathcal{V}} J^0 dV$ is the conserved charge, dV is the curved volume element $dV = \sqrt{-g}d^4x$. In QFT this charge is identified with the number of fermions or

with the electric charge of the system. In flat space-time, we have $B = \tilde{\gamma}^0$, so that $J^0 = \psi^\dagger\psi = n$ represents the number density of fermion particles. In curved space-time J^0 (which is determined by γ^0 and by generalized gamma matrices) has a different interpretation, which includes the geometry of space-time. The form of B given by eqs. (4.100) and (4.106) for each metric are related to the gamma matrices and the tetrad formalism.
Maxwell´s equations take the form

$$\nabla_\nu F^{\nu\mu} = J^{E\mu}, \tag{4.109}$$

$$F_{\mu\nu} = \nabla_\mu A_\nu - \nabla_\nu A_\mu. \tag{4.110}$$

where $J^{E\mu}$ is the four-electromagnetic current.
It is possible to rewrite the Dirac equation in the Weyl representation.
In terms of the Pauli matrices σ^μ the 4×4 gamma matrices γ^μ can be written as two 2×2 block matrices

$$\gamma^0 = N\tilde{\gamma}^0 = N\begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}, \tag{4.111}$$

$$\gamma^j = \hat{e}^j{}_i(\tilde{\gamma}^i + N^i\tilde{\gamma}^0) = \begin{pmatrix} 0 & -\hat{e}^j{}_i(\tilde{\sigma}^i - N^i\mathbb{I}) \\ \hat{e}^j{}_i(\tilde{\sigma}^i + N^i\mathbb{I}) & 0 \end{pmatrix}, \tag{4.112}$$

where $\tilde{\sigma}^i$ are the 2×2 Pauli matrices in flat space-time

$$\tilde{\sigma}^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tilde{\sigma}^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tilde{\sigma}^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4.113}$$

and $\mathbb{I}$ is the 2×2 identity matrix. The γ^μ matrices satisfy $(\gamma^0)^\dagger = \gamma^0$ and $(\gamma^j)^\dagger = -\gamma^j + 2N^j\gamma^0/N$. The standard representation is adopted for the gamma matrices in a flat space-time $\tilde{\gamma}^\mu$ as follows

$$\tilde{\gamma}^0 = \begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}, \quad \tilde{\gamma}^j = \begin{pmatrix} 0 & -\tilde{\sigma}^j \\ \tilde{\sigma}^j & 0 \end{pmatrix}. \tag{4.114}$$

Thus, in the Weyl representation a Dirac fermion is written as a four-spinor ψ made of two spinors, each of which having two components

$$\psi = \begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix}, \tag{4.115}$$

where ψ_R and ψ_L are the right- and the left- handed Weyl spinors, respectively. If we write the adjoint spinor $\bar{\psi}$ and use the Weyl representation, it follows that

$$\bar{\psi} = \psi^\dagger B = \left(\psi_R^\dagger, \psi_L^\dagger\right) B, \tag{4.116}$$

where B is the matrix from eqs. (4.106) and (4.106). If we use the relation (4.100) it is straightforward to see that the matrix B must have the following form

$$B = \begin{pmatrix} 0 & B_\zeta \\ B_\zeta & 0 \end{pmatrix}, \tag{4.117}$$

where the 2×2 matrix B_ζ is a diagonal matrix, $B_\zeta = b\mathbb{I}$, with $b = b(x^\mu)$. Therefore, we get $B = b\tilde{\gamma}^0$ we transform into

$$\begin{aligned} \nabla_0(Nb) + \nabla_j(\hat{e}_i^j N^i b) &= 0, & (4.118)\\ \nabla_j(\hat{e}_i^j b)\tilde{\sigma}^i &= 0. & (4.119)\end{aligned}$$

Using the definition of the spinor and its adjoint, we can write the Dirac quadri-current J^μ from eq. (4.102) as

$$J^\mu = \left(\psi_R^\dagger, \psi_L^\dagger\right) B\gamma^\mu \left(\begin{array}{c} \psi_R \\ \psi_L \end{array}\right), \tag{4.120}$$

where the gamma matrices are defined by eqs. (4.111) and (4.112) and, in general, B is given by the conditions mentioned above. This yields

$$\begin{aligned} J^0 &= Nb(\psi_R^\dagger\psi_R + \psi_L^\dagger\psi_L), & (4.121)\\ J^j &= b\hat{e}^j{}_i(\psi_R^\dagger(\tilde{\sigma}^i + N^i\mathbb{I})\psi_R - \psi_L^\dagger(\tilde{\sigma}^i - N^i\mathbb{I})\psi_L). & (4.122)\end{aligned}$$

To simplify the notation, we now define the vectors of the 2×2 matrices $\mathbb{S}^a = (\mathbb{I}, \tilde{\sigma}^j + N^j\mathbb{I})$ and $\bar{\mathbb{S}}^a = (-\mathbb{I}, \tilde{\sigma}^j - N^j\mathbb{I})$ in terms of the Pauli matrices. $\mathbb{S}^a$ and $\bar{\mathbb{S}}^a$ are the (generalized) Pauli matrices in flat space-time. In terms of these new definitions, the density current reads

$$\begin{aligned} J^\mu &= b\hat{e}^\mu{}_i(\psi_R^\dagger\mathbb{S}^i\psi_R - \psi_L^\dagger\bar{\mathbb{S}}^i\psi_L),\\ &= b(\psi_R^\dagger\sigma^\mu\psi_R - \psi_L^\dagger\bar{\sigma}^\mu\psi_L), & (4.123)\end{aligned}$$

where we have defined the 2×2 Pauli matrices in a curved space-time by $\sigma^\mu = e^\mu{}_a\mathbb{S}^a$ and $\bar{\sigma}^\mu = e^\mu{}_a\bar{\mathbb{S}}^a$. With this definition, the matrices γ^j read

$$\gamma^j = \begin{pmatrix} 0 & -\bar{\sigma}^j \\ \sigma^j & 0 \end{pmatrix}. \tag{4.124}$$

Furthermore, observe that the σ^j matrices follow the same commutation relations as the flat space-time Pauli matrices $[\tilde{\sigma}_i, \tilde{\sigma}_j] = 2i\varepsilon_{ijk}\tilde{\sigma}_k$.
In the Weyl representation the Dirac equation (4.97) can be written as

$$\left(\begin{array}{c} i\sigma^\mu\left(\bar{\nabla}_\mu + iqA_\mu\right)\psi_R - m\psi_L \\ i\bar{\sigma}^\mu\left(\nabla_\mu + iqA_\mu\right)\psi_L - m\psi_R \end{array}\right) = \left(\begin{array}{c} 0 \\ 0 \end{array}\right). \tag{4.125}$$

These are the Weyl equations for a spinor in a curved space-time coupled to an electromagnetic field.
By choosing $B = b\tilde{\gamma}^0$, the current density reads

$$J^\mu = b\left(\psi_R^\dagger\sigma^\mu\psi_R - \psi_L^\dagger\bar{\sigma}^\mu\psi_L\right). \tag{4.126}$$

Explicitly, we have, for the spatial part, the following

$$J^j = b\hat{e}_i^j\left(\psi_R^\dagger\tilde{\sigma}^i\psi_R - \psi_L^\dagger\tilde{\sigma}^i\psi_L + \frac{N^i}{Nb^2}J^0\right). \tag{4.127}$$

On the other hand, it is possible to rewrite in this representation the following identities as

$$\gamma^\mu\gamma^\nu F_{\mu\nu}\psi = \begin{pmatrix} (2NN^k F_{0k} + i\hat{F}_{ij}\epsilon^{ij}{}_k\tilde{\sigma}^k)\psi_R \\ -(2NN^k F_{0k} - i\hat{F}_{ij}\epsilon^{ij}{}_k\tilde{\sigma}^k)\psi_L \end{pmatrix}, \tag{4.128}$$

and using definition (4.124), we find that

$$\begin{aligned} \gamma^\mu(\nabla_\mu\gamma^\nu)(D_\nu\psi) &= \begin{pmatrix} -\bar{\mathbb{S}}^a\mathbb{S}^b(\hat{\nabla}_a\hat{e}^\nu_b)(D_\nu\psi_R) \\ -\mathbb{S}^a\bar{\mathbb{S}}^b(\hat{\nabla}_a\hat{e}^\nu_b)(D_\nu\psi_L) \end{pmatrix}, \\ &= \begin{pmatrix} (N\nabla_0 N - \bar{\sigma}^j\nabla_j N)D_0\psi_R + (N\nabla_0\sigma^i - \bar{\sigma}^j\nabla_j\sigma^i)D_i\psi_R \\ (N\nabla_0 N + \sigma^j\nabla_j N)D_0\psi_L - (N\nabla_0\bar{\sigma}^i - \sigma^j\nabla_j\bar{\sigma}^i)D_i\psi_L \end{pmatrix}, \\ &= \begin{pmatrix} (\hat{\nabla}_0 N - \bar{\mathbb{S}}^k\hat{\nabla}_k N)D_0\psi_R + (\mathbb{S}^k\hat{\nabla}_0\hat{e}^i_k - \bar{\mathbb{S}}^k\mathbb{S}^l\hat{\nabla}_k\hat{e}^i_l)D_i\psi_R \\ (\hat{\nabla}_0 N + \mathbb{S}^k\hat{\nabla}_k N)D_0\psi_L - (\bar{\mathbb{S}}^k\hat{\nabla}_0\hat{e}^i_k - \mathbb{S}^k\bar{\mathbb{S}}^l\hat{\nabla}_k\hat{e}^i_l)D_i\psi_L \end{pmatrix}, \end{aligned} \tag{4.129}$$

where $\epsilon^{ij}{}_k$ is the 3d Levi-Civita tensor, $\hat{F}_{ij} = \hat{e}^l_i\hat{e}^m_j F_{lm}$ is the directional Maxwell tensor $\hat{F}_{ij} = (\hat{e}^l_i\hat{\nabla}_j - \hat{e}^l_j\hat{\nabla}_i)A_l$, and $\hat{\nabla}_a = \hat{e}^\alpha_a\nabla_\alpha$ is the directional covariant derivative which defines the Cartan connection $\hat{\nabla}_c\hat{e}^\nu_b = \Gamma^a_{bc}\hat{e}^\nu_a$. The Cartan connection $\Gamma^a_{bc} = \hat{e}^a_\nu\hat{\nabla}_c\hat{e}^\nu_b$ determines the Cartan first fundamental form $d\hat{e}^a + \Gamma^a_b \wedge \hat{e}^b$ for the connections $\Gamma^a_b = \Gamma^a_{bd}\hat{e}^d$ with the property that $\Gamma_{ab} + \Gamma_{ba} = 0$, where $\Gamma_{ab} = \eta_{ad}\Gamma^d_b$.

4.6 Polymer quantum mechanics

Polymeric quantization is an alternative quantization scheme [98–101] based on the techniques developed for loop quantum gravity (LQG). It can help us to better understand progress and problems in systems with greater degrees of complexity. These techniques differ from standard quantization in some fundamental aspects; an important result is that in this scheme the Stone-von Neumann theorem [102, 103] does not hold due to the fact that there exists non continuous representation, and the polymeric and standard quantization are not unitary equivalent; another important difference is the algebra used between the fundamental operators, that is, the commutation relation on the Hilbert space. Nevertheless, it is possible to find a limit in which we can recover the standard quantization. In this section, we show some aspects for this alternative quantization which are illuminating for the symmetry reduced gravitational models.
Let us consider a particle in 1-dimension. For standard QM, the Hilbert space $\mathcal{H} = L^2(\mathbb{R}, \mathrm{d}x)$ is the set of complex square integral functions over $\mathbb{R}$, with the standard Lebesgue measure $\mathrm{d}x$, the position x and the momentum p of a particle follow the canonical commutation relations

$$[\hat{x},\hat{x}] = i\hbar\widehat{\{x,x\}} = \hat{0}, \quad [\hat{p},\hat{p}] = i\hbar\widehat{\{p,p\}} = \hat{0}, \quad [\hat{x},\hat{p}] = i\hbar\widehat{\{x,p\}} = i\hbar\hat{\mathbb{I}}. \tag{4.130}$$

Now, in the polymeric scheme, it is convenient to work with the exponential versions of $\hat{x}$ and $\hat{p}$, that is, the one-parametric families of unitary operators

$$\widehat{U}_\mu = e^{i\mu\hat{x}} = \sum_{n=0}^{\infty}\frac{1}{n!}(i\mu\hat{x})^n, \quad \widehat{V}_\nu = e^{i\nu\hat{p}/\hbar} = \sum_{n=0}^{\infty}\frac{1}{n!}(i\nu\hat{p}/\hbar)^n, \tag{4.131}$$

where μ, ν are arbitrary real parameters. The action of these operators in an arbitrary state $\psi \in \mathcal{H}$ is

$$\widehat{U}_\mu \psi(x) = e^{i\mu x}\psi(x), \quad \widehat{V}_\nu \psi(x) = \psi(x+\nu). \tag{4.132}$$

Both operators are well-defined on the Hilbert space and they obey the following relations

$$\widehat{U}_{\mu_1}\widehat{U}_{\mu_2} = \widehat{U}_{\mu_1+\mu_2}, \quad \widehat{V}_{\nu_1}\widehat{V}_{\nu_2} = \widehat{V}_{\nu_1+\nu_2}, \quad \widehat{U}_\mu \widehat{V}_\nu = e^{-i\mu\nu}\widehat{V}_\nu \widehat{U}_\mu. \tag{4.133}$$

In addition, the hermiticity conditions are satisfied.

$$\widehat{U}^\dagger_\mu = \widehat{U}_{-\mu}, \quad \widehat{V}^\dagger_\nu = \widehat{V}_{-\nu}. \tag{4.134}$$

In the canonical representation, the relations (4.133) are unitary equivalent to the canonical relations (4.130), this algebra is called the Weyl algebra. Nevertheless, it is possible to relax the conditions in the Stone-von Neumann theorem.
The main difference between both quantizations is the choice of a non-separable Hilbert space $\mathcal{H}_{pol}$. This Hilbert space with an uncountable orthonormal basis is described by kets $|\mu\rangle$, with μ real numbers, with inner product between both kets $\langle\mu|\nu\rangle = \delta_{\mu,\nu}$. It is possible to check that the operators $\hat{U}_\mu$ and $\hat{V}_\nu$ are well defined in $\mathcal{H}_{pol}$, they obey also the relation (4.133). The position operator $\hat{x}$ is defined as $\hat{x}\,|\mu\rangle = \mu\,|\mu\rangle$. However, in polymeric representation, in Hilbert space there does not exist a Hermitian operator $\hat{p}$, this operator is not well defined in $\mathcal{H}_{pol}$.
Since the momentum operator $\hat{p}$ it is not well defined in $\mathcal{H}_{pol}$ we need to look for a replacement for a system withh classical Hamiltonian

$$H = \frac{p^2}{2m} + V(x). \tag{4.135}$$

One considers a length scale μ_0 approximates the $\widehat{p^2}$ operator from the classical relation

$$e^{i\mu_0 p/\hbar} + e^{-i\mu_0 p/\hbar} \approx 2 - \mu_0^2 p^2/\hbar^2, \tag{4.136}$$

valid in the following manner for $p << \hbar/\mu_0$. The operators $\hat{V}_{\mu_0}$ and $\hat{V}_{-\mu_0}$ are used

$$\widehat{p^2_{\mu_0}} := \frac{\hbar^2}{\mu_0^2}\left[2 - \widehat{V}_{\mu_0} - \widehat{V}_{-\mu_0}\right], \tag{4.137}$$

The algebra with the commutator that is used in this quantization is the flux and holonomy algebra instead of the canonical algebra in the standard Schrödinger representation, namely

$$\left[\hat{x}, \hat{V}_{\mu_0}\right] = -\mu_0 \hat{V}_{\mu_0}. \tag{4.138}$$

As in canonical quantization, we have a Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}_{\mu_0}\Psi, \tag{4.139}$$

where the stationary solution is given by $\Psi = \psi e^{-iEt/\hbar}$. the energy eigenvalue problem $\widehat{H}_{\mu_0}\psi = E\psi$, becomes the difference equation in the x-representation

$$\psi(x+\mu_0) + \psi(x-\mu_0) = \left(2 - \frac{2m\mu_0^2}{\hbar^2}(E - V(x))\right)\psi(x). \tag{4.140}$$

In the p-representation it is equivalent to a differential equation

$$\left[V\left(-i\hbar\frac{\partial}{\partial p}\right)+\frac{\hbar^2}{m\mu_0^2}\left(1-\cos\left(\frac{\mu_0 p}{\hbar}\right)\right)-E\right]\tilde{\psi}(p)=0, \tag{4.141}$$

for $-\frac{\pi\hbar}{\mu_0}\leq p\leq\frac{\pi\hbar}{\mu_0}$ and for a free particle $V(x)=0$ the energy spectrum takes the form

$$E=\frac{\hbar^2}{m\mu_0^2}\left[1-\cos\left(\frac{p\mu_0}{\hbar}\right)\right]. \tag{4.142}$$

Note that for $\mu_0\to 0$ we have $E\approx p^2/(2m)$. When $\mu_0\to 0$ the separation of the lattice goes to zero the continuous limit is regained and we recover the standard energy spectrum. Although polymeric QM is not a unitary equivalent representation to QM due to the Stone-von Neumann theorem, it is possible to recover the standard QM description in a certain limit, when the discreteness of position disappears.

This alternative quantization has been extensively studied and applied in reduced-symmetry models such as QM and in gravitational cases such as cosmology or interior of black holes. These techniques have been applied to symmetry-reduced gravitational models.

CHAPTER

FIVE

HYDRODYNAMIC REPRESENTATION

The hydrodynamic representation of some particles has been useful for multiple calculations and interpretations. The hydrodynamics of classical particles has been studied using the Navier-Stokes equation, which does not have analytical solutions. However, it is possible to obtain numerical simulations and solutions of fluids. This representation describes a system as a fluid or a large number of particles. In QM, particles can be cataloged by bosons and fermions; additionally, the spin value for each kind of particles is determined depending on what statistics are used. In this section, we discuss some important concepts and results on hydrodynamic representation for classical particles and for quantum particles for non-relativistic and relativistic systems, extending it to fermions in curved spacetimes, which are described by the Dirac equation in curved spacetime. For quantum particles, the Madelung transformation is implemented to obtain this hydrodynamic representation.

5.1 Classical particles

The hydrodynamic representation of classical particles is based on the Navier-Stokes equation, which treats a fluid on a scale where it can be considered to be continuous rather than as constituted by individual discrete particles. Thus,

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)=-\nabla p+\nabla\cdot\left[\mu\left(\nabla\mathbf{u}+(\nabla\mathbf{u})^{\top}\right)\right]+\nabla\cdot[\lambda(\nabla\cdot\mathbf{u})\mathbb{I}]+\rho\mathbf{g}, \quad (5.1)$$

where ρ is the mass density, $\mathbf{u}$ is the flow velocity, p is the mechanical pressure. Furthermore, μ and λ are the first and second viscosity coefficients, respectively. However, when the viscosity coefficients are negligible ($\mu=\lambda=0$) the equation obtained is called the Euler equation; in this case the fluid can be described by

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)=-\nabla p+\rho\mathbf{g}. \quad (5.2)$$

For the case where the Euler equation (5.2) is physically realizable, the fluid would continue flowing forever and would never dissipate its energy and reach equilibrium. The Navier-Stokes equations are derived from basic principles such as continuity of mass, conservation of momentum, and conservation of energy.

Furthermore, using the conservative forces and taking into account the Bernoulli principle, which is applied to steady flow with small fluctuations by keeping time derivative terms and expanding the applied forces with some fluctuations, it is possible to rewrite this as

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = \mathbf{F} - \frac{1}{\rho}\nabla p. \tag{5.3}$$

The assumptions on the conservative forces and irrotational (laminar) flow, respectively, are given by

$$\mathbf{F} = -\nabla U, \tag{5.4}$$

$$\nabla \times \mathbf{u} = 0, \implies \mathbf{u} = -\nabla \varphi, \tag{5.5}$$

where U and φ are potentials. Substituting these assumptions in the Euler equation (5.2) it is possible to rewrite it as

$$\nabla \left(-\frac{\partial \varphi}{\partial t} + \frac{u^2}{2} + U + \frac{p}{\rho} \right) = 0. \tag{5.6}$$

Applying the steady-flow assumption reduces the time derivative term to zero. Therefore, we arrive at the Bernoulli equation, which is

$$\frac{u^2}{2} + U + \frac{p}{\rho} = \text{ cte.} \tag{5.7}$$

Note that the Bernoulli equation is the first integral of the Euler equation, which is a particular case of the Navier-Stokes equation that describes the dynamics of a fluid.

5.2 Quantum Mechanics

The hydrodynamic representation in QM can be found by applying the Madelung transformation [7] to the Schrödinger equation (4.5) to get the Navier-Stokes equation. The Madelung transformation can be written as

$$\psi(\mathbf{x}, t) = \sqrt{\rho(\mathbf{x}, t)} e^{\frac{i}{\hbar} S(\mathbf{x}, t)}, \tag{5.8}$$

which is the polar form of the wave-function, where the probability density is denoted by $\rho = \psi\psi^*$, the mass density is $\rho_m = m\rho$ and $S(\mathbf{x}, t)$ is a phase, that is related to the flow velocity $\mathbf{u}(\mathbf{x}, t)$ by

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{m}\nabla S. \tag{5.9}$$

Furthermore, the probability current $\mathbf{j}$ in standard QM in these variables is written as

$$\mathbf{j} = \rho \mathbf{u} = \frac{\hbar}{2mi} \left[\psi^* (\nabla \psi) - \psi \left(\nabla \psi^* \right) \right]. \tag{5.10}$$

Thus, we apply the Madelung transformation to the continuity equation and the Schrödinger equation, respectively, which yield

$$\partial_t \rho_m + \nabla \cdot (\rho_m \mathbf{u}) = 0, \tag{5.11}$$

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{m}\nabla(Q + V), \tag{5.12}$$

where V is the potential coming from the Schrödinger equation and Q denotes the Bohm quantum potential, also referred to as the quantum potential

$$Q = -\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}. \tag{5.13}$$

Note that the expressions (5.11) and (5.12) are the Madelung equations, which can describe the hydrodynamic representation of quantum mechanics due to eq.(5.12) being the Euler equation (5.2), which comes from the Navier-Stokes equation. Thus, using the Madelung transformation to the Schrödinger equation, it is possible to find a hydrodynamic representation given by a quantum Navier-Stokes equation.

The expressions obtained by the Madelung transformation applied to standard quantum mechanics are similar to the de Broglie-Bohm formulation [9–11], which is an alternative formulation and interpretation of quantum theory to the standard interpretation, or Copenhagen interpretation. The de Broglie-Bohm interpretation solves the measure or collapse problem in QM because it is a statistical proposal, and this interpretation is an example of hidden variables which can provide a deterministic description. In addition, this alternative formulation can be extended from quantum mechanics to quantum field theory.

5.3 Bosons in curved space-times

The hydrodynamic description for bosons in curved space-times coupled to an electromagnetic field is studied in [12, 104], where the KG equation in curved space-times is used as in Section 4.5. Thus,

$$\begin{aligned} \Box_{\mathrm{E}}\Phi - \frac{\mathrm{d}V}{\mathrm{d}\Phi^*} &= 0, \\ \nabla_\nu F^{\nu\mu} &= J^{E\mu}, \end{aligned} \tag{5.14}$$

where the D'Alembert operator is defined as $\Box_{\mathrm{E}} \equiv (\nabla^\mu + ieA^\mu)(\nabla_\mu + ieA_\mu)$, with e being the unit charge and A_μ denoting the gauge vector field corresponding to the Maxwell four-potential. The Faraday tensor describes the electromagnetism field as in (4.110), the potential $V(\Phi,\Phi^*)$ and the 4-current J^E_μ given by

$$V(\Phi,\Phi^*) = m^2|\Phi|^2 + \frac{\lambda}{2}|\Phi|^4, \tag{5.15}$$

$$J^E_\mu = i\frac{e}{2m^2}\left[\Phi\left(\nabla_\mu - ieA_\mu\right)\Phi^* - \Phi^*\left(\nabla_\mu + ieA_\mu\right)\Phi\right]. \tag{5.16}$$

The hydrodynamic representation is derived using the Madelung transformation as follows

$$\Phi(t,\mathbf{x}) = \sqrt{n}\exp(i\theta) = \sqrt{n}\exp\left[i\left(S - \omega_0 t\right)\right], \tag{5.17}$$

where the scalar field is decomposed into density $n(t,\mathbf{x}) = |\Phi(t,\mathbf{x})|^2$ and a phase $S(t,\mathbf{x})$. Applying this transformation into the KG equation, it is possible to get an imaginary and a real part, respectively, such as

$$\nabla_\mu \sqrt{n}\,(2\nabla^\mu \theta + eA^\mu) + e\nabla_\mu \left(A^\mu \sqrt{n}\right) + \sqrt{n}\Box\theta = 0, \tag{5.18}$$

$$\Box\sqrt{n} - \sqrt{n}\left[\nabla_\mu \theta\,(\nabla^\mu \theta + 2eA^\mu) + e^2 A^2 + m^2 + \lambda n\right] = 0, \tag{5.19}$$

where $A^2 = A^\mu A_\mu$, applying the Madelung transformation to (5.16) yields

$$J^E_\mu = \frac{ne}{m^2}\left(\nabla_\mu \theta + eA_\mu\right). \tag{5.20}$$

In terms of the current density, expressions (5.18) and (5.19) can be rewritten as

$$\nabla^\mu J^E_\mu = 0, \tag{5.21}$$

$$J^E{}_\mu J^{E\mu} + \frac{n^2 e^2}{m^4}\left(m^2 + \lambda n - \frac{\Box\sqrt{n}}{\sqrt{n}}\right) = 0. \tag{5.22}$$

The 4-velocity of an individual particle is defined as

$$m v_\mu = \nabla_\mu S + eA_\mu. \tag{5.23}$$

In terms of the four-velocity the continuity relation (5.21) and the quantum Hamilton-Jacobi equation (5.22) can be expressed as

$$\nabla^\mu (n v_\mu) - \frac{\omega_0}{m}\left(\nabla^0 n + n\Box t\right) = 0, \tag{5.24}$$

$$v_\mu v^\mu - \frac{2\omega_0}{m} v^0 - \frac{\omega_0^2}{m^2 N^2} + 1 + \frac{\lambda}{m^2} n - \frac{1}{m^2}\frac{\Box\sqrt{n}}{\sqrt{n}} = 0. \tag{5.25}$$

Applying the covariant derivative ∇_α to eq.(5.25) it is possible to obtain that

$$-\frac{\omega_0}{m}\nabla^0 v_\alpha + v_\mu \nabla^\mu v_\alpha = F^E_\alpha + F^G_\alpha + F^Q_\alpha + F^n_\alpha. \tag{5.26}$$

Note that eq.(5.26) is the Euler equation that describes the hydrodynamics of a boson gas, where the right hand of this equation is the balance of forces, which are defined as

$$F^E_\alpha = -\frac{e}{m}\left(v_\mu F_\alpha{}^\mu - \frac{\omega_0}{m} F^0_\alpha\right), \tag{5.27}$$

where F^E_α is the Lorentz force in covariant form in curved space-times. Furthermore, F^G_α is the gravitational force that measures the curvature associated with the gravitational strength quantified by the time-time component of the metric

$$F^G_\alpha = -2\nabla_\alpha U^G; \quad U^G = -\frac{\omega_0^2}{4N^2 m^2}, \tag{5.28}$$

and U^G is the gravitational potential contribution. Another force F^Q_α is given by the quantum four-potential U^Q in curved space-times, which is defined as

$$F^Q_\alpha = -\nabla_\alpha U^Q; \quad U^Q = -\frac{1}{2m^2}\frac{\Box\sqrt{n}}{\sqrt{n}}. \tag{5.29}$$

Finally, F^n_α is related to the self-interaction parameter

$$F^n_\alpha = -\nabla_\alpha h; \quad h = \frac{\lambda n}{2m^2}, \tag{5.30}$$

where h is the enthalpy. This description helps us to find the hydrodynamic representation of the fermion system in a curved space-time.

5.4 Fermions in curved space-times

It is convenient to rewrite the Dirac equation in curved space-times by applying the operator $i\gamma^\mu D_\mu = i\gamma^\mu \nabla_\mu - q\gamma^\mu A_\mu$ to the Dirac equation (4.97) written in the form $i\gamma^\mu \nabla_\mu \psi = q\gamma^\mu A_\mu \psi + m\psi$. Thus, it is possible to obtain the following

$$\Box_E \psi + m^2\psi + \frac{i}{2} q\gamma^\mu\gamma^\nu F_{\mu\nu}\psi + \gamma^\mu(\nabla_\mu \gamma^\nu)(D_\nu \psi) = 0. \tag{5.31}$$

Analogously to the hydrodynamic representation of the Schrödinger equation and of the KG equation in curved spacetimes, which was introduced using the Madelung transformation [7, 12], it is possible to derive the hydrodynamic representation of the Dirac equation [1]. Each component of the spinor $\psi = \psi(x^\mu)$ has the following form,

$$\psi = \exp(i\theta\mathbb{I})R, \tag{5.32}$$

where $\mathbb{I}$ is the identity matrix, R is a spinor and θ is a complex function. Observe that the spinor ψ has eight degrees of freedom, and the spinor $R\exp(i\theta\mathbb{I})$ has ten. A similar situation appeared for the boson case, where the scalar field $\Phi = \Psi\exp(i\theta)$ has two degrees of freedom and the right-hand side has three. This extra degree of freedom is interpreted as the velocity potential. Here we will have a similar situation. In what follows, the notation $\theta\mathbb{I} \to \theta$, unless specified, is used. For the case where a Dirac electron-like fermion is considered, we write the spinor ψ as

$$\psi = \begin{pmatrix} R_{\dot{1}} \\ R_{\dot{2}} \\ R_{\dot{3}} \\ R_{\dot{4}} \end{pmatrix} \exp(i\theta) = R\exp(i\theta), \tag{5.33}$$

where $\dot{\mu}$, $\dot{\nu}$, ...$= \dot{1}, \cdots, \dot{4}$ for the spinor indices such that

$$R = \begin{pmatrix} R_{\dot{1}} \\ R_{\dot{2}} \\ R_{\dot{3}} \\ R_{\dot{4}} \end{pmatrix} = \begin{pmatrix} \sqrt{n_{\dot{1}}} \\ \sqrt{n_{\dot{2}}} \\ \sqrt{n_{\dot{3}}} \\ \sqrt{n_{\dot{4}}} \end{pmatrix}. \tag{5.34}$$

Note that the covariant derivative of the spinor ψ in terms of its decomposition (5.33) is $\nabla_\mu(\psi_{\dot{\nu}}) = \partial_\mu(R_{\dot{\nu}}e^{i\theta}) + \Gamma^{\dot{\alpha}}_{\mu\dot{\nu}}(R_{\dot{\alpha}}e^{i\theta}) = (\partial_\mu R_{\dot{\nu}})e^{i\theta} + i(\partial_\mu\theta)R_{\dot{\nu}}e^{i\theta} + \Gamma^{\dot{\alpha}}_{\mu\dot{\nu}}(R_{\dot{\alpha}}e^{i\theta})$, which implies that $\nabla_\mu\theta = \partial_\mu\theta$.

As for the Klein-Gordon equation [12, 13, 104], we define the diagonal matrix four-velocity v_μ by

$$mv_\mu = \nabla_\mu S + qA_\mu\mathbb{I}. \tag{5.35}$$

Here, $S(x^\mu)$ is a phase with components $S = (\theta - \omega t)\mathbb{I}$, where ω are constants that can be related to the mass of the fermion particle by $\omega = mc^2/\hbar$. In this manner, we can write

$$\nabla_\mu\theta\mathbb{I} = mv_\mu - \omega\delta^0{}_\mu\mathbb{I} - qA_\mu\mathbb{I}. \tag{5.36}$$

We will interpret $n_{\dot{\nu}}$ as the number of fermion density and v_μ as its velocity. In what follows, the abbreviated notation $\omega \to \omega\mathbb{I}$ shall be utilized, unless.

According to [12, 13] if the transformation (5.32) into equation. (5.31), as in the KG equation, the continuity equation for the imaginary part and the Bernoulli equation for the real part could be obtained. However, in the case of the Dirac equation, the four components are mixed in the presence of the four-dimensional spinor ψ. Hence, it is possible to obtain the following expression

$$\begin{aligned} i\left[2(mv^\mu-\omega\delta^\mu_0)\nabla_\mu R - qA_\mu + q\nabla_\mu(A^\mu R) + \nabla_\mu(mv^\mu-\omega\delta^\mu_0 - qA^\mu)R\right] &+ \\ \left(m^2 v_\mu v^\mu + 2m\omega v^0 + \frac{\omega^2}{N^2} + m^2\right)R - \Box R &+ \\ \frac{i}{2}q\gamma^\mu\gamma^\nu F_{\mu\nu}R + \gamma^\mu(\nabla_\mu\gamma^\nu)(i(mv_\nu + \omega\nabla_\nu t)R + D_\nu R) &= 0, \end{aligned} \tag{5.37}$$

where $\Box = \nabla^\nu\nabla_\nu$. For bosons, the real and imaginary parts are separated into two independent equations, namely, the continuity equation and the Bernoulli equation [12, 13]. But in the spinor case, the last line of equation (5.37) mixes the imaginary and real parts, and there is no natural separation into real and imaginary parts. The system remains coupled.
On the other hand, in the Weyl representation the Madelung transformation is proposed as

$$\psi = \begin{pmatrix} \psi_R \\ \psi_L \end{pmatrix} = \begin{pmatrix} R_R \\ R_L \end{pmatrix} e^{i\theta}. \tag{5.38}$$

Since ψ_R and ψ_L are two spinors, R_R and R_L are two two-dimensional vectors. The Weyl representation of the adjoint spinor $\bar{\psi}$ when $B = b\tilde{\gamma}^0$ is

$$\bar{\psi} = b\left(\psi_R^\dagger, \psi_L^\dagger\right)\tilde{\gamma}^0 = \left(R_R^\dagger, R_L^\dagger\right)e^{-i\theta}, \tag{5.39}$$

where R_L and R_R are complex two spinors and θ is a complex function. Therefore, using the Madelung transformation (5.38) in the Weyl equations (4.125), they can be rewritten as

$$\begin{pmatrix} -\sigma^\mu\left(\bar{\nabla}_\mu\theta\right)R_R + i\sigma^\mu\left(\bar{\nabla}_\mu R_R\right) - q\sigma^\mu A_\mu R_R \\ -\bar{\sigma}^\mu\left(\nabla_\mu\theta\right)R_L + i\bar{\sigma}^\mu\left(\nabla_\mu R_L\right) - q\bar{\sigma}^\mu A_\mu R_L \end{pmatrix} = \begin{pmatrix} mR_L \\ mR_R \end{pmatrix}. \tag{5.40}$$

Furthermore, the Madelung transformation (5.38) and (5.39) can be applied to the current density (4.126). Thus obtaining

$$J^\mu = b\left(R_R^\dagger\bar{\sigma}^\mu R_R - R_L^\dagger\sigma^\mu R_L\right), \tag{5.41}$$

where each component reads

$$J^0 = Nb(R_R^\dagger R_R + R_L^\dagger R_L) = Nbn, \tag{5.42}$$

$$J^j = b\left(\hat{e}^j_3(n_{\dot{1}} - n_{\dot{2}} - n_{\dot{3}} + n_{\dot{4}}) + 2\hat{e}^j_1(\sqrt{n_{\dot{1}}n_{\dot{2}}} - \sqrt{n_{\dot{3}}n_{\dot{4}}}) + \hat{e}^j_i N^i n\right). \tag{5.43}$$

Note that the zero component, where $n = \sum_{\dot{\nu}=\dot{1}}^{\dot{4}} n_{\dot{\nu}}$ is the density number of fermions in the system, gives the number of both right and left-handed particles. It is possible to write the following expressions $|\psi_R|^2 = \psi_R^\dagger\psi_R = R_R^\dagger R_R = n_R$ and $|\psi_L|^2 = \psi_L^\dagger\psi_L = R_L^\dagger R_L = n_L$ for the right and left-handed spinors, as in the Dirac representation. Thus, n_R, n_L are the particle numbers of the right and left- hand and $n = n_R + n_L$ is the total density number.

Furthermore, using the Weyl representation, which has been discussed in this section, equation (5.37) becomes

$$\begin{aligned}
i\frac{m}{\sqrt{n_{\dot\nu}}}\left[-\frac{\omega}{m}\nabla_0 n_{\dot\nu} + \nabla_\mu(n_{\dot\nu}v^\mu) + \frac{\omega}{m}\Box t\right] & + \\
\sqrt{n_{\dot\nu}}\left[m^2 v_\mu v^\mu + 2m\omega v^0 + \frac{\omega^2}{N^2} + m^2 - \frac{\Box\sqrt{n_{\dot\nu}}}{\sqrt{n_{\dot\nu}}}\right] & + \\
(2NN^k F_{0k} + i\epsilon^{lj}{}_k \hat{F}_{lj}\tilde{\sigma}^k)R_R & + \\
-(\hat{\nabla}_a \hat{e}^\alpha_b)\bar{\mathbb{S}}^a\mathbb{S}^b((mv_\alpha - \omega\delta^0_\alpha)R_R + D_\alpha R_R) & = 0.
\end{aligned} \tag{5.44}$$

Note that expression (5.44) mixes the analogous eqs. (5.24) and (5.25), for the fermion case. The separation between the real and imaginary parts cannot be considered, because in the Madelung transformation (5.32), R and θ are assumed as complex parameters. Additionally, the first line of equation. (5.44) represents the hydrodynamic part of the fermionic fluid. The second line in eq. (5.44) is the Bernoulli equation. Then, the last lines of eq. (5.44) are the source of the fermionic fluid, something that is not present in the case of bosons. This is because the Dirac equation was introduced [105] to eliminate the negative probability problem of the KG equation. As a result, the Dirac equation involves only first derivatives while the KG equation is a second order equation.
From equation (5.44), it is possible to identify the different energy contributions to the Fermi gas, and obtain an energy balance equation for fermions analogous to the one obtained for bosons in [12, 13, 104]. To simplify notation, equation (5.44) can be rewritten in terms of the $\dot\nu$ coefficients with the understanding that the subindex R refers to each component $R = \dot{1}, \dot{2}$ individually. We get

$$\begin{aligned}
i\left[-\omega\nabla_0 \ln(n_{\dot\nu}) + \frac{m\nabla_\mu(n_{\dot\nu}v^\mu)}{n_{\dot\nu}} + \frac{\omega}{n_{\dot\nu}}\Box t\right] & + \\
2m^2\left(K + \frac{1}{m}\omega v^0 + \frac{1}{2}U^N + U^Q\right) + E + U^S & = 0.
\end{aligned} \tag{5.45}$$

The first line in eq. (5.45) describes the evolution of the free density of the fermions, while the contribution of the different energy terms appears in the second line. Its first term is the kinetic energy K defined as

$$K = \frac{1}{2}v_\mu v^\mu. \tag{5.46}$$

The lapse potential U^N is given by

$$U^N = \frac{\omega^2}{m^2}\frac{1}{N^2} + 1. \tag{5.47}$$

It represents the energy contribution due to the chosen lapse function N. The quantum potential U^Q is defined as

$$U^Q = -\frac{1}{2m^2}\frac{\Box\sqrt{n_{\dot\nu}}}{\sqrt{n_{\dot\nu}}}. \tag{5.48}$$

The contribution of the electromagnetic interaction E is given by

$$
\begin{aligned}
E &= (2NN^k F_{0k} + i\epsilon^{lj}{}_k \hat{F}_{lj}\tilde{\sigma}^k), \qquad (5.49)\\
&= 2N(F_{01}N^1 + F_{02}N^2 + F_{03}N^3) - e_{1\dot{\nu}}F_{13}\sqrt{\frac{n_{\ddot{\nu}}}{n_{\dot{\nu}}}} + i\left(e_{1\dot{\nu}}F_{12} + F_{23}\sqrt{\frac{n_{\ddot{\nu}}}{n_{\dot{\nu}}}}\right).
\end{aligned}
$$

It depends on the Faraday tensor, shift vector and lapse function that are related to the Pauli matrices. This relationship is due to the interaction between the electromagnetic field and the fermionic spin. Finally, the potential $U^S_{\dot{\nu}}$ describes the interaction between spin and the geometry of space-time. It is given by

$$
\begin{aligned}
U^S &= -\left((m\hat{v}_{Rd} - \omega_{\dot{\nu}}\hat{\delta}^0_d) + \frac{\hat{D}_\alpha\sqrt{n_{\dot{\nu}}}}{\sqrt{n_{\dot{\nu}}}}\right)\Gamma^d_{ba}\bar{\mathbb{S}}^a\mathbb{S}^b, \qquad (5.50)\\
&= \left[\Gamma^a_{11}(1-(N^1)^2) + \Gamma^a_{22}(1-(N^2)^2) + \Gamma^a_{33}(1-(N^3)^2)\right.\\
&+ \left. 2e_{2\dot{\nu}}(\Gamma^a_{31}N^1 + \Gamma^a_{32}N^2 + \Gamma^a_{30}) - \Gamma^a_{00}\right]\left((m\hat{v}_a - \omega\hat{\delta}^0_a) + \frac{\hat{D}_a\sqrt{n_{\ddot{\nu}}}}{\sqrt{n_{\dot{\nu}}}}\right)\\
&+ (-2e_{3\dot{\nu}}(\Gamma^a_{21}N^2 + \Gamma^a_{31}N^3 - \Gamma^a_{10}) + 2e_{1\dot{\nu}}\Gamma^a_{31})\left((m\hat{v}_a - \omega\hat{\delta}^0_a)\sqrt{\frac{n_{\ddot{\nu}}}{n_{\dot{\nu}}}} + \frac{\hat{D}_a\sqrt{n_{\ddot{\nu}}}}{\sqrt{n_{\dot{\nu}}}}\right)\\
&+ i\left[-2e_{1\dot{\nu}}\Gamma^a_{21}\left((m\hat{v}_a - \omega\hat{\delta}^0_a) + \frac{\hat{D}_a\sqrt{n_{\dot{\nu}}}}{\sqrt{n_{\dot{\nu}}}}\right)\right.\\
&- \left. 2(\Gamma^a_{21}N^1 - \Gamma^a_{32}N^3 + \Gamma^a_{20} + e_{2\dot{\nu}}\Gamma^a_{32})\left((m\hat{v}_a - \omega\hat{\delta}^0_a)\sqrt{\frac{n_{\ddot{\nu}}}{n_{\dot{\nu}}}} + \frac{\hat{D}_a\sqrt{n_{\ddot{\nu}}}}{\sqrt{n_{\dot{\nu}}}}\right)\right]. \qquad (5.51)
\end{aligned}
$$

Note that U^S disappears if we assume a flat space-time or if we consider particles without spin. Furthermore, U^S is constructed with the generalized gamma matrices (4.124), which are related to spin (Pauli matrices) and to space-time geometry (tetrads).

Spin is a fundamental outcome of the Dirac equation [105], which combines elements of special relativity and quantum mechanics. It was introduced to solve the problem of negative probability present in the KG equation, first proposed as a relativistic generalization of the Schrödinger equation. Here, we observe that the general relativistic Dirac equation involves an additional contribution due to geometry and spin through the generalized gamma and Pauli matrices. These terms arise from endowing a quantum field with curvature (geometry) given by a metric in General Relativity. Such a contribution is absent in flat space-time and in a system without spin, for example, a scalar field.

This hydrodynamic description is a general representation for an arbitrary geometry. To obtain a better physical interpretation, the strategy we should follow it to explore specific cases such as cosmological or black hole geometries as a fixed background. Taking into account the results obtained for each example, we can find a better understanding of the hydrodynamic representation of fermions in a curved space-time. As future work, some geometries and different representations of spinors can be considered following the formalism presented in this section. With this we can compare between the classical description and relativistic quantum particles in different geometries.

CHAPTER

SIX

LOOP QUANTUM COSMOLOGY

We refer to loop quantum cosmology (LQC) as a reduced-symmetry cosmological model in which analogous techniques developed for loop quantum gravity (LQG), a non-perturbative and background-independent approach. This formalism is based on general relativity (GR), which is our best theory of gravity today. However, this theory is not complete, it presents some conceptual and technical problems, such as the problem of time in quantum gravity and the reduction of degrees of freedom, where the symmetric sector of LQG can emerge.

In LQC the symmetric reduction starts from the classical description; in this case, it is considered an isotropic and homogeneous universe described by the FLRW metric and we can work with finite degrees of freedom. In fact, there is only one degree of freedom. The goal with this reduction is to apply and learn more about techniques and concepts of LQG in a simpler model. This so-called loop quantum cosmology is expected to be recovered in some limit from LQG. Thus, we could have corrections due to this.

In this chapter we recall the basic elements of LQC for spatially flat model to consider next an extension of it incorporating both Euclidean and Lorentzian terms with a relative weight in the Hamiltonian constraint. Its possible unitary evolution is addressed. Finally, the negatively and positively curved FLRW models are revisited.

6.1 Flat Universe

Isotropic and homogeneous models are studied in this section, and the simplest LQC model is a spatial flat universe. In this section, a brief review of the LQC models with zero curvature is presented. As a first step in the quantization of the model using Ashtekar-Barbero variables (Sec. 3.3 and Ref. [17–22], as well as [23–30]) we describe the volume representation. In loop quantization fluxes and holonomies are the fundamental variables, then these classical variables are promoted to quantum operators.

The Hamiltonian constraint in LQG is expressed by the extrinsic curvature K_a^i and the gravitational connection A_a^i, which appears through its curvature F_{ab}^i. Since the operator corresponding to c does not exist because the Stone-von Neumann theorem is not fulfilled, this operator is only well defined in holonomy terms. Thus, the curvatures and the constraint can then be expressed as holonomies. Therefore, in the $\bar{\mu}$-scheme, the holonomies (2.64) along the edges e_i^a starting from the base point of the elemental call $\mathcal{V}$ using the physical length $\sqrt{\Delta}$, which are given by

$$\begin{aligned} h_i^{(\bar{\mu})} &= \mathcal{P}\exp\left(\int_{e_i} A\right) = \mathcal{P}\exp\left(\int_0^{\bar{\mu}V_0^{1/3}} A_a^i \tau_i \dot{e}^a\right) = e^{\bar{\mu}c\tau_i} \\ &= \cos\left(\frac{\bar{\mu}c}{2}\right)\mathbb{I} + 2\sin\left(\frac{\bar{\mu}c}{2}\right)\tau_i = \cos\left(\frac{b}{2}\right)\mathbb{I} + 2\sin\left(\frac{b}{2}\right)\tau_i, \end{aligned} \tag{6.1}$$

where $\tau_j = -\frac{i}{2}\sigma_j$ with σ_j are the Pauli matrices, these holonomies take a simpler form without the path ordering due to the homogeneous symmetry of the cosmological model. In addition, we take into account the improved variables [27, 38] because in these variables there do not exist quantum effects at large scales, as we can observe. These variables are given by the conjugate pair (b, v) related by the following canonical expression

$$v = \frac{\mathrm{sgn}(p)|p|^{3/2}}{2\pi\gamma\ell_p^2\sqrt{\Delta}}, \qquad b = \bar{\mu}c, \tag{6.2}$$

where $\bar{\mu} = \sqrt{\Delta/|p|}$, ℓ_p is the Planck length ($\ell_p^2 = G\hbar$), the area gap is indicated by $\Delta = 4\sqrt{3}\pi\gamma G\hbar$, that is, the minimum nonzero eigenvalue of the area operator, and $\hbar$ is the reduced Planck constant; these variables obey the Poisson brackets.

$$\{b, v\} = \frac{2}{\hbar}. \tag{6.3}$$

Moreover, the inverse of the holonomy is given by

$$h_i^{(\bar{\mu})-1} = \cos\left(\frac{b}{2}\right)\mathbb{I} - 2\sin\left(\frac{b}{2}\right)\tau_i. \tag{6.4}$$

Previously to build the quantum description in LQC and to express the classical Hamiltonian constraint (2.55) as holonomies, we need to include the matter part in the Hamiltonian with a massless scalar field matter ϕ. The Hamiltonian part of the matter field is given by

$$H_\phi = \frac{p_\phi^2}{2|p|^{3/2}} = \frac{p_\phi^2}{2V} = \frac{p_\phi^2}{4\pi\gamma\ell_p^2\sqrt{\Delta}|v|}, \tag{6.5}$$

where p_ϕ denotes the momentum of ϕ. The matter field obeys the Poisson bracket as follows:

$$\{\phi, p_\phi\} = 1. \tag{6.6}$$

The equations of motion of the Hamiltonian part of matter are given by

$$\dot{p}_\phi = \{p_\phi, H_\phi\} = 0, \tag{6.7}$$

$$\dot{\phi} = \{\phi, H_\phi\} = \frac{p_\phi}{|p|^{3/2}}, \tag{6.8}$$

from the eq.(6.7) we have that $p_\phi = \text{cte}$. The inclusion of the scalar matter field is an important ingredient of the construction of the LQC model, due to the fact that this matter field works as the evolution parameter or internal time; this is because ϕ is a monotonic function, it plays an important role in the dynamics of the quantum evolution, as we will see. On the other hand, we can include an extra term in the Hamiltonian constraint that has a contribution of an explicit cosmological constant Λ, which is given by

$$H_\Lambda(N) = \frac{1}{16\pi G}\int_{\mathcal{V}} d^3x N\sqrt{q}\Lambda, \tag{6.9}$$

where the contribution in the full Hamiltonian constraint H of each term take the following form

$$H_F = H_g + H_\Lambda + H_\phi. \tag{6.10}$$

Therefore, the classical dynamical equation is given by the Hamiltonian constraint using the improved canonical pair for a model with arbitrary curvature k

$$H_F = -\frac{3\hbar|v|}{\gamma\sqrt{\Delta}}\left[b^2 + kV_0^{2/3}\left(\frac{\gamma^2\Delta}{16\pi G\hbar|v|}\right)^{2/3}\right] + \frac{p_\phi^2}{4\pi\gamma\ell_p^2\sqrt{\Delta}|v|}, \tag{6.11}$$

where the gravitational part of the Hamiltonian constraint H_g in Eq.(6.10) is given by

$$H_g = -\frac{3\hbar|v|}{\gamma\sqrt{\Delta}}\left[b^2 + kV_0^{2/3}\left(\frac{\gamma^2\Delta}{16\pi G\hbar|v|}\right)^{2/3}\right]. \tag{6.12}$$

Therefore, the full constraint in these variables for $N = 1$ and $k = 0$ is given by

$$p_\phi^2 - 3\pi G\hbar^2 b^2 v^2 + \frac{\pi\gamma^2\Delta G\hbar^2 v^2}{2}\Lambda \approx 0. \tag{6.13}$$

To introduce the quantum description of a cosmological model in LQC formalism. We need to define the kinematical Hilbert space for the gravitational and matter parts as $\mathcal{H}^{kin} = \mathcal{H}_g^{kin}\otimes\mathcal{H}_\phi$, where $\mathcal{H}_g^{kin} = L^2(\mathbb{R}_{\text{Bohr}}, \mathrm{d}\mu_{\text{Bohr}})$, being $\mathbb{R}_{\text{Bohr}}$ and $\mathrm{d}\mu_{\text{Bohr}}$ the Bohr compactification of the real line $\mathbb{R}$ and the Haar measure, respectively. In addition, $\mathcal{H}_\phi = L^2(\mathbb{R}, \mathrm{d}\phi)$ is the Hilbert space in the standard Schrödinger representation.
For the matter field, the elementary operators $\hat{\phi}$ and $\hat{p}_\phi$ act as follows over an arbitrary state

$$\hat{\phi}\psi(v,\phi) = \phi\psi(v,\phi), \tag{6.14}$$

$$\hat{p}_\phi\psi(v,\phi) = -i\hbar\frac{d}{d\phi}\psi(v,\phi). \tag{6.15}$$

Furthermore, for the gravitational part, the fundamental operators $\widehat{\mathcal{N}}_\mu = \widehat{e^{i\mu c/2}}$ and $\hat{v}$, in the v-representation, act on the basis $|v\rangle$ of $\mathcal{H}_g^{kin}$ as follows

$$\widehat{\mathcal{N}}_\mu |v\rangle = |v+\mu\rangle, \qquad \hat{v}|v\rangle = v|v\rangle, \tag{6.16}$$

as in the polymeric quantum mechanics, the action of the operator $\widehat{\mathcal{N}}$ is by translation and the operator $\hat{v}$ is diagonal. These operators obey the holonomy and flux algebra commutator (4.138)

$$\left[\hat{v}, \widehat{\mathcal{N}}_\mu\right] = -\mu\widehat{\mathcal{N}}_\mu. \tag{6.17}$$

Another important operator is the volume $\hat{V}$, which acts on this basis as

$$\hat{V}|v\rangle = 2\pi\gamma\ell_p^2\sqrt{\Delta}|v||v\rangle, \tag{6.18}$$

where γ is the Barbero-Immirzi parameter, $\ell_p = \sqrt{G\hbar}$ is the Planck length and the non-zero minimum eigenvalue of the area operator is denoted by $\Delta = 4\sqrt{3}\pi\gamma G\hbar$. It is also so-called gap of area [106–108].

To proceed with the quantum description of LQC it is needed to express the Hamiltonian constraint in terms of holonomies and fluxes; this procedure is based on [23–25, 27–30, 35, 38] using the Thiemann regularization [14]. For the case $k = 0$, we see that the Ashtekar-Barbero connection (2.45) is only $A_i^a = \gamma K_a^i$ due to $\Gamma_a^i = 0$ for a flat space. It is convenient to rewrite the Euclidean term (3.36) as

$$\begin{aligned} H_0^E &= \frac{1}{16\pi G}\int_{\mathcal{V}} \mathrm{d}^3x \frac{E_i^a E_j^b}{\sqrt{\det(q)}}\epsilon^{ij}{}_l{}^{(A)}F^l_{ab}, \\ &= \frac{1}{16\pi G}\int_{\mathcal{V}} \mathrm{d}^3x \frac{E_i^a E_j^b}{\sqrt{\det(q)}}\epsilon^{ij}{}_l{}^{(\gamma K)}F^l_{ab}, \\ &= \frac{1}{16\pi G}\int_{\mathcal{V}} \mathrm{d}^3x \frac{E_i^a E_j^b}{\sqrt{\det(q)}}\epsilon^{ij}{}_l\left[2\partial_{[a}\gamma K^l_{b]} + \epsilon^l{}_{nm}\gamma K_a^n\gamma K_b^m\right], \\ &= \frac{1}{16\pi G}\int_{\mathcal{V}} \mathrm{d}^3x \frac{E_i^a E_j^b}{\sqrt{\det(q)}}\epsilon^{ij}{}_l\epsilon^l{}_{nm}\gamma K_a^n\gamma K_b^m, \end{aligned} \tag{6.19}$$

where in the fourth line it is used the fact that the first term in the third line vanishes, due to an internal gauge fixing is employed. Moreover, we use the notation of a curvature ${}^{(X)}F^i_{ab}$ of the connection X as

$${}^{(X)}F^i_{ab} = 2\partial_{[a}X^i_{b]} + \epsilon^i{}_{nm}X_a^n X_b^m. \tag{6.20}$$

Here we need to consider the so-called Thiemann regularization [14], which is based on the identity

$$\frac{E_i^a E_j^b}{\sqrt{\det(q)}}\epsilon^{ij}_k = \frac{2}{\kappa\gamma}\tilde{\epsilon}^{abc}\left\{A_c^k, V\right\} = \frac{2}{\kappa\gamma}\tilde{\epsilon}^{abc}\left\{\gamma K_c^k, V\right\}, \tag{6.21}$$

where $\tilde{\epsilon}^{abc} = \sqrt{\det(q)}\epsilon^{abc}$ is the Levi-Civita density and $V = |p|^{3/2}$. Thus, the Hamiltonian term can be rewritten as

$$\begin{aligned} H_0^E &= \frac{1}{\kappa^2\gamma}\int_{\mathcal{V}} \mathrm{d}^3x\tilde{\epsilon}^{abc}\epsilon^n{}_{lm}\gamma K_a^l\gamma K_b^m\left\{\gamma K_c^n, V\right\}, \\ &= -\frac{4}{\kappa^2\gamma}\int_{\mathcal{V}} \mathrm{d}^3x\tilde{\epsilon}^{abc}\,\mathrm{Tr}\left(\gamma K_a\gamma K_b\left\{\gamma K_c, V\right\}\right). \end{aligned} \tag{6.22}$$

Here the identity $\mathrm{Tr}(\tau_i\tau_j\tau_k) = -\frac{1}{4}\epsilon_{ijk}$ was used. By continuing this regularization process, it is possible to express the extrinsic curvature in holonomy terms; the strategy is to take integrals along curves of the vector fields ${}^o e_i^a$ and ${}^o e_j^b$ that form closed loops $\Box_{ij}$. The curvature ${}^{(\gamma K)}F^i_{ab}$ can be recast as holonomies $h^{(\bar{\mu})}_{\Box_{ij}}$ of γK_a^i due to the fact that invariant vector fields on the left and right ${}^o e_i^a$ commute with each other. Note that for the (c, p) variables we have

$$c\tau_i = \lim_{\bar{\mu}\to 0}\frac{1}{2\bar{\mu}}\left[h_i^{(\bar{\mu})} - h_i^{(\bar{\mu})^{-1}}\right], \tag{6.23}$$

where the holonomies are defined as in (6.1). Thus, we can obtain the following expressions

$$\gamma K_a = \lim_{\bar{\mu}\to 0} \frac{h_i^{(\bar{\mu})} - h_i^{(\bar{\mu})-1}}{4\bar{\mu}V_o^{1/3}} {}^o\omega_a^i, \tag{6.24}$$

$$\{\gamma K_a, V\} = -\frac{1}{\bar{\mu}V_o^{1/3}} \sum_j h_j^{(\bar{\mu})} \left\{h_j^{(\bar{\mu})-1}, V\right\} {}^o\omega_a^j. \tag{6.25}$$

Note that the expressions that are valid in the limit when $\bar{\mu} \to 0$, are considered as regularized expressions in the $\bar{\mu}$-scheme, where the Euclidean term is written as the regularized Euclidean term $H_0^{E,\bar{\mu}}$

$$H_0^E = \lim_{\bar{\mu}\to 0} H_0^{E,\bar{\mu}}. \tag{6.26}$$

Therefore, the Euclidean contribution to the constraint is given by

$$H_0^{E,\bar{\mu}} = \frac{\mathrm{sgn}(p)}{4\kappa^2\gamma\bar{\mu}^3} \sum_{i,j,l} \epsilon^{ijk} \,\mathrm{Tr}\left[\left(h_i^{(\bar{\mu})} - h_i^{(\bar{\mu})-1}\right)\left(h_j^{(\bar{\mu})} - h_j^{(2\bar{\mu})-1}\right) h_l^{(\bar{\mu})} \left\{h_l^{(\bar{\mu})-1}, V\right\}\right], \tag{6.27}$$

here, the equality $\tau_i\tau_j = \frac{1}{2}\epsilon_{ijk}\tau^k - \frac{1}{4}\delta_{ij}$ has been applied. Analogously, as in LQG where both terms are independently quantized, the Lorentzian term can be expressed by holonomies using Thiemann regularization [14] for a cosmological model [27, 30, 38]. Thus, we use the classical identities

$$\begin{aligned} K_a^i\tau_i &= \frac{1}{\kappa\gamma}\left\{A_a^i\tau_i, K\right\}, \\ &= \frac{1}{\kappa\gamma}\left\{\gamma K_a^i\tau_i, K\right\}, \\ &= -\frac{2}{3\kappa\gamma}\frac{1}{\bar{\mu}V_o^{1/3}} \sum_i h_i^{(\bar{\mu})} \left\{h_i^{(\bar{\mu})-1}, K\right\} {}^o\omega_a^i, \end{aligned} \tag{6.28}$$

where the integrated densitized trace of the extrinsic curvature K is defined as

$$K = \int \mathrm{d}^3x K_a^i E_i^a, \tag{6.29}$$

for the symmetry-reduced model in cosmology. As noticed in [27], the following relation holds

$$\{c\tau_i, K\} = -\frac{2}{3\bar{\mu}} h_i^{(\bar{\mu})} \left\{h_i^{(\bar{\mu})-1}, K\right\}. \tag{6.30}$$

This equation is valid only in a scheme where $\bar{\mu}$ is a function of p, but it is not valid when $\bar{\mu}$ is a constant. We use the expressions as in the full theory, to get

$$\begin{aligned} K &= \frac{1}{\gamma^2}\left\{{}^{(A)}H_0^E, V\right\} = \frac{1}{\gamma^2}\left\{{}^{(\gamma K)}H_0^E, V\right\}, \\ &= \frac{1}{\gamma^2}\left\{H_0^E, V\right\}, \end{aligned} \tag{6.31}$$

where, making an analogy with the notation as in (6.20) but now for the Euclidean term of a connection X, we have

$$^{(X)}H^{\mathrm{E}} = \frac{1}{16\pi G}\int_{\mathcal{V}} \mathrm{d}^3x \frac{E^a_i E^b_j}{\sqrt{\det(q)}}\epsilon^{ij}{}_l{}^{(X)}F^l_{ab}. \tag{6.32}$$

Thus, we can rewrite the Lorentzian term (3.37) as follows

$$\begin{aligned} H_0^L &= \frac{1}{16\pi G}\int_{\mathcal{V}} \mathrm{d}^3x \frac{E^a_i E^b_j}{\sqrt{\det(q)}} K^i_{[a}K^j_{b]}, \\ &= \frac{1}{32\pi G}\int_{\mathcal{V}} \mathrm{d}^3x \frac{E^a_i E^b_j}{\sqrt{\det(q)}} \epsilon^{ij}{}_n \epsilon^n{}_{lm} K^l_a K^m_b, \\ &= -\frac{2}{\kappa^2\gamma}\int_{\mathcal{V}} \mathrm{d}^3x \tilde{\epsilon}^{abc}\,\mathrm{Tr}\left(K_a K_b \left\{\gamma K_c, V\right\}\right). \end{aligned} \tag{6.33}$$

The Lorentzian part of the constraint thus takes the form

$$\begin{aligned} H_0^{L,\bar{\mu}} =& \frac{8\,\mathrm{sgn}(p)}{9\kappa^4\gamma^7\bar{\mu}^3}\sum_{i,j,k}\epsilon^{ijk}\,\mathrm{Tr}\left(h_i^{(\bar{\mu})}\left\{h_i^{(\bar{\mu})^{-1}}, \left\{H^{E,\bar{\mu}}(1), V\right\}\right\}\right. \\ & \left.\times h_j^{(\bar{\mu})}\left\{h_j^{(\bar{\mu})^{-1}}, \left\{H^{E,\bar{\mu}}, V\right\}\right\} h_k^{(\bar{\mu})}\left\{h_k^{(\bar{\mu})^{-1}}, V\right\}\right), \end{aligned} \tag{6.34}$$

that is connected with the local form as follows

$$H_0^L = \lim_{\bar{\mu}\to 0} H_0^{L,\bar{\mu}}. \tag{6.35}$$

Therefore, the regularized Hamiltonian constraint $H_g^{\bar{\mu}}$ is written as

$$H_g^{\bar{\mu}} = H_0^{E,\bar{\mu}} - 2\left(1+\gamma^2\right) H_0^{L,\bar{\mu}}. \tag{6.36}$$

Now, we restrict ourselves to the case of a flat universe. Then, we can promote this regularized gravitational constraint to an operator using Dirac quantization, where we can replace classical variables C, D by quantum operators $\hat{C}, \hat{D}$ in the following form $\widehat{\{C, D\}} \to (i\hbar)^{-1}[\hat{C}, \hat{D}]$. The Euclidean operator reads

$$\begin{aligned} \hat{H}_0^E &= -\frac{i\hbar\gamma}{4\sqrt{\Delta}}\widehat{\sin(b)}\left(\hat{v}\sum_j \mathrm{Tr}\left(\tau_j \widehat{h_j^{(\bar{\mu})}}\left[\widehat{h_j^{(\bar{\mu})-1}}, |\hat{v}|\right]\right)\right)\widehat{\sin(b)}, \\ &= -\frac{i3\hbar\gamma}{4\sqrt{\Delta}}\widehat{\sin(b)}\left(\hat{v}\hat{A}_{|\hat{v}|}\right)\widehat{\sin(b)}, \end{aligned} \tag{6.37}$$

where the identities $\tau_j\tau_j = -\frac{1}{4}\mathbb{I}$, $\sum_j \mathrm{Tr}\left(\tau_j\tau_j\right) = -\frac{3}{2}$ and $\mathrm{Tr}\left(\tau_j\right) = 0$ were used. Furthermore, the Lorentzian operator is given by

$$\begin{aligned} \hat{H}_0^L =& -\frac{i\sqrt{\Delta}}{288\hbar\gamma^3}\sum_{i,j,k}\epsilon^{ijk}\,\mathrm{Tr}\left(\widehat{h_i^{(\bar{\mu})}}\left[\widehat{h_i^{(\bar{\mu})-1}}, \left[\hat{H}_0^E, |\hat{v}|\right]\right]\widehat{\hat{v}h_j^{(\bar{\mu})}}\right. \\ & \left.\times\left[\widehat{h_j^{(\hat{\bar{\mu}})-1}}, |\hat{v}|\right]\widehat{h_k^{(\bar{\mu})}}\left[\widehat{h_k^{(\bar{\mu})-1}}, \left[\hat{H}_0^E, |\hat{v}|\right]\right]\right), \\ =& -\frac{i\sqrt{\Delta}}{24\hbar\gamma^3}\hat{A}_{[\hat{H}_0^L, |\hat{v}|]}\left(\hat{v}\hat{A}_{|\hat{v}|}\right)\hat{A}_{[\hat{H}_0^E, |\hat{v}|]}. \end{aligned} \tag{6.38}$$

To get this expression we used the following $\sum_{ijk}\epsilon^{ijk}=0$, $\sum_{ijk}\epsilon^{ijk}\,\mathrm{Tr}\,(\tau_k)=0$, and $\sum_{ijk}\epsilon^{ijk}\,\mathrm{Tr}\,(\tau_i\tau_j)=-\frac{1}{2}\sum_{ijk}\epsilon^{ijk}\delta_{ij}=0$, also the identity $\sum_{i,j,k}\epsilon^{ijk}\,\mathrm{Tr}\,(\tau_i\tau_j\tau_k)=-\frac{1}{4}\sum_{i,j,k}\epsilon^{ijk}\epsilon_{ijk}=-\frac{3}{2}$. Furthermore, the operator $\hat{A}_{\hat{B}}$ is defined as

$$\hat{A}_{\hat{B}}=\widehat{\sin(b/2)}\hat{B}\widehat{\cos(b/2)}-\widehat{\cos(b/2)}\hat{B}\widehat{\sin(b/2)}, \tag{6.39}$$

for a given operator $\hat{B}$. The Euclidean and Lorentzian operators act on the basis $|v\rangle$ of the gravitational Hilbert space $\mathcal{H}_g^{kin}$. Thus, in the v-representation, we have

$$\hat{H}_0^E|v\rangle=f_+(v)|v+4\rangle+f_0(v)|v\rangle+f_-(v)|v-4\rangle, \tag{6.40}$$

$$\hat{H}_0^L|v\rangle=g_+(v)|v+8\rangle+g_0(v)|v\rangle+g_-(v)|v-8\rangle, \tag{6.41}$$

where the definition of the functions $f_*(v)$, with $*=-,0,+$, are [24, 27–29, 38]

$$f_+(v)=\frac{3\gamma\hbar}{32\sqrt{\Delta}}(v+2)M_v(1,3), \tag{6.42}$$

$$f_-(v)=f_+(v-4), \tag{6.43}$$

$$f_0(v)=-f_+(v)-f_-(v), \tag{6.44}$$

$$M_v(a,b)=|v+a|-|v+b|. \tag{6.45}$$

Moreover, the functions $g_*(v)$, for $*=-,0,+$ are given by

$$g_+(v)=-\frac{\sqrt{\Delta}}{192\gamma^3\hbar}(v+4)M_{v+4}(-1,1)G_-(v+4)G_+(v+4), \tag{6.46}$$

$$g_-(v)=g_+(v-8), \tag{6.47}$$

$$g_0(v)=-\frac{\sqrt{\Delta}}{192\gamma^3\hbar}\left\{(v+4)M_{v+4}(-1,1)\left[G_+(v)\right]^2\right. \tag{6.48}$$

$$\left.+(v-4)M_{v-4}(-1,1)\left[G_-(v)\right]^2\right\}, \tag{6.49}$$

where

$$G_\pm(v)=f_\pm(v-1)M_{v-1}(0,\pm4)-f_\pm(v+1)M_{v+1}(0,\pm4). \tag{6.50}$$

Furthermore, the Hamiltonian constraint for a matter field H_ϕ is promoted to a quantum operator as

$$\hat{H}_\phi=\frac{1}{2}\widehat{|p|^{-3/2}}\widehat{p_\phi^2}. \tag{6.51}$$

This operator acts on states $|v,\phi\rangle=|v\rangle\otimes|\phi\rangle$ belonging to the total Hilbert space $\mathcal{H}^{kin}=\mathcal{H}_g^{kin}\otimes\mathcal{H}_\phi^{kin}$. Therefore,

$$\hat{H}_\phi\psi(v,\phi)=-\frac{\hbar^2}{4\pi\gamma\sqrt{\Delta}\ell_{\mathrm{p}}^2}B(v)\partial_\phi^2\psi(v,\phi), \tag{6.52}$$

where $\psi(v,\phi)=\langle v,\phi|\psi\rangle$ and the function $B(v)$ is defined as [24]

$$B(v)=\left(\frac{3}{2}\right)^3|v|\left||v+1|^{1/3}-|v-1|^{1/3}\right|^3. \tag{6.53}$$

On the other hand, the Hamiltonian part associated with the cosmological constant H_Λ is promoted to quantum operator by

$$\hat{H}_\Lambda = \frac{\Lambda}{8\pi G}\hat{V}. \tag{6.54}$$

The total Hamiltonian operator $\hat{H}_F$ coming from Eq. (6.10) becomes

$$\hat{H}_F\psi(v,\phi) = \left(\hat{H}_g + \hat{H}_\Lambda + \hat{H}_\phi\right)\psi(v,\phi), \tag{6.55}$$

where the gravitational one includes Euclidean and Lorentzian parts; for $k=0$ we have $\hat{H}_g = \hat{H}_0^E - 2(1+\gamma^2)\hat{H}_0^L$. The evolution of the quantum system is obtained by the internal time, which is given by the scalar field ϕ. This fact is relevant for obtaining the dynamical description in the next section.
As we can see, the expressions of the operators in LQC can be obtained from the classical constraint by the holonomy and flux terms. However, these quantum operators are described by functions with absolute values, and note that the eq.(6.55) is not easy to deal with. We can take some simplifying assumptions given in [25] to get a tractable form by eliminating the absolute values. The model obtained under these assumptions is simpler and solvable; then, the model is denoted by sLQC. Thus, the total Hamiltonian operator $\hat{\Theta}_F$ can be written as

$$\hat{\Theta}_F = \mathbb{I}\otimes\partial_\phi^2 + \hat{\Theta}_g\otimes\mathbb{I}, \qquad \hat{\Theta}_g = \hat{\Theta}_0 - \pi G\gamma^2\Delta\Lambda v^2, \tag{6.56}$$

where the flat Hamiltonian operator $\hat{\Theta}_0$ in this sLQC model, which includes both the Euclidean and Lorentzian terms takes the form

$$\begin{aligned}\hat{\Theta}_0\psi(v) = \frac{3\pi G\gamma^2}{4}\Big[&\xi\tilde{f}_8(v)\psi(v+8) - \tilde{f}_4(v)\psi(v+4) - 2(\xi-1)\tilde{f}_0(v)\psi(v)\\ &- \tilde{f}_{-4}(v)\psi(v-4) + \xi\tilde{f}_{-8}(v)\psi(v-8)\Big],\end{aligned} \tag{6.57}$$

with functions $\tilde{f}_a(v) = \sqrt{|v(v+a)|}|v+a/2|$ and $\xi = (1+\gamma^2)/(4\gamma^2)$, being a an integer. The inner product in the representation v is defined as a sum in the selected superselection sector of sets $\mathcal{L}_4$, in which the gravitational Hilbert space is divided, these lattices $\mathcal{L}_\varepsilon = \varepsilon + 4\mathbb{Z}$, with $\varepsilon \in (0,4]$ are preserved by the action of $\hat{\Theta}_0$

$$\langle\psi \mid \psi'\rangle = \sum_{v\in\mathcal{L}_4}\bar{\psi}(v)\psi'(v). \tag{6.58}$$

Fixing a superselected sector the domain of definiteness of the gravitational operator is

$$D(\hat{\Theta}_0) = \left\{|\psi\rangle \in \mathcal{H}_g^{kin}; |\psi\rangle = \sum_{n=1}^{N} c_n|4n\rangle, c_n\in\mathbb{C}, N\in\mathbb{N}\right\}. \tag{6.59}$$

The difficulty in working with the Hamiltonian operator $\hat{\Theta}_F$ in the representation v comes from the fact that it produces a difference equation. The theory to solve this kind of equations is not as standard as that for differential equations. There exist well-established methods for solving difference equations with constant coefficients. Nevertheless, for variable coefficients the difficulty increases. Some papers [109, 110] propose a method to solve analytically this problem by a factorization method,

but this is not always possible in practice.
In LQC, various representations have been used depending on the problem to solve: for the v-representation there exist some numerical methods that have been applied [28, 29, 32, 111], but our work focus on (semi)-analytical methods, where another more convenient representation is introduced.
Since the conjugated momentum variable b is a compact variable with domain in a circle of radius 1/2, in b-representation, one takes a difference equation into a second order differential equation by Fourier transformation

$$\tilde{\psi}(b) = [\mathcal{F}\psi](b) = \sum_{v\in\mathcal{L}_4} \frac{1}{\sqrt{|v|}}\psi(v)e^{ivb/2}. \tag{6.60}$$

The inverse Fourier transformation is given by

$$\psi(v) = [\mathcal{F}^{-1}\tilde{\psi}](b) = \frac{\sqrt{|v|}}{\pi}\int_0^\pi db\tilde{\psi}(b)e^{-ivb/2}, \tag{6.61}$$

the parity reflection symmetry in the v-representation becomes in b-representation $\tilde{\psi}(b) = \tilde{\psi}(\pi - b)$. This transformation in b is periodic with a period of π, where $b \in [0, \pi]$, and we have $[\mathcal{F}\psi](0) = [\mathcal{F}\psi](\pi)$. In the b-representation, the fundamental operators act on the b-states as

$$\hat{v}\,|b\rangle = 2i\partial_b\,|b\rangle\,, \quad \text{and} \quad \hat{\mathcal{N}}_\mu\,|b\rangle = e^{-i\mu b/2}\,|b\rangle\,. \tag{6.62}$$

Therefore, the flat gravitational Hamiltonian operator $\hat{\Theta}_g$ in the momentum representation has a differential form that includes both the Euclidean, Lorentzian, and the cosmological constant part given by

$$\hat{\Theta}_g\tilde{\psi}(b) = 12\pi G\gamma^2\left[(\sin(b)\partial_b)^2 - \xi(\sin(2b)\partial_b)^2 + \frac{b_\Lambda^2}{\gamma^2}\partial_b^2\right]\tilde{\psi}(b), \tag{6.63}$$

where $b_\Lambda = \gamma\sqrt{\Delta\Lambda/3} = \sqrt{\Lambda/\Lambda_c}$ and the critical cosmological constant is defined as $\Lambda_c = 3/(\Delta\gamma^2)$. This critical cosmological constant will play an important role in the unitary evolution of the model, as we will see in the following sections.

6.1.1 Effective models

Once the quantum description is built in the LQC context, it is possible to find an effective model defined in the classical phase space but incorporating quantum corrections. In LQC different strategies have been taken to find these effective models ranging from heuristic to expectation values, and path integral methods.
In the heuristic strategy [28, 29], $\hat{C} \to C_{\text{eff}}^{\text{heu}}$, the operators are replaced as $\hat{p}_\phi \to p_\phi$, $\hat{\mathcal{N}} \to \mathcal{N} = e^{ib/2}$ and $\hat{V} \to V$, where the quantities without hat are effective classical quantities, which commute. In this way, for instance, (6.55) takes the form

$$C_{\text{eff}}^{\text{heu}} = \frac{p_\phi^2}{2V} - \frac{3}{8\pi G\Delta\gamma^2}V\left[\sin^2(b)\left(1 - \left(1+\gamma^2\right)\sin^2(b)\right) + b_\Lambda^2\right]. \tag{6.64}$$

Alternatively an effective constraint can be obtained from the expectation value of the Hamiltonian operator (6.55) [27, 30, 38]. Here the expectation value uses

Gaussian states peaked at a point $(b_0, v_0, \phi_0, p_\phi)$ of the gravitational classical phase space and the semi-classical state of matter part, which are

$$(\Psi_{(b_o,v_o)}| = \sum_{v\in\mathbb{R}} e^{-\left[\frac{1}{2d^2}(v-v_o)^2\right]} e^{ib_o(v-v_o)}(v\,|, \tag{6.65}$$

$$(\Psi_{(\phi_0,p_\phi)}| = \int \mathrm{d}\phi e^{-\left[\frac{1}{2\sigma^2}(\phi-\phi_0)^2\right]} e^{ip_\phi(\phi-\phi_0)/\hbar}(\phi|, \tag{6.66}$$

where d and σ are the widths of the coherent state. The total semi-classical state is then $(\Psi_{(b_0,v_0,\phi_0,p_\phi)}| = (\Psi_{(b_o,v_o)}| \otimes (\Psi_{(\phi_0,p_\phi)}|$. However, for the calculations the "shadow" of the semi-classical state $(\Psi_{(b_0,v_0)}|$ is used on a regular lattice with spacing one reads by

$$\begin{aligned}|\Psi\rangle &= \int \mathrm{d}\phi \sum_{n\in\mathbb{Z}} e^{-\frac{\epsilon^2}{2}(n-v_o)^2} e^{-\mathrm{i}b_o(n-v_o)} e^{-\frac{\sigma^2}{2}(\phi-\phi_o)^2} e^{-\frac{\mathrm{i}}{\hbar}p_\phi(\phi-\phi_o)}|n\rangle\otimes|\phi\rangle \\ &\equiv |\Psi_g\rangle\otimes|\Psi_\phi\rangle\,,\end{aligned} \tag{6.67}$$

where $\epsilon = 1/d$ and fixing $v_0 = N \in \mathbb{Z}$. Assuming large volumes and late times, the relative quantum fluctuations in the volume of the universe must be very small, since it is considered a large quantity and late time, where there exist some restrictions such as $1/N << \epsilon << 1$ and $b_0 << 1$. Hence, we can calculate the expectation value of the Euclidean and Lorentzian operators using these gaussian states. We have

$$\begin{aligned}H^E_{0,\text{eff}} = \left\langle \hat{H}^E_0 \right\rangle &= \frac{3\hbar\gamma v}{4\sqrt{\Delta}}\left[\sin^2(b) + O\left(\epsilon^2\right)\right] \\ &\times\left[1 + O\left(e^{-\frac{\pi^2}{\epsilon^2}}\right) + O\left(\frac{1}{(v\epsilon)^2}\right)\right],\end{aligned} \tag{6.68}$$

$$\begin{aligned}H^L_{0,\text{eff}} = \left\langle \hat{H}^L_0 \right\rangle &= \frac{3\hbar v}{32\gamma\sqrt{\Delta}}\left[\sin^2(2b) + O\left(\epsilon^2\right)\right] \\ &\times\left[1 + O\left(e^{-\frac{\pi^2}{\epsilon^2}}\right) + O\left(\frac{1}{(v\epsilon)^2}\right)\right].\end{aligned} \tag{6.69}$$

Thus, the total effective Hamiltonian constraint $C^{\text{ev}}_{\text{eff}} = \left\langle \hat{H}_F \right\rangle$ using the expectation value reads

$$C^{\text{ev}}_{\text{eff}} = \frac{p_\phi^2}{4\pi\gamma G\hbar\sqrt{\Delta}v} - \frac{3\hbar v}{4\gamma\sqrt{\Delta}}\left[\sin^2(b)\left[1 - \left(1+\gamma^2\right)\sin^2(b)\right] + b_\Lambda^2\right], \tag{6.70}$$

where $V = 2\pi\gamma G\hbar\sqrt{\Delta}v$ is the classical physical volume. Therefore, the effective constraints (6.64) and (6.70) are consistent with each other.
Finally one can obtain the effective constraint using path integral [99–101, 111–113]. Using the group averaging, it is possible to obtain the physical states as

$$\psi_f(v,\phi) = \lim_{\alpha_0\to\infty}\int_{-\alpha_0}^{\alpha_0} \mathrm{d}\alpha e^{i\hat{\Theta}_F} f(v,\phi), \tag{6.71}$$

where $f(v,\phi)$ belongs to the Hilbert space $\mathcal{H}^{kin}$. The transition amplitude in the timeless framework between initial and final states, which is given by using the physical inner product as

$$A_{tls}(v_f,\phi_f|v_i,\phi_i) = \langle v_f,\phi_f|v_i,\phi_i\rangle_{phy} = \lim_{\alpha_0\to\infty}\int_{-\alpha_0}^{\alpha_0}\mathrm{d}\alpha\,\langle v_f,\phi_f|\,e^{i\alpha\hat{\Theta}_F}\,|v_i,\phi_i\rangle\,, \tag{6.72}$$

where $|v_i, \phi_i\rangle$ and $|v_f, \phi_f\rangle$ are the eigenstates in $\mathcal{H}^{kin}$. In addition, the physical inner product between two states is defined as

$$\langle f|g\rangle_{phy} = \langle \psi_f|g\rangle = \lim_{\alpha_0\to\infty}\int_{-\alpha_0}^{\alpha_0} \mathrm{d}\alpha \, \langle f| e^{i\alpha\hat{\Theta}_F} |g\rangle \, . \tag{6.73}$$

Furthermore, Equation (6.56) is written as the Klein-Gordon equation

$$\partial_\phi^2 \psi(v,\phi) + \hat{\Theta}_g \psi(v,\phi) = 0, \tag{6.74}$$

which suggests that ϕ can be used as an internal time. To implement path integration let us divide the exponential into identical pieces N in the equation (6.72) and the completeness of the basis [111–113]. Therefore, we take $\tilde{\alpha}_n = \epsilon\alpha_n$ where $\epsilon = 1/N$

$$\begin{aligned} A_{tls}(v_f,\phi_f|v_i,\phi_i) = & \lim_{\alpha_{N_0},\ldots,\alpha_{1_0}\to\infty} \frac{1}{2\alpha_{N_0}} \int_{-\alpha_{N_0}}^{\alpha_{N_0}} \mathrm{d}\alpha_N \ldots \frac{1}{2\alpha_{2_0}} \int_{-\alpha_{2_0}}^{\alpha_{2_0}} \mathrm{d}\alpha_2 \\ & \times\epsilon \int_{-\alpha_{1_0}}^{\alpha_{1_0}} \mathrm{d}\alpha_1 \, \langle v_f,\phi_f| \exp\left(i\sum_{n=1}^{N} \epsilon\alpha_n \hat{\Theta}\right) |v_i,\phi_i\rangle \, . \end{aligned} \tag{6.75}$$

The completeness relation in $\mathcal{H}^{kin}$ is given by

$$\mathbb{I}_{kin} = \mathbb{I}_{kin}^{g} \otimes \mathbb{I}_{kin}^{\phi} = \sum_v |v\rangle\langle v| \int \mathrm{d}\phi \, |\phi\rangle\langle\phi| \, . \tag{6.76}$$

It is convenient to set $v_f = v_N$, $\phi_f = \phi_N$, $v_i = v_0$, and $\phi_i = \phi_0$. The quantum constraint $\hat{\Theta}_F$ can be separated into a gravitational part and a matter part. Thus, it is possible to calculate the exponential separately. Hence, the matter part is given by

$$\begin{aligned} \langle\phi_n| \exp\left(i\epsilon\alpha_n \frac{\hat{p}_\phi^2}{\hbar^2}\right) |\alpha_{n-1}\rangle = & \int \mathrm{d}p_{\phi_n} \, \langle\alpha_n|p_{\alpha_n}\rangle \langle p_{\phi_n}| \exp\left(i\epsilon\alpha_n \frac{\hat{p}_\phi^2}{\hbar^2}\right) |\alpha_{n-1}\rangle \\ = \frac{1}{2\pi\hbar} & \int \mathrm{d}p_{\phi_n} \exp\left[i\epsilon\left(\frac{p_{\phi_n}}{\hbar}\frac{\phi_n - \phi_{n-1}}{\epsilon} + \alpha_n \frac{p_{\phi_n}^2}{\hbar^2}\right)\right]. \end{aligned} \tag{6.77}$$

On the other hand, in the limit $N \to \infty (\epsilon \to 0)$ for the gravitational part, the operator $e^{i\epsilon\alpha_n\hat{\Theta}_g}$ can be expressed as an expansion in series, where in the first order it is obtained

$$\langle v_n| e^{i\epsilon\alpha_n\hat{\Theta}_g} |v_{n-1}\rangle = \delta_{v_n,v_{n-1}} - i\epsilon\alpha_n \langle v_n| \hat{\Theta}_g |v_{n-1}\rangle + \mathcal{O}(\epsilon^2). \tag{6.78}$$

To calculate the matrix elements, one uses the expression (6.56) to get

$$\begin{aligned} \langle v_n| \hat{\Theta}_g |v_{n-1}\rangle = & \frac{3\pi G\gamma^2}{4}\left[\sqrt{v_n v_{n-1}} \frac{v_n + v_{n-1}}{2} (\delta_{v_n,v_{n-1}+4} - 2\delta_{v_n,v_{n-1}} - \delta_{v_n,v_{n-1}-4})\right] \\ & - \frac{3\pi G(1+\gamma^2)}{16}\left[\sqrt{v_n v_{n-1}} \frac{v_n + v_{n-1}}{2} (\delta_{v_n,v_{n-1}+8} - 2\delta_{v_n,v_{n-1}} - \delta_{v_n,v_{n-1}-8})\right] \\ & - 3\pi G b_\Lambda^2 \sqrt{v_n v_{n-1}} \frac{v_n + v_{n-1}}{2} \delta_{v_n,v_{n-1}}. \end{aligned} \tag{6.79}$$

Next, taking into account the identity

$$\delta_{v_n,v_m} = \frac{1}{\pi}\int_0^{\pi} \mathrm{d}b_n e^{-ib_n(v_n-v_m)}, \tag{6.80}$$

from the eqs.(6.79), (6.78) and (6.80) it is possible to get

$$\begin{aligned}\langle v_n| e^{i\epsilon\alpha_n\hat{\Theta}_g} |v_{n-1}\rangle &= \frac{1}{\pi}\int_0^{\pi} \mathrm{d}b_n e^{-ib_n(v_n-v_{n-1})}\\ \times &\left[1 - i\epsilon\alpha_n(3\pi G)\sqrt{v_n v_{n-1}}\frac{v_n+v_{n-1}}{2}\left[\sin^2(b_n)[1-(1+\gamma^2)\sin^2(b_n)]\right.\right.\\ + &\left.\left. 4b_\Lambda^2\right]\right] + \mathcal{O}(\epsilon^2).\end{aligned} \tag{6.81}$$

Using Equations (6.77) and (6.81) in the transition amplitude yields

$$\begin{aligned}A^F_{tls}(v_f,\phi_f|v_i,\phi_i) &= \lim_{N\to\infty}\lim_{\alpha_{N_0},\ldots,\alpha_{1_0}\to\infty}\left(\epsilon\prod_{n=2}^{N}\frac{1}{2\alpha_{n_0}}\right)\int_{-\alpha_{N_0}}^{\alpha_{N_0}}\mathrm{d}\alpha_N\ldots\int_{-\alpha_{1_0}}^{\alpha_{1_0}}\mathrm{d}\alpha_1\\ \times\int_{\infty}^{\infty}\mathrm{d}\phi_{N-1}\ldots\mathrm{d}\phi_1&\left(\frac{1}{2\pi\hbar}\right)^N\int_{\infty}^{\infty}\mathrm{d}p_{\phi_{N-1}}\ldots\mathrm{d}p_{\phi_1}\sum_{v_{N-1},\ldots,v_1}\left(\frac{1}{\pi}\right)^N\int_0^{\pi}\mathrm{d}b_N\ldots\mathrm{d}b_1\\ &\times\prod_{n=1}^{N}\exp i\epsilon\left[\frac{p_{\phi_n}}{\hbar}\frac{\phi_n-\phi_{n-1}}{\epsilon} - b_n\frac{v_n-v_{n-1}}{\epsilon}\right.\\ +\alpha_n\left(\frac{p^2_{\phi_n}}{\hbar^2} - 3\pi G\sqrt{v_n v_{n-1}}\right.&\left.\left.\frac{v_n+v_{n-1}}{2}(\sin^2(b_n)[1-(1+\gamma^2)\sin^2(b_n)]+b_\Lambda^2)\right)\right].\end{aligned} \tag{6.82}$$

Furthermore, use will be made of replacement $\sum_{n=1}^{N}\epsilon$ by $\int_0^1\mathrm{d}\tau$. Thus, in the path-integral formulation, we can rewrite this expression as follows

$$\begin{aligned}A^F_{tls}(v_f,\phi_f|v_i,\phi_i) = \beta\int\mathcal{D}\alpha\int\mathcal{D}\phi\int\mathcal{D}p_\phi\int\mathcal{D}v\int\mathcal{D}b\exp\left\{\frac{i}{\hbar}\int_0^1\mathrm{d}\tau\left[p_\phi\dot{\phi} - \hbar b\dot{v}\right.\right.\\ \left.\left.+\hbar\alpha\left(\frac{p^2_\phi}{\hbar^2} - 3\pi G v^2\left[\sin^2(b)(1-(1+\gamma^2)\sin^2(b)) + b_\Lambda^2\right]\right)\right]\right\},\end{aligned} \tag{6.83}$$

where β is a constant, the notation of a dot on a letter means the derivative with respect to the time variable τ. The path integral (6.183) is the "sum over histories", where this sum is over the same family of v paths. In fact, if we perform the integral over b_i, it is possible to recover the sum over histories expansion. We use the Jacobi identity

$$\sum_{m\in\mathbb{Z}}\int_0^{2\pi} d\theta f(\theta,m)e^{im\theta} = \int_{-\infty}^{\infty} dx\int_{-\infty}^{\infty} d\theta f(\theta,x)e^{ix\theta}, \tag{6.84}$$

for any continuous function $f(\theta,x)$ with a period of 2π in θ. This identity transforms from a discrete sum over m to a continuous integral over x. Additionally, we can use the following expression rewriting each sum over v_n and integral over b_n as

$$\pi\sum_{\nu_n}\int_0^{\pi} db_n\ldots\to\int_{-\infty}^{\infty} d\nu_n\int_{-\infty}^{\infty} db_n\ldots \tag{6.85}$$

where $n = 1, ..., N-1$. For path integral is possible to take the formal limit $N \to \infty$. Therefore,

$$A\left(\nu_f, \phi_f | \nu_i, \phi_i\right) = \int d\alpha \int [\mathcal{D}v(\tau)][\mathcal{D}b(\tau)][\mathcal{D}p_\phi(\tau)][\mathcal{D}\phi(\tau)]e^{(i/\hbar)S}. \tag{6.86}$$

Hence, we can reorganize the effective Hamiltonian constraint $\tilde{C}^{\rm pi}_{\rm eff}$, which is obtained by path integral

$$\tilde{C}^{\rm pi}_{\rm eff} = \frac{p_\phi^2}{\hbar^2} - 3\pi G v^2 \left[\sin^2(b)(1-(1+\gamma^2)\sin^2(b)) + b_\Lambda^2\right]. \tag{6.87}$$

This effective constraint is consistent with what the authors obtained in [111–113]. However, this effective constraint comes from the sLQC model that uses the Hamiltonian $\hat{\Theta}$ instead of $\hat{H}$, which we can be regained by rescaling $\tilde{C}^{\rm pi}_{\rm eff} = 4\pi\gamma\ell_p^2\sqrt{\Delta}vC^{\rm pi}_{\rm eff}/\hbar^2$. Therefore,

$$C^{\rm pi}_{\rm eff} = \frac{p_\phi^2}{2V} - \frac{3}{8\pi G\Delta\gamma^2}V\left[\sin^2(b)\left(1-\left(1+\gamma^2\right)\sin^2(b)\right) + b_\Lambda^2\right]. \tag{6.88}$$

Note that the three methods are consistent with each other; we can obtain the same effective constraint at the dominant order of approximation. The advantage of path-integral and the expectation value is that further corrections can be obtained as opposed to the heuristic method. We will use the effective constraint $C_{\rm eff} = C^{\rm heu}_{\rm eff} = C^{\rm ev}_{\rm eff} = C^{\rm pi}_{\rm eff}$ to find the effective equations of motion [27–30, 38].
From the effective constraint (6.88) we can identify the energy density as $\rho_0 = \frac{p_\phi^2}{2V^2}$. Thus,

$$\rho_0 - \frac{\Lambda}{8\pi G} = \frac{3}{8\pi G\Delta\gamma^2}\sin^2(b)\left[1-\left(1+\gamma^2\right)\sin^2(b)\right], \tag{6.89}$$

where the total energy density is defined as $\rho = \rho_0 - \frac{\Lambda}{8\pi G}$. It is straightforward to find the solution for b_+ and b_- from eq.(6.89)

$$\sin^2(b_\pm) = \frac{1 \pm \sqrt{1-\frac{\rho}{\rho_c}}}{2\left(1+\gamma^2\right)}, \tag{6.90}$$

where the critical energy density is given by

$$\rho_c = \frac{\rho_c^E}{4(1+\gamma^2)} = \frac{3}{32\pi G\left(1+\gamma^2\right)\gamma^2\Delta}, \tag{6.91}$$

with $\rho_c^E = \frac{3}{8\pi G\gamma^2\Delta}$ is the critical energy density for an effective cosmological model that includes only the Euclidean part in the LQC scheme [23–26]. Now, we find the Hamilton equations corresponding to (6.88) as the effective equations of motion with

$$\dot{v} = \{v, C_{\rm eff}\} = \frac{3}{2\gamma\sqrt{\Delta}}v\sin(2b)\left[1-2\left(1+\gamma^2\right)\sin^2(b)\right], \tag{6.92}$$

$$\begin{aligned}\dot{b} = \{b, C_{\rm eff}\} = &-\frac{p_\phi^2}{2\pi G\hbar^2\gamma\sqrt{\Delta}v^2} \\ &-\frac{3}{2\gamma\sqrt{\Delta}}\left(\sin^2(b)\left[1-\left(1+\gamma^2\right)\sin^2(b)\right] + b_\Lambda^2\right). \end{aligned}\tag{6.93}$$

As for the massless scalar field are given by

$$\dot{\phi} = \{\phi, C_{\text{eff}}\} = \frac{p_\phi}{V}, \tag{6.94}$$

$$\dot{p}_\phi = \{p_\phi, C_{\text{eff}}\} = 0, \tag{6.95}$$

and p_ϕ is a constant of motion.
Additionally, note that when $\dot{v} = 0$ we have $\sin^2(b_c) = \frac{1}{2(1+\gamma^2)}$, that is, the maximum of ρ_0, this condition corresponds to the bounce at b_c. On the other hand, from the equations of motion we can get the modified Friedmann equation and the Raychaudhuri equation, respectively, which can be read as

$$H^2 = \left(\frac{\dot{a}}{a}\right)^2 = \left(\frac{\dot{v}}{3v}\right)^2$$

$$= \frac{1}{\gamma^2\Delta}\sin^2(b)\left(1-\sin^2(b)\right)\left[1-2\left(1+\gamma^2\right)\sin^2(b)\right]^2, \tag{6.96}$$

$$\frac{\ddot{a}}{a} = H^2 + \frac{1}{\gamma\sqrt{\Delta}}\dot{b}\left[1-2\sin^2(b)-2\left(1+\gamma^2\right)\sin^2(b)\left(3-4\sin^2(b)\right)\right], \tag{6.97}$$

where the Hubble parameter is denoted by H and a is the scale factor.
Equations of motion (6.92), (6.93), (6.94) and (6.95) are with respect to the cosmological time t. However, these equations of motion can be calculated with respect to physical time ϕ. As we see in the equations of motion for the scalar field (6.94) and (6.95) where $\dot{\phi}$ has a definite sign, then if we choose, for example, p_ϕ to be positive, $\dot{\phi} > 0$ and ϕ grow monotonically with respect to the cosmological time t. This fact makes ϕ an appropriate evolution parameter. The election of different time or evolution parameters comes from the time reparametrization of the theory [14–16, 73–75]. The equations of motion with respect to the physical time ϕ take the form

$$\frac{dV}{d\phi} = \frac{3}{\gamma\sqrt{\Delta}}\frac{V^2}{p_\phi}\sin(b)\sqrt{1-\sin^2(b)}\left[1-2\left(1+\gamma^2\right)\sin^2(b)\right], \tag{6.98}$$

$$\frac{db}{d\phi} = -2\pi G\gamma\sqrt{\Delta}\frac{p_\phi}{V} - \frac{3}{2\gamma\sqrt{\Delta}}\frac{V}{p_\phi}\sin^2(b)\left[1-\left(1+\gamma^2\right)\sin^2(b)\right]. \tag{6.99}$$

The solutions for the conjugated momentum, which are give by the variable as $\chi = \sin^2(b)$, the volume V and the energy density ρ in terms of physical time ϕ can be written as

$$\chi(\phi) = \frac{1}{1+\gamma^2\cosh^2\left(\sqrt{12\pi G}\,(\phi-\phi_o)\right)}, \tag{6.100}$$

$$\rho(\phi) = \frac{3}{8\pi G\Delta}\left[\frac{\sinh\left(\sqrt{12\pi G}\,(\phi-\phi_o)\right)}{1+\gamma^2\cosh^2\left(\sqrt{12\pi G}\,(\phi-\phi_o)\right)}\right]^2, \tag{6.101}$$

$$V(\phi) = \sqrt{\frac{4\pi G\Delta p_\phi^2}{3}}\frac{1+\gamma^2\cosh^2\left(\sqrt{12\pi G}\,(\phi-\phi_o)\right)}{\left|\sinh\left(\sqrt{12\pi G}\,(\phi-\phi_o)\right)\right|}, \tag{6.102}$$

where ϕ_0 is a constant of integration. The Hubble parameter in terms of the physical time is given by

$$H = \frac{1+\gamma^2\left[1-\sinh^2\left(\sqrt{12\pi G}\,(\phi-\phi_o)\right)\right]\cosh\left(\sqrt{12\pi G}\,(\phi-\phi_o)\right)}{\sqrt{\Delta}\left[1+\gamma^2\cosh^2\left(\sqrt{12\pi G}\,(\phi-\phi_o)\right)\right]^2}. \tag{6.103}$$

Furthermore, the cosmological time t is related to the physical time ϕ by

$$\begin{aligned} t(\phi)-t_o = \frac{\gamma^2\,\mathrm{sgn}\,(p_\phi\,(\phi-\phi_o))}{\sqrt{12\pi G}}&\left[\cosh\left(\sqrt{12\pi G}\,(\phi-\phi_o)\right)\right.\\ &\left.-\left(1+\gamma^2\right)\ln\left|\coth\left(\sqrt{3\pi G}\,(\phi-\phi_o)\right)\right|\right], \end{aligned} \tag{6.104}$$

where t_0 is a constant of integration.
Note that from eq.(6.104) the infinite past and infinite future of t take these values when $\phi \to \phi_0^+$ and $\phi \to +\infty$, respectively. In addition, the two universes or branches are in the range $0 < \sin^2 b_- \leq \frac{1}{2(1+\gamma^2)}$ and $\frac{1}{2(1+\gamma^2)} \leq \sin^2 b_+ < \frac{1}{1+\gamma^2}$. These two universes or branches are connected by the bounce in b_c. Therefore, the asymptotic limit is given by $v \to +\infty$, which occurs when $(\phi-\phi_0) \to +\infty$, or equivalently when $b \to 0$, or $(\phi-\phi_0) \to 0^+$, which corresponds to $b \to b_0 = \arcsin\left(\frac{1}{\sqrt{(1+\gamma^2)}}\right)$. Thus, the asymptotic limit of the Hubble parameter is given by

$$H^2 = \frac{8\pi G}{3}\rho, \quad \text{for} \quad b \to 0, \tag{6.105}$$

$$H^2 = \left(\frac{1-5\gamma^2}{1+\gamma^2}\right)\frac{8\pi G\rho}{3} + \frac{\Lambda_{\text{eff}}}{3}, \quad \text{for} \quad b \to b_0. \tag{6.106}$$

Note that in this limit (6.105) corresponds to a FLRW spatially flat Universe, and (6.106) to a de Sitter Universe with a effective cosmological constant

$$\Lambda_{\text{eff}} \equiv \frac{3}{(1+\gamma^2)^2\,\Delta}. \tag{6.107}$$

Furthermore, the asymptotic Raychaudhuri equations are given by

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}(\rho+3P), \quad \text{for } b \to 0, \tag{6.108}$$

$$\frac{\ddot{a}}{a} = -\left(\frac{1-5\gamma^2}{1+\gamma^2}\right)\frac{4\pi G}{3}(\rho+3P) + \frac{\Lambda_{\text{eff}}}{3}, \quad \text{for} \quad b \to b_0, \tag{6.109}$$

where $P = -\frac{\partial H_\phi}{\partial V}$ is the matter pressure.
An effective cosmological constant is found working with a regularization based on the loop quantization scheme such as in the full theory, where the Lorentzian term is also included in the Hamiltonian constraint. The Thiemann regularization applied in a reduced-cosmological model can lead to an effective cosmological constant, which emerges from the theory itself due to discrete space-time. However, as noted in [27–30] the theoretical and observable values of the cosmological constant differ by 120 orders of magnitude; this is a catastrophic discrepancy. The authors

in [30] propose the inclusion of a weight parameter λ between the Euclidean and Lorentzian terms in the Hamiltonian constraint. With this extra parameter, they adjust the effective cosmological constant from the LQC scheme, to match the observational value. This can be criticized of course as an undesirable fine tunning. However, it is tempting to further explore this avenue by considering the possible unitary evolution with this motivation we analyze how this weight parameter affects the dynamics.
With weight parameter λ between the Euclidean and Lorentzian terms in the gravitational constraint H_g one gets

$$H_g(N) = \lambda H^E(N) - 2(1+\lambda\gamma^2)H^L(N) + (-1+\lambda)\int_\Sigma d^3x\sqrt{q}^{(3)}R, \tag{6.110}$$

where ${}^{(3)}R$ is the 3-dimensional spatial curvature of Σ. However, for a flat space, this term vanishes. Different limit values of λ can be used, for example, with $\lambda = 1$ returns both terms in the gravitational constraint. On the other hand, for the $\lambda = -\frac{1}{\gamma^2}$, we only have the Euclidean part; these models have been extensively studied mostly because classically both H^E and H^L are proportional.
Applying the Thiemann regularization as already described in this section, the simplified Hamiltonian operator $\hat{\Theta}_\lambda$ takes the same form as without weight parameter

$$\hat{\Theta}_\lambda = \mathbb{I}\otimes\partial_\phi^2 + \hat{\Theta}_{\lambda,g}\otimes\mathbb{I}, \qquad \hat{\Theta}_{\lambda,g} = \hat{\Theta}_{\lambda,0} - \pi G\gamma^2\Delta\Lambda v^2, \tag{6.111}$$

where the gravitational operator $\hat{\Theta}_{\lambda,g}$ in sLQC context is defined by the flat simplified gravitational operator $\hat{\Theta}_{\lambda,0}$ as

$$\begin{aligned}\hat{\Theta}_{\lambda,0}\psi(v) \;&= \frac{3\pi G\gamma^2}{4}\Big[\xi_\lambda\tilde{f}_8(v)\psi(v+8) - \lambda\tilde{f}_4(v)\psi(v+4) - 2(\xi_\lambda-\lambda)\tilde{f}_0(v)\psi(v)\\ &\qquad - \lambda\tilde{f}_{-4}(v)\psi(v-4) + \xi_\lambda\tilde{f}_{-8}(v)\psi(v-8)\Big],\end{aligned} \tag{6.112}$$

where the functions $\tilde{f}_a(v)$ are defined in (6.57) and $\xi_\lambda = (1+\lambda\gamma^2)/(4\gamma^2)$. Furthermore, we can find the representation of the b variable using the Fourier transformation (6.60), where we have

$$\hat{\Theta}_{\lambda,g}\tilde{\psi}(b) = 12\pi G\gamma^2\left[\lambda(\sin(b)\partial_b)^2 - \xi_\lambda(\sin(2b)\partial_b)^2 + \frac{b_\Lambda^2}{\gamma^2}\partial_b^2\right]\tilde{\psi}(b). \tag{6.113}$$

If the weight parameter is $\lambda = -1/\gamma^2$, then $\xi_\lambda = 0$. Therefore, we have the case that includes only the Euclidean term [24–26]. On the other hand, if $\lambda = 1$, we have $\xi_\lambda = \xi$, that is, the case shown in (6.57) in [27–29]. In addition, because of eq.(6.111) we can write a Klein-Gordon (KG) equation

$$\partial_\phi^2\tilde{\psi}(b,\phi) + \hat{\Theta}_{\lambda,g}\tilde{\psi}(b,\phi) = 0, \tag{6.114}$$

this equation will be relevant in the unitary evolution description of this quantum system. Additionally, from this quantum behavior it is possible to find an effective model, such as described previously; it does not matter which method we use, the effective Hamiltonian constraint is given, to lowest order, by

$$C_{\lambda,\text{eff}} = \frac{p_\phi^2}{2V} - \frac{3}{8\pi G\Delta\gamma^2}V\left(\sin^2(b)\left[1-\left(1+\lambda\gamma^2\right)\sin^2(b)\right] + b_\Lambda^2\right). \tag{6.115}$$

The asymptotic limit of the Hubble parameter H_λ can be obtained as previously shown

$$H_\lambda^2 = \frac{8\pi G}{3}\rho, \quad \text{for} \quad b \to 0, \tag{6.116}$$

$$H_\lambda^2 = \left(\frac{1-5\lambda\gamma^2}{1+\lambda\gamma^2}\right)\frac{8\pi G\rho}{3} + \frac{\Lambda_{\text{eff}}}{3}, \quad \text{for} \quad b \to b_0. \tag{6.117}$$

Note that in this limit (6.116) corresponds to a FLRW universe and (6.117) to a de Sitter universe with an effective cosmological constant

$$\Lambda_{\lambda,\text{eff}} = \frac{3\lambda}{(1+\lambda\gamma^2)^2\,\Delta}. \tag{6.118}$$

Moreover, the effective Newton constant can be set as

$$G_\lambda = \frac{1-5\lambda\gamma^2}{1+\lambda\gamma^2}G. \tag{6.119}$$

To match the observational and theoretical cosmological constant, we find two solutions $\lambda_1 \sim \frac{3}{\gamma^4\Delta\Lambda_{\text{obs}}}$ and $\lambda_2 \sim \frac{\Delta\Lambda_{\text{obs}}}{3}$, because the solution λ_1 makes G_λ inconsistent with the experimental results it is discarted. However, the fixed parameter λ_2 is sufficiently small to reproduce an acceptable G_λ. Therefore, the choice $\lambda = \frac{\Delta\Lambda_{\text{obs}}}{3} \sim 10^{-122}$. Thus, this value is so very small and close to zero, but positive. With this fixed parameter, eq.(6.117) takes the following form

$$H_\lambda^2 = \frac{8\pi G\rho}{3} + \frac{\Lambda_{\text{obs}}}{3}. \tag{6.120}$$

This was found in [30]. We adopt this model to investigate its unitary evolution and possible limitations on λ.

6.2 Unitary Evolution

The unitary time evolution of the gravitational operator in LQC is studied by the self-adjoint character and its possible extensions using the index deficiency method described in Section 4.2. The operator (6.112) leads to a generalized description of the LQC models, which contains a weight parameter between the Euclidean and Lorentzian parts and an effective cosmological constant contribution. The possible extensions can be analyzed by solving the complex eigenvalue problem (4.13). We can use this to solve the index method using the operator (6.112) in the representation v. However, this representation, as has been discussed previously, produces a difference equation and the methods for solving this kind of equation are less studied in comparison with the differential equation theory. Although there exist some methods [109, 110] to explore these solutions, not all cases may have an analytic answer.

In LQC some authors have studied this problem numerically in the asymptotic limit where some convergence criteria are used, but in this section we do not focus on these numerical methods; it is possible to see more information on [28, 29, 31, 32]. On the other hand, there exist some examples in which self-adjointness is not consistent in the asymptotic limit as in the full description, as shown by the authors in [114]. Unitary evolution is given by the massless scalar field as an evolution parameter, such as it is describe in eq.(6.114). Before solving the complex eigenvalue problem for the quantum Hamiltonian constraint, we show some important properties of the gravitational operator in b-representation (6.113). This differential representation is used to transform into another convenient representation that help us to investigate this problem. By using [26, 28, 29] the transformation

$$\partial_x = (\partial_x b)\partial_b = f(b)\partial_b, \tag{6.121}$$

equivalent to the integral expression

$$\int \frac{\mathrm{d}b}{f(b)} = \int \mathrm{d}x, \tag{6.122}$$

allows to simplify the analysis. Note that $f(b)$ can take positive and negative values, that is, $f(b) < 0$ or $f(b) > 0$. Thus, we can have different regions depending on the sign of this function. The generalized gravitational operator (6.113) can be explicitly rewritten as in [2]

$$\begin{aligned}\hat{\Theta}_{\lambda,g}\tilde{\psi}(b) = 12\pi G\gamma^2 \Bigg\{ &\left(\lambda \sin^2(b) - \xi_\lambda \sin^2(2b) + \frac{b_\Lambda^2}{\gamma^2}\right)\partial_b^2 \\ &+ \left(\lambda \sin(b)\cos(b) - 2\xi_\lambda \sin(2b)\cos(2b)\right)\partial_b \Big\}\, \tilde{\psi}(b),\end{aligned} \tag{6.123}$$

where

$$f^2(b) = -\gamma^2 \left(\lambda \sin^2(b) - \xi_\lambda \sin^2(2b) + \frac{b_\Lambda^2}{\gamma^2}\right), \tag{6.124}$$

$$g(b) = -\gamma^2 \left(\lambda \sin(b)\cos(b) - 2\xi_\lambda \sin(2b)\cos(2b)\right). \tag{6.125}$$

Note that the function $g(b)$ obeys the following relation $g(b) = f(b)\partial_b f(b)$, this expression is fulfilled due to the structure of the gravitational operator in LQC. Before showing the explicit variable changes given by (6.122), we show illustrative graphs on the behavior of different functions $f^2(b)$ for different values of λ and b_Λ, these values have been studied in previous works [26, 28, 29, 31, 32]. We present some previous conclusions without doing explicit calculations on self-adjointness and its possible extensions below. For all graphics, the Barbero-Immirzi parameter is set to $\gamma = 0.2$.

6.2.1 Qualitative analysis

The first example that we will analyze, Figure 6.2.1, where the function $f^2(b)$ is evaluated in $\lambda = -\frac{1}{\gamma^2}$ and $b_\Lambda = 0$, that is, the specific case where the LQC model includes only the Euclidean term (3.36) in the Hamiltonian constraint with cosmological constant equal to zero $\Lambda = 0$. Note that in Figure 6.2.1 $f^2(b) > 0$, for all $b \in (0, \pi)$. On the other hand, when the function $f^2(b)$ changes sign, this condition becomes the boundary condition. Thus, for this case we have that the gravitational operator is essentially self-adjoint, because we do not have new boundary condition, then there exists only a unique extension. This example was analyzed

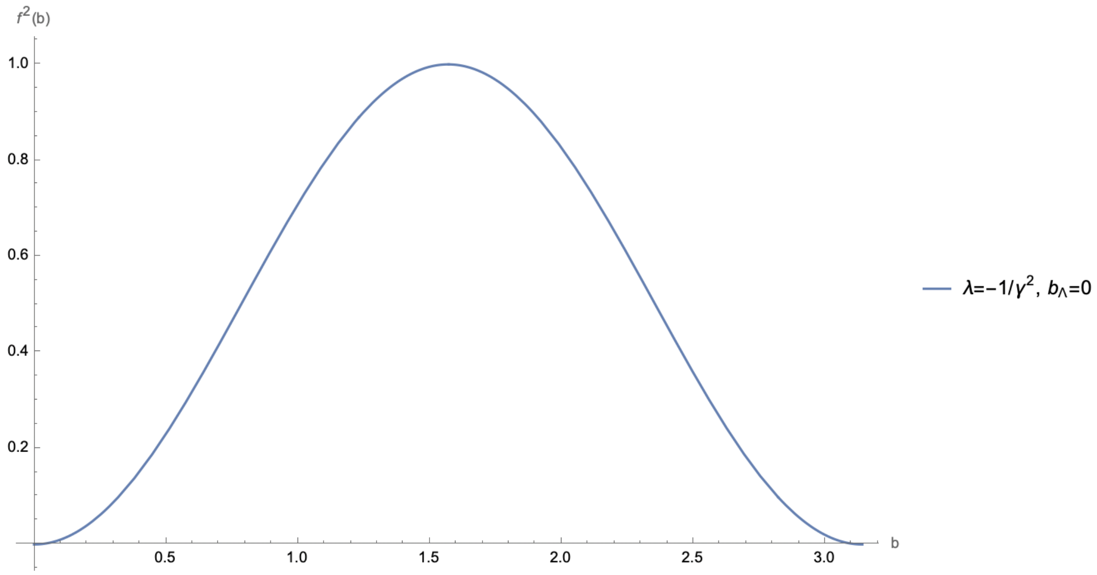

Figure 6.2.1: This plot shows the behavior of the function $f^2(b)$ for $\lambda = -\frac{1}{\gamma^2}$ and $b_\Lambda = 0$, where $\gamma = 0.2$, that is the gravitational operator that includes only the Euclidean term without explicit cosmological constant.

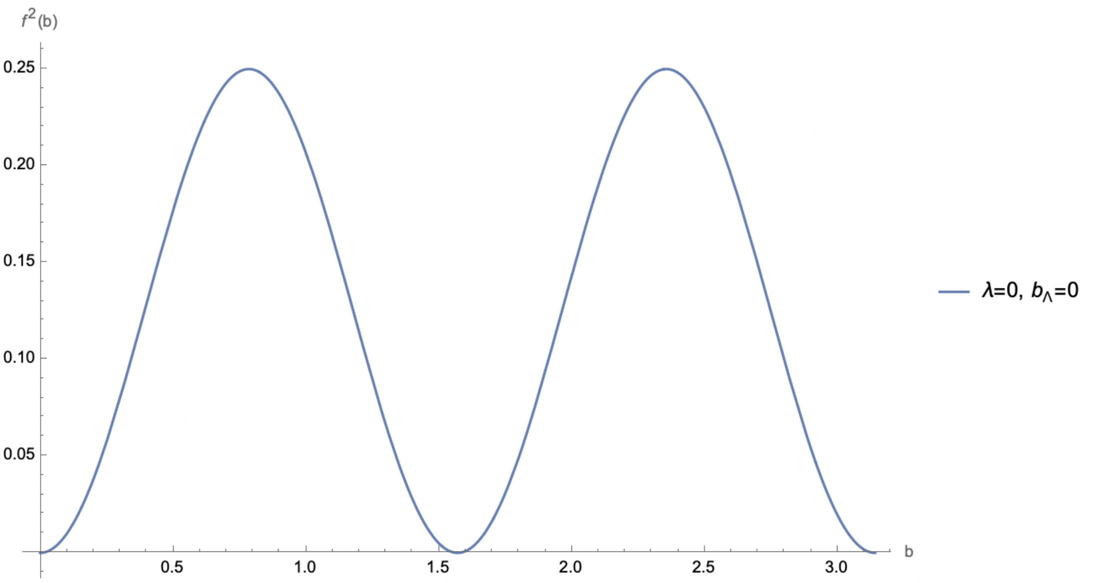

Figure 6.2.2: This plot shows the behavior of the function $f^2(b)$ for $\lambda = 0$ and $b_\Lambda = 0$, where $\gamma = 0.2$, that is the gravitational operator that includes only the Lorentzian term without explicit cosmological constant.

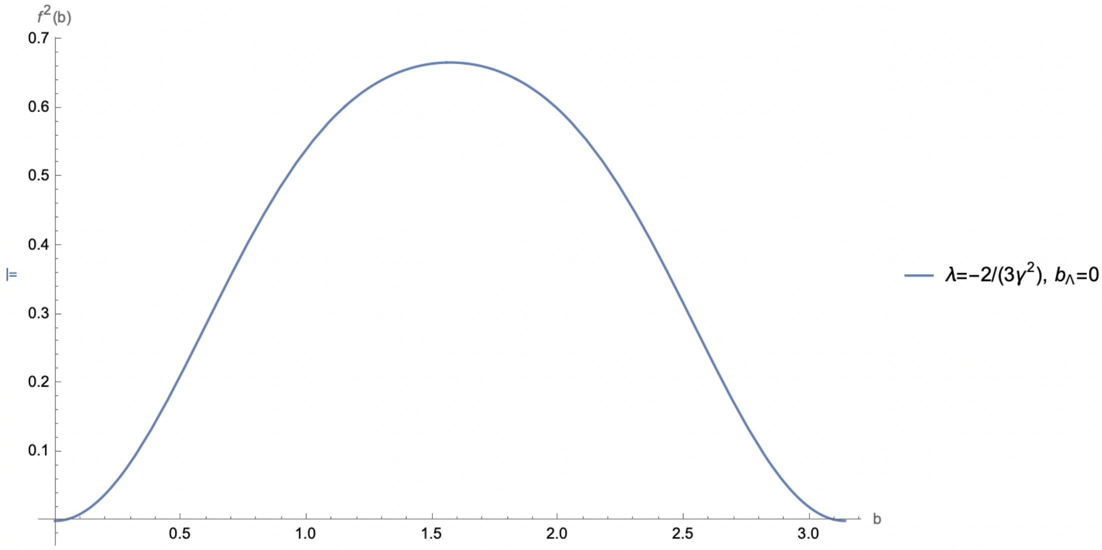

Figure 6.2.3: This plot shows the behavior of the function $f^2(b)$ for $\lambda = -\frac{2}{3\gamma^2}$ and $b_\Lambda = 0$, where $\gamma = 0.2$, that is the gravitational operator that includes both terms with a weight parameter $\lambda = -\frac{2}{3\gamma^2}$ and without explicit cosmological constant.

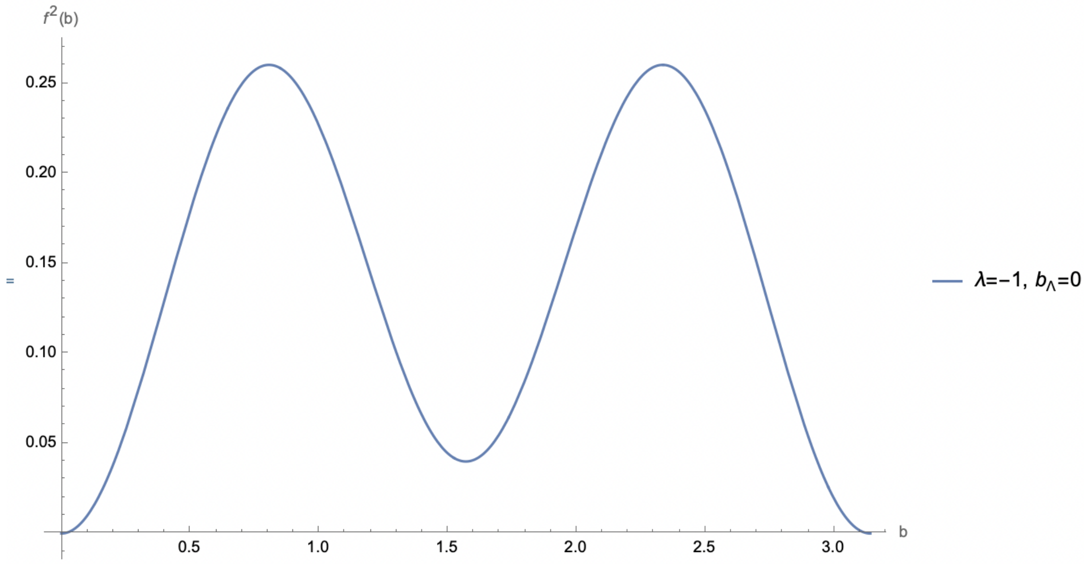

Figure 6.2.4: This plot shows the behavior of the function $f^2(b)$ for $\lambda = -1$ and $b_\Lambda = 0$, where $\gamma = 0.2$, that is the gravitational operator that includes both terms with a weight parameter $\lambda = -1$ and without explicit cosmological constant.

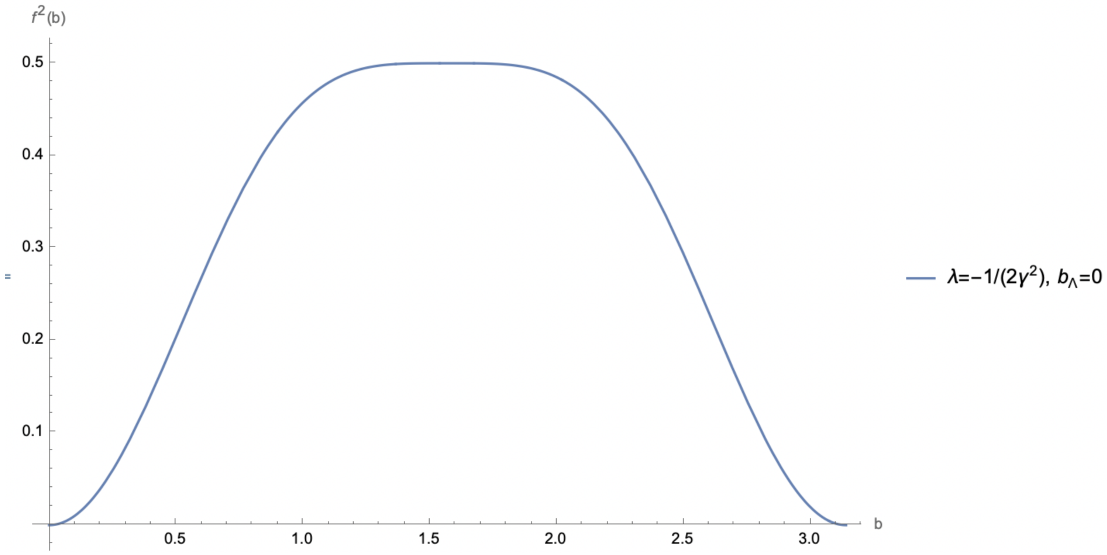

Figure 6.2.5: This plot shows the behavior of the function $f^2(b)$ for $\lambda = -\frac{1}{2\gamma^2}$ and $b_\Lambda = 0$, where $\gamma = 0.2$, that is the gravitational operator that includes both terms with a weight parameter $\lambda = -\frac{1}{2\gamma^2}$ and without explicit cosmological constant.

by the authors in [31].

Another particular example is when we have only the Lorentzian term (3.37) in the gravitational operator (3.38) without cosmological constant contribution, that is $b_\Lambda = 0$. In this case, as we see in Figure 6.2.2, we have three minima in $b = 0, \pi/2, \pi$, for these values of the function $f^2(b) = 0$. However, as in the previous case, when we have only the Euclidean term in the constraint, we can conclude that this case is also essentially self-adjoint because the function $f(b)$ does not change the sign for any value of b. Note that with the minimum value at $b = \pi/2$ we could recover a couple of behaviors of the function $f^2(b)$ for the case where the constraint includes only the Euclidean term.

To explore different values of the weight parameter λ in our model, now we take $b_\Lambda = 0$. As shown in Figure 6.2.3, Figure 6.2.4 and Figure 6.2.5 the weight parameter is negative. In fact, for all $\lambda < 0$, the function $f^2(b) > 0$. Note that in Figure 6.2.3 the behavior of the curve is similar to the behavior in Figure 6.2.1 where there is only a maximum in $\pi/2$. On the other hand, Figure 6.2.4 has two maxima. This behavior is more similar to Figure 6.2.2 than to Figure 6.2.1, where the Lorentzian term dominates over the Euclidean term. This dominance of one term over another is identified by a critical value of the weight parameter in $\lambda = -\frac{1}{2\gamma^2}$. This behavior is illustrated in Figure 6.2.5. However, for $\lambda < 0$ and also for $\lambda = 0$, the gravitational operator is essentially self-adjoint, because there is no change of sign and the function $f^2(b) \geq 0$.

For the positive values of the weight parameter ($\lambda > 0$) and a cosmological constant vanishes ($b_\Lambda = 0$) such as Figure 6.2.6 and Figure 6.2.7 illustrate, where the function $f^2(b)$ changes of sign. Thus, in both graphs we have three regions, where two of these regions $f^2(b) > 0$ and another $f^2(b) < 0$, then we have two roots for $b \in (0, \pi)$. Figure 6.2.6 is the specific case in which the Euclidean and Lorentzian are included in the Hamiltonian constraint in the standard description without the weight parameter ($\lambda = 1$) as is studied by the authors in [27–30, 38]. However,

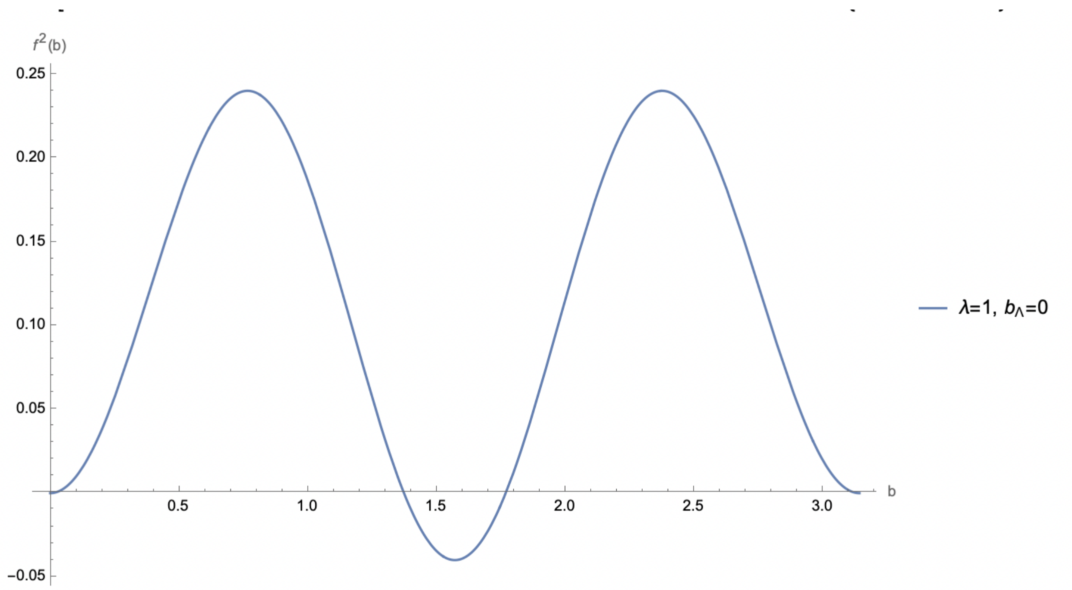

Figure 6.2.6: This plot shows the behavior of the function $f^2(b)$ for $\lambda = 1$ and $b_\Lambda = 0$, where $\gamma = 0.2$, that is the gravitational operator that includes both terms without weight parameter and without explicit cosmological constant.

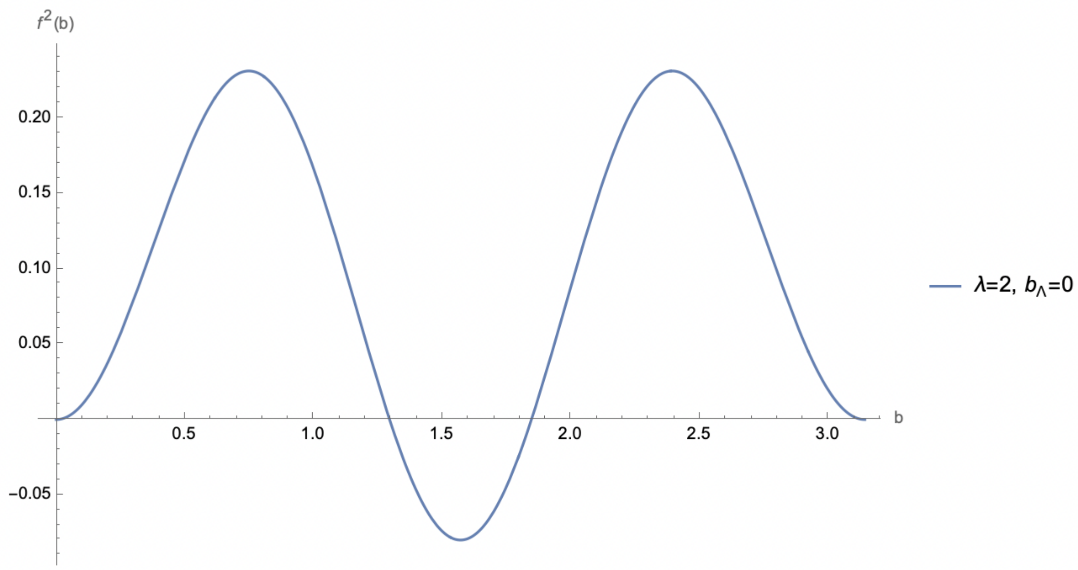

Figure 6.2.7: This plot shows the behavior of the function $f^2(b)$ for $\lambda = 2$ and $b_\Lambda = 0$, where $\gamma = 0.2$, that is the gravitational operator that includes both terms with a weight parameter $\lambda = 2$ and without explicit cosmological constant.

the self-adjoint character of the gravitational operator in this case is analyzed in [28, 29], and this behavior continues for any positive weight parameter. Since the function $f^2(b)$ can be positive or negative, this can be translated into a new boundary condition. In this case, the quantum Hamiltonian operator has a family of infinite self-adjoint extensions. In fact, these extensions are related to the the group $U(1)$.

Up to now, we have only worked with LQC models that do not contain an explicit cosmological constant. Now, we study its inclusion this. The model in LQC

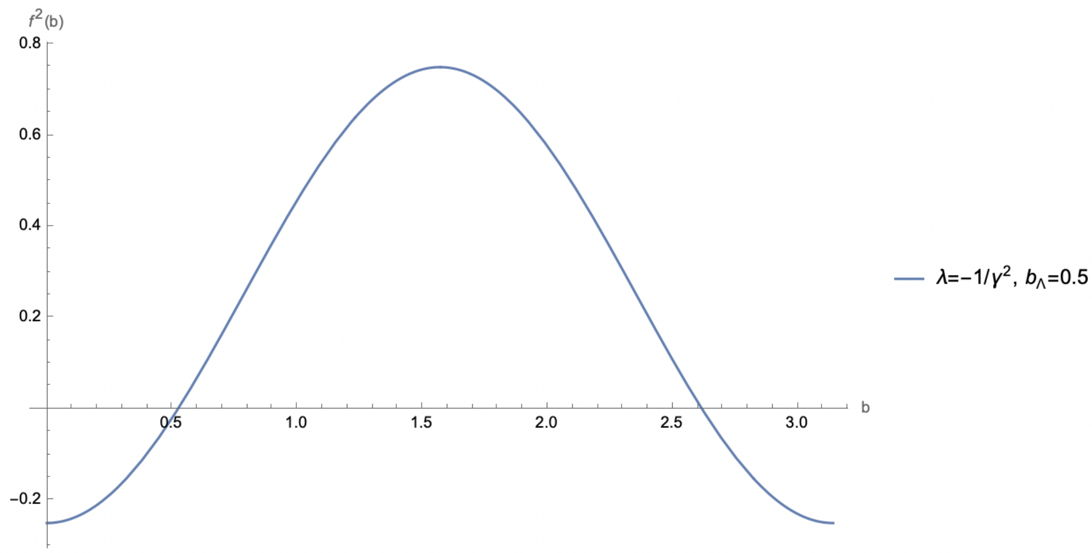

Figure 6.2.8: This plot shows the behavior of the function $f^2(b)$ for $\lambda = -\frac{1}{\gamma^2}$ and $b_\Lambda = 0.5$, where $\gamma = 0.2$, that is the gravitational operator that includes only the Euclidean term with an explicit cosmological constant $b_\Lambda = 0.5$.

that contains only the Euclidean term ($\lambda = -\frac{1}{\gamma^2}$) with a cosmological constant distinct from zero, self-adjointness for this problem, was studied in [26, 32]. They obtained that one can have two different regions, subcritical ($\Lambda < \Lambda_c$, that is, when $0 < b_\Lambda < 1$), and supercritical ($\Lambda \geq \Lambda_c$, or $b_\Lambda \geq 1$). Note that in Figure 6.2.8 for the subcritical case the function $f^2(b)$ presents a sign change, which can yield three regions, two where $f^2(b)$ is negative and another where $f^2(b)$ is positive. Therefore, the gravitational operator for the subcritical case has a family of self-adjoint extensions because this change of sign produces a new boundary condition.

On the other hand, as we see in Figure 6.2.9 the supercritical case does not have this change of sign. Thus, in this case, the quantum operator is essentially self-adjoint; there is a unique extension. However, in this example, there is a fundamental distinction with respect to the previous examples, that is, $f^2(b) < 0$, for all $b \in (0, \pi)$. Due to the fact that we consider only the positive spectrum of the Hamiltonian operator, the Hilbert space is empty. This is not physically relevant because the solutions are not normalizable.

If we include also the Lorentzian term and an explicit cosmological constant to the Hamiltonian operator, where the function $f^2(b)$ can have a form of those already shown without the effect of the cosmological constant, such as it is possible to see in Figure 6.2.10. The contribution of this cosmological constant is encoded in different roots of $f^2(b)$. For the more extreme cases where $\lambda > -1/\gamma^2$ in combination with some values of b_Λ it is possible to have four roots of $f^2(b)$, we then have five regions, two of these where $f^2(b)$ is positive and three where $f^2(b)$ is negative; in this case, we would expect to have self-adjoint extensions in our operator. However, these extensions would be related to the elements of the group $SU(2)$ because there exists a double change of sign, one more by the weight parameter also having this change. Therefore, the deficiency space admits more solutions, and the dimension of the deficiency subspaces increases to two.

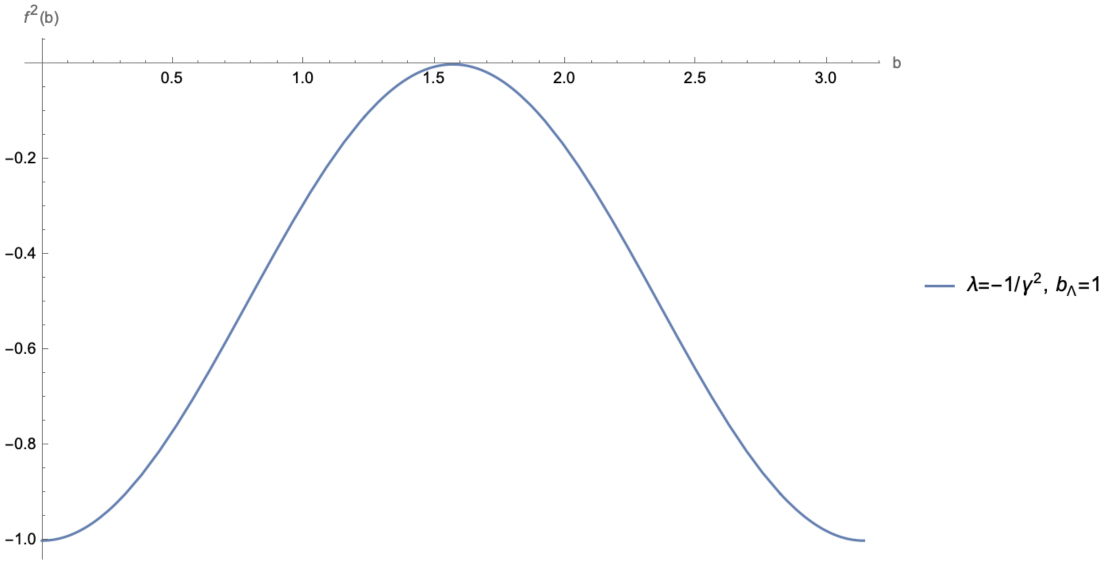

Figure 6.2.9: This plot shows the behavior of the function $f^2(b)$ for $\lambda = -\frac{1}{\gamma^2}$ and $b_\Lambda = 1$, where $\gamma = 0.2$, that is the gravitational operator that includes only the Euclidean term with an explicit cosmological constant $b_\Lambda = 1$.

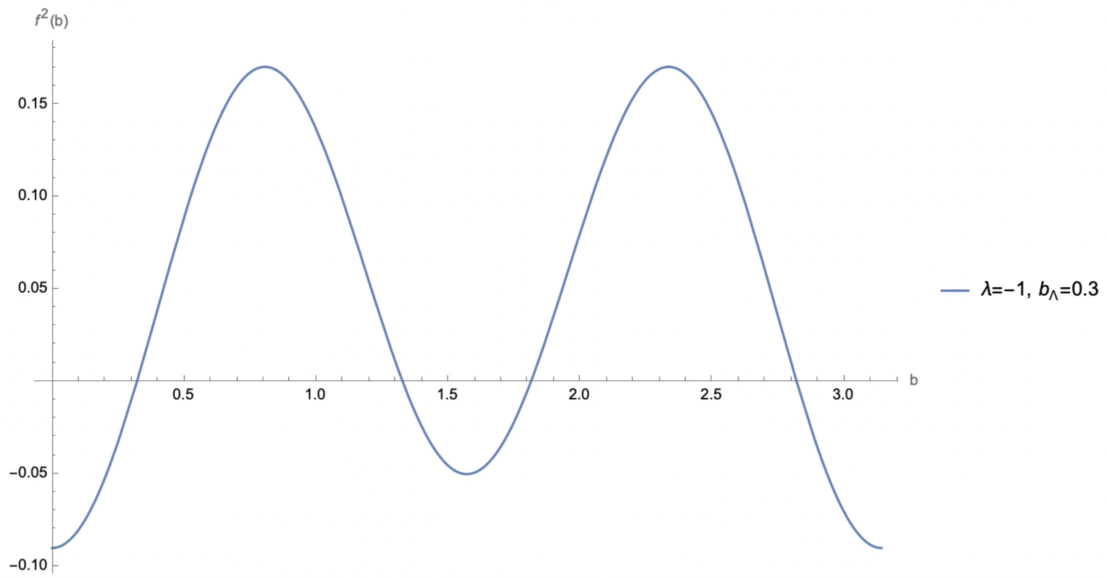

Figure 6.2.10: This plot shows the behavior of the function $f^2(b)$ for $\lambda = -1$ and $b_\Lambda = 0.3$, where $\gamma = 0.2$, that is the gravitational operator that includes both terms with a weight parameter $\lambda = -1$ and an explicit cosmological constant $b_\Lambda = 0.3$.

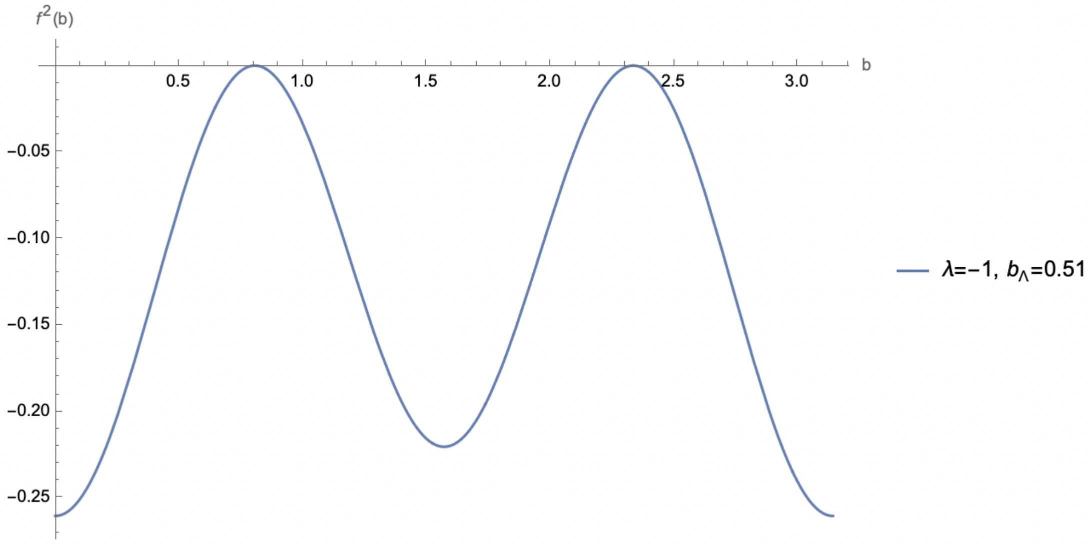

Figure 6.2.11: This plot shows the behavior of the function $f^2(b)$ for $\lambda = -1$ and $b_\Lambda = 0.51$, where $\gamma = 0.2$, that is the gravitational operator that includes both terms with a weight parameter $\lambda = -1$ and an explicit cosmological constant $b_\Lambda = 0.51$.

However, there could be cases where $b_\Lambda < 1$, but the function $f^2(b) < 0$, in these cases, the operator is essentially self-adjoint, but the Hilbert space is empty, as can be seen in Figure 6.2.11. In this generalized model that includes both the Euclidean and Lorentzian terms and the cosmological constant, we could have many cases, from the gravitational operator being essentially self-adjoint, with and without a Hilbert space empty, that this operator admits self-adjoint extensions with elements related to either the group $U(1)$ or $SU(2)$. This will depend on the values that we use for λ and b_Λ in our model.

After this qualitative description of the different LQC models and some conclusions on the self-adjoint property and its possible extensions of the quantum Hamiltonian operator we proceed the explicit details of the calculations on self-adjointness in this formalism using the index deficiency method given in Section 4.2. As we saw, a new representation x is needed to solve the complex eigenvalue problem of this operator. Furthermore, the graphs shown in this section help us to resolve the relationship between the variables b and x, and the change of sign is crucial to adapt the new boundary condition for self-adjoint extensions. We study some cases that have been relevant in LQC models below.

6.2.2 Self-adjoint extensions

For simplicity, first we consider the LQC models without a cosmological constant part ($b_\Lambda = 0$) but with a weight parameter between both terms in the quantum constraint, whose x-representation when the function $f^2(b)$ does not present a sign change, this behavior is presented when $\lambda \leq 0$. The operator $\hat{\Theta}_{\lambda,g}$ takes the following differential form based on (6.121)

$$\hat{\Theta}_{\lambda,g}\psi(x) = -12\pi G \partial_x^2 \psi(x). \tag{6.126}$$

Although for $\lambda < 0$ and $\lambda = 0$ the gravitational operator has the same x representation, there exist two different changes in the variable that solve the equation (6.122). Thus, the relation between x and b for $\lambda = 0$ is given by

$$x(b) = \ln|\tan(b)|, \tag{6.127}$$

in this case $b \in (0, \pi)$, we can get the following limits from eq.(6.127) where

$$\lim_{b\to 0} x(b) = -\infty, \quad \lim_{b\to\pi} x(b) = +\infty, \quad x(\pi/2) = +\infty. \tag{6.128}$$

For the negative weight parameter ($\lambda < 0$), the relation between x and b in the range $b \in (0, \pi)$ is written as

$$x(b) = -\operatorname{arctanh}\left(\frac{\cos(b)}{(1+\lambda\gamma^2)\sin^2(b) - 1}\right), \tag{6.129}$$

the new coordinate $x(b)$ in eq.(6.129) is defined over the real line, where the following limits are obtained

$$\lim_{b\to 0} x(b) = -\infty, \quad \lim_{b\to\pi} x(b) = +\infty. \tag{6.130}$$

Note the specific cases, where the gravitational operator is proportional to the Euclidean term when $\lambda = -1/\gamma^2$ and it is proportional to the Lorentzian part when $\lambda = 0$. However, the weight parameter gives a combination between the Euclidean and Lorentzian terms, where $-1/\gamma^2 < \lambda < -1/(2\gamma^2)$ the Euclidean term dominates over the Lorentzian term in the Hamiltonian operator, in the region where $-1/(2\gamma^2) < \lambda$ the dominant behavior is the Lorentzian term in the quantum constraint. Thus, the critical point where both terms have the same weight is given by $\lambda = -1/(2\gamma^2)$.
On the other hand, for the case where $\lambda > 0$ exists a sign change, this is crucial to the boundary condition in the self-adjoint extensions, which is presented as a boundary in b_0 given by

$$b_0 = \arccos\left(\sqrt{\frac{\lambda}{1+\lambda\gamma^2}}\right). \tag{6.131}$$

Therefore, the Hamiltonian operator in this new representation takes the following form.

$$\hat{\Theta}_{\lambda,g}\psi(x) = -12\pi G \operatorname{sgn}(|x| - x_0)\partial_x^2\psi(x), \tag{6.132}$$

where $x_0 = -x(b_0)$ and using the symmetry of this function, the relation for $x(b)$ is given by

$$x(b) = \begin{cases} \frac{1}{2}\ln\left[1 - \frac{2\sqrt{1-(1+\lambda\gamma^2)\sin^2(b)}}{\cos(b)+\sqrt{1-(1+\lambda\gamma^2)\sin^2(b)}}\right] - \frac{\pi}{2}, & b \in (0, b_0)\,, \\ -\arctan\left(\frac{\cos(b)}{\sqrt{(1+\lambda\gamma^2)\sin^2(b)-1}}\right), & b \in (b_0, \pi - b_0)\,, \\ \frac{1}{2}\ln\left[1 - \frac{2\sqrt{1-(1+\lambda\gamma^2)\sin^2(b)}}{\cos(b)+\sqrt{1-(1+\lambda\gamma^2)\sin^2(b)}}\right] + \frac{\pi}{2}, & b \in (\pi - b_0, \pi)\,. \end{cases} \tag{6.133}$$

The case $\lambda = 1$ has been studied in [28, 29]. As in the cases analyzed in [28, 29] we obtain some limits where this new coordinate spans the entire real line

$$\lim_{b\to 0} x(b) = -\infty, \quad \lim_{b\to\pi} x(b) = +\infty, \quad x(\pi/2) = 0,$$
$$x(b_0) = -\frac{\pi}{2}, \quad x(\pi - b_0) = \frac{\pi}{2}. \tag{6.134}$$

Note that for the cases where λ is negative or zero, we do not have change sign in the transformation to representation x. However, for $\lambda = 0$, we observe that $x(b)$ goes to infinity when b goes to $\pi/2$, in this case we can observe that the transformation gives a couple of copies of the model in which the Euclidean term is dominant, one of these copies is associated with $b \in (0, \pi/2)$ and the other to the range $b \in (\pi/2, \pi)$. This property is due to the fact that at this weight parameter value, the sign changes, as we see in case $\lambda > 0$, where this change of sign becomes a boundary condition because at the point $x = \pm\pi/2$ it is continuous but not differentiable. This property is crucial to the structure of self-adjoint extensions
To explore the self-adjointness property of the Hamiltonian operator, the deficiency index method can be implemented as discussed in Section 4.2, this method consists of identifying the deficiency subspaces $\mathcal{K}^{\pm}$, which are the spaces of the normalizable solutions $\psi^{\pm}$ of the following complex eigenvalue equation

$$\hat{\Theta}_{\lambda,g}\psi^{\pm}(x) = \pm 12\pi G i \psi^{\pm}(x). \tag{6.135}$$

This method focuses on the dimension of these subspaces of deficiency $n_{\pm} = \dim(\mathcal{K}^{\pm})$, which helps to determine the self-adjoint extension. For simplicity, we take the eigenvalues $\pm 12\pi G i$. This choice does not have an effect on the dimension of the deficiency subspaces, which is the main objective of this method.
This method is applied to our case (6.113), where the Hamiltonian operator without cosmological constant ($b_\Lambda = 0$) in the representation x the gravitational operator can take two forms as in the eq.(6.126) for $\lambda \leq 0$ and in the eq.(6.132) for $\lambda > 0$. However, the change in variable $x(b)$ can have three possibilities depending on whether $\lambda < 0$, $\lambda = 0$ or $\lambda > 0$.
The parameters of the model are hidden in the change of variable. Thus, to solve the deficiency method (6.135) for the case $\lambda \leq 0$, we get the solutions

$$\psi^{\pm}(x) = c_{\pm}\left(\exp\left(\frac{1 \pm i}{\sqrt{2}}x\right) + \exp\left(-\frac{1 \pm i}{\sqrt{2}}x\right)\right), \tag{6.136}$$

where $c_{\pm} \in \mathbb{C}$. Nevertheless, the solutions are not normalizable on the Hilbert space $\mathcal{H}_g^{kin}$. Therefore, the scalar product of $\psi^{\pm}(x)$ is not finite; then $c_{\pm} = 0$. Thus, the deficiency subspaces contain only the null vector, that is, $n_{\pm} = \dim(\mathcal{K}^{\pm}) = 0$. Therefore, it is possible to conclude that the Hamiltonian operator (6.126) is essentially self-adjoint for $\lambda \leq 0$. Specifically, in the range that contains this analysis ($\lambda \leq 0$) includes the cases where the quantum Hamiltonian constraint is proportional only to the Euclidean part ($\lambda = -1/\gamma^2$) or the Lorentzian part ($\lambda = 0$), and when the Euclidean part dominates over the Lorentzian part, these cases are studied in [31, 32].
For the case where the weight parameter is positive, the solutions by the deficiency index method will take solutions that have a similar expression with respect to

the case $\lambda = 1$ that the authors studied in [28, 29]. The solution of the complex eigenvalue problem from the eq.(6.132) is given by

$$\psi^{\pm}(x) = C \begin{cases} \frac{1}{A_{\pm}}(e^{(1\mp i)x/\sqrt{2}} + e^{-(1\mp i)x/\sqrt{2}}), & |x| < x_0, \\ \frac{1}{B_{\pm}}(e^{(1\pm i)(\pi - x)/\sqrt{2}} + e^{-(1\pm i)(\pi - x)/\sqrt{2}}), & |x| > x_0, \end{cases} \tag{6.137}$$

where the normalization constants read

$$A_{\pm} = e^{(1\mp i)x_0/\sqrt{2}} + e^{-(1\mp i)x_0/\sqrt{2}}, \tag{6.138}$$

$$B_{\pm} = e^{(1\pm i)(\pi - x_0)/\sqrt{2}} + e^{-(1\pm i)(\pi - x_0)/\sqrt{2}}. \tag{6.139}$$

Since the solutions (6.137) are normalizable, the deficiency spaces $\mathcal{K}^{\pm}$ are 1-dimensional, the gravitational operator admits a family of infinite self-adjoint extensions, which are associated with a unitary transformation $U^{\alpha} : \mathcal{K}^{+} \to \mathcal{K}^{-}$ where each extension belongs to the group $U(1)$, which acts in the following form

$$U^{\alpha}\psi^{+} = e^{i\alpha}\psi^{-}. \tag{6.140}$$

The uniparametric family of self-adjoint extensions is labeled by the parameter $\alpha \in (0, 2\pi]$. Furthermore, using Theorem X.2, which is found in [83] where the extended domain $D_{\alpha}(\hat{\Theta}_{\lambda,g})$ of the Hamiltonian operator and the corresponding extension $\widehat{\Theta}_{\alpha}$ are written as

$$D_{\alpha}(\hat{\Theta}_{\lambda,g}) = \{\psi + \psi^{+} + U^{\alpha}\psi^{+};\ \psi \in D,\ \psi^{\pm} \in \mathcal{K}^{\pm}\}, \tag{6.141}$$

$$\hat{\Theta}_{\alpha}(\psi + \psi^{+} + U^{\alpha}\psi^{+}) = \hat{\Theta}_{\alpha}\psi + i\psi^{+} - iU^{\alpha}\psi^{+}. \tag{6.142}$$

It is possible to define $\psi^{\alpha} = \psi^{+} + U^{\alpha}\psi^{+}$ as an element of D_{α} which can characterize the self-adjoint extensions that can be calculated as

$$\psi^{\alpha}(x) = C_1 \begin{cases} h(\alpha, x, x_0), & |x| < x_0, \\ h(\alpha, \pi - x, \pi - x_0), & |x| > x_0, \end{cases} \tag{6.143}$$

where $C_1 \in \mathbb{C}$ and the function $h(\alpha, x, x_0)$ is defined as

$$h(\alpha, x, x_0) = \frac{e^{i\alpha/2}}{\cosh(\sqrt{2}x_0) + \cos(\sqrt{2}x_0)} \times \sum_{r,s=\pm 1} e^{(x + r x_0)s/\sqrt{2}} \cos\left(\frac{x - r x_0}{\sqrt{2}} + \frac{s\alpha}{\sqrt{2}}\right). \tag{6.144}$$

The ratios of the left and right derivatives of each extension at the boundary $x = \pm x_0$ depend only on the extension. That is,

$$\frac{\lim_{x \to^{+} x_0} \partial_x \psi^{\alpha}}{\lim_{x \to^{-} x_0} \partial_x \psi^{\alpha}} = \tan(x_0)\frac{\cos(\alpha/2) + \sin(\alpha/2)}{\cos(\alpha/2) - \sin(\alpha/2)} = -\tan(\beta). \tag{6.145}$$

Thus, it is possible to replace β with α as a label of the extension, where $\beta \in [0, \pi)$, $\tan(\beta)$ is a convenient and consistent choice that is bijective to U^{α}. As in previous papers [26, 28, 29] this condition can be interpreted as a glue condition at $b = \pm b_0$.

Furthermore, to solve the eigenvalue problem for a general eigenvalue ω^2 for the gravitational operator (6.132) where the solutions are given by

$$\psi_{\omega^2}(x) = \begin{cases} A(e^{i\omega x} + e^{-i\omega x}), & |x| < x_0, \\ B(e^{\omega(\pi - x)} + e^{-\omega(\pi - x)}), & |x| > x_0, \end{cases} \tag{6.146}$$

where $A, B \in \mathbb{C}$. Since $\hat{\Theta}_\beta$ has discrete spectre, the physical states $\Psi_\beta(x, \phi)$ of each self-adjoint extension $\hat{\Theta}_\beta$ of the quantum constraint $\hat{\Theta}$ have the following form

$$\psi_\beta(x, \phi) = \sum_{n=0}^{\infty} \Phi_n \Psi_{\beta,n}(x) e^{i\omega_{\beta,n}(\phi - \phi_0)}, \tag{6.147}$$

where Φ_n are the square-summable sequences, $\Psi_{\beta,n}$ are the normalized eigenfunctions of $\hat{\Theta}_\beta$ with eigenvalue $\omega^2_{\beta,n}$, which is related to k_n through $\omega_n^2 = 12\pi G k_n^2$. Taking into account the relation (6.145) the normalized eigenfunctions can be written as

$$\Psi_{\beta,n}(x) = N_{\beta,n} \begin{cases} \cosh(k_n(\pi - x_0)) \cos(k_n x), & |x| < x_0, \\ \cos(k_n x_0) \cosh(k_n(\pi - x)), & |x| > x_0, \end{cases} \tag{6.148}$$

where the normalizable constants are given by $N_{\beta,n}$ and $k_{\beta,n}$ take their values fixed by the following transcendental equation

$$\tan(k_n x_0) + \tanh(k_n(\pi - x_0)) \tan(\beta) = 0. \tag{6.149}$$

The dynamical evolution of the Hamiltonian operator is generated using the scalar field as an evolution parameter and the square root of the positive part of the self-adjoint extension of this operator $\hat{\Theta}_\beta$. Thus,

$$\psi_\beta(x, \phi) = e^{i(\phi - \phi_0)\sqrt{|\Theta_\beta|}} \psi_\beta(x, \phi_0) \tag{6.150}$$

where $\psi_\beta(x, \phi) \in \mathcal{H}^{phy}_\beta = P^+_\beta \mathcal{H}^g_{kin}$ taking P^+ as the projection onto the positive part of the operator $\hat{\Theta}_\beta$.

The Hamiltonian operator (6.113) without an explicit cosmological constant is essentially self-adjoint for values of $\lambda \leq 0$, therefore there is only a unique extension and the dimension of the deficiency subspaces is equal zero. Furthermore, for values $\lambda > 0$, the gravitational operator admits a family of self-adjoint extensions that are related to the elements of the group $U(1)$. The strategy to explore analytically the self-adjoint property of this operator was the same one that has been adopted in [26, 28, 29, 114]. To find the deficiency subspaces it is necessary to build a new representation x, where the gravitational operator takes the KG form, this form is adopted due to the operator form in LQC, also this is convenient to solve the eigenvalue problem. The parameters that contain the LQC model hide in the change of variable $x(b)$, for example, the expressions for $x(b)$ are different for the cases $\lambda = 0$ and $\lambda < 0$, but the conclusions and calculations after this transformation are the same because it has the same mathematical structure. This makes it difficult to obtain physical information in this representation. Since each value λ is a different model in LQC.

As we saw at the end of Section 6.1.1, the main result of the paper [30] is to match the observational and theoretical cosmological constants; this occurs when the weight parameter takes the following value $\lambda_2 = \frac{\Delta\Lambda_{ob}}{3} \sim 10^{-122}$. Note that $\lambda_2 > 0$, but it is a very small quantity, close to zero. We can revisit the different models analyzed in this section, where for models with positive weight parameters, the quantum constraint operator admits a family of self-adjoint extensions, each extension being related to an element of the group $U(1)$. Therefore, the gravitational operator for this value of λ_2 requires an extension in the domain, and the contribution of the Euclidean part to the constraint is almost negligible because λ_2 is close to zero. Indeed, when $\lambda = 0$ the Hamiltonian constraint is only proportional to the Lorentzian term and the geometric operator is essentially self-adjoint, for this case, we have only a unique extension in contrast to models with positive weight parameter.

Since the Hamiltonian operator in x-representation has the same functional form, that is, the KG equation, it would seem that this analysis is the same no matter what parameters are fixed on the Hamiltonian operator. However, there is a substantial difference in each choice of the fixed parameters that are used. This lies in the change of the variable between x and b, which is different for each case. To distinguish physical regions of the cosmological constant, these parameters, including the self-adjoint extensions, can have a specific weight. However, the self-adjoint parameter that characterizes the extensions until have not been included in an LQC effective model, this is due to the difficult to build an extended Hamiltonian operator, because the operator in x-representation is only a means to find the dimension of the deficiency subspaces, which are used to explore self-adjointness. Furthermore, another important outcome is the ambiguity in the quantization program regardless of whether the same regularization program is used in this analysis; these ambiguities in LQC have been studied in [27], also in [115] where the authors found a different Hamiltonian operator without this weight parameter that includes both terms but is essentially self-adjoint, only using these ambiguities in the regularization program.

6.3 Hyperbolic Universe

Another possible shape of the universe from the classical description is described by hyperbolic geometry such as in Section 3.1. This open universe is obtained when the curvature $k = -1$ in the FLRW metric. In LQC the hyperbolic universe has been studied in [34, 35, 38].

This section presents a brief review of this model without the cosmological constant ($b_\Lambda = 0$) and weight parameter $\lambda = 1$. For models where the spatial curvature is distinct from zero, it is necessary to consider the effect due to the spin connection, namely, $A^i_a = \gamma K^i_a + \Gamma^i_a$.

The line element for an isotropic and homogeneous model reads

$$\begin{aligned} \mathrm{d}s^2 &= -N(t)^2\mathrm{d}t^2 + a(t)^2\left[\frac{\mathrm{d}r^2}{1-kr^2} + r^2(\mathrm{d}\theta^2 + \sin^2(\theta)\mathrm{d}\phi^2)\right], \\ &= -N(t)^2\mathrm{d}t^2 + \alpha_{ij}(t)\,{}^o\omega^i_a\,{}^o\omega^j_b\mathrm{d}x^a\mathrm{d}x^b, \end{aligned} \tag{6.151}$$

where $\alpha_{ij}(t)$ are the dynamical components of the metric, with $k = -1$ the universe takes a hyperbolic shape. It is necessary to introduce an elementary cell $\mathcal{V}$ because this model is spatially open. Moreover, the fiducial metric is chosen as ${}^oq_{ab} =$

${}^o\omega_a^i {}^o\omega_b^j \delta_{ij}$ they are one-forms invariant to the left for $k = -1$, and satisfy the Maurer-Cartan relation

$$\mathrm{d}{}^o\omega^i = -\frac{1}{2} C^i_{jk} {}^o\omega^j \wedge {}^o\omega^k, \tag{6.152}$$

where C^i_{jk} are the structure constants of the isometry group, that characterize the Bianchi V model, for $k = -1$,

$$C^i{}_{jk} = \delta^i_j \delta_{k1} - \delta^i_k \delta_{j1}. \tag{6.153}$$

For flat models the structure constants are zero, in $k = -1$ model they are distinct from zero, which implies the Bianchi V model is class B. On the other hand, the fiducial left-invariant vector fields ${}^o e^a_i$, which are dual to ${}^o\omega^i_a$, satisfy ${}^o e^a_i {}^o\omega^j_a = \delta^j_i$ and ${}^o e^a_i {}^o\omega^i_b = \delta^a_b$. Thus, the left-invariant vectors obey the following commutator, which provides a representation of the Lie algebra as

$$[{}^o e_i, {}^o e_j] = C^k{}_{ij} {}^o e_k. \tag{6.154}$$

The spin connection Γ^i_a takes the following form

$$\Gamma^i_a = -\frac{1}{2} \epsilon^{ijk} e^b_j \left(\partial_a e^k_b - \partial_b e^k_a + e^c_k e^l_a \partial_c e^m_b \delta_{lm} \right), \tag{6.155}$$

where the physical triads obey $e^i_a e^i_b = q_{ab}$ and this physical triads are related to the densitized triad E^a_i

$$E^a_i = \sqrt{\det(q)} e^a_i = p V_o^{-\frac{2}{3}} \sqrt{\det({}^o q)} {}^o e^a_i. \tag{6.156}$$

Using the symmetry reduction form in (6.156) and replacing into (6.155), one gets

$$\Gamma^i_a = \Gamma^i_j {}^o\omega^j_a = -\epsilon^{1ij} {}^o\omega^j_a, \tag{6.157}$$

where

$$\Gamma^i_j = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{6.158}$$

Note that Γ^i_j is non-diagonal. Then, the Ashtekar-Barbero connection in the symmetry reduced model reads

$$A^i_a = -\epsilon^{1ij} {}^o\omega^j_a + c V_o^{-\frac{1}{3}} {}^o\omega^i_a = A^i_j V_o^{-\frac{1}{3}} {}^o\omega^j_a, \tag{6.159}$$

where

$$A^i_j = \begin{pmatrix} c & 0 & 0 \\ 0 & c & -V_o^{\frac{1}{3}} \\ 0 & V_o^{\frac{1}{3}} & c \end{pmatrix}. \tag{6.160}$$

Here the pair (c, p) are the conjugated variables as in flat model in Section 6.1, which obey the Poisson bracket (3.33). However, as in that section, the improved variables (b, v) are used.

The gravitational constraint (2.54) including the effect due to the curvature takes the form [30]

$$H_g(N) = H^E(N) - 2(1+\gamma^2)H^L(N), \tag{6.161}$$

the Euclidean term $H^E(N)$ and the Lorentzian term $H^L(N)$ are defined as in (3.36) and (3.37), respectively

$$\begin{aligned} H^E(N) &= \frac{1}{16\pi G}\int_\Sigma d^3x N F^j_{ab}\frac{\epsilon_{jkl}E^a_k E^b_l}{\sqrt{q}}, \\ H^L(N) &= \frac{1}{16\pi G}\int_\Sigma d^3x N \epsilon^j_{mn} K^m_a K^n_b \frac{\epsilon_{jkl}E^a_k E^b_l}{\sqrt{q}}. \end{aligned}$$

It is convenient to introduce the notation [38] where ${}^{(X)}H^E(N)$ is the Euclidean term for an arbitrary connection X which can be read as in (6.32)

$${}^{(X)}H^E(N) = \frac{1}{16\pi G}\int_\Sigma d^3x N {}^{(X)}F^j_{ab}\frac{\epsilon_{jkl}E^a_k E^b_l}{\sqrt{q}}.$$

Note that $F^i_{ab} = {}^{(A)}F^i_{ab}$ hence by definition $H^E(N) = {}^{(A)}H^E(N)$ and $H^E(N) = {}^{(\Gamma)}H^E(N) + {}^{(\gamma K)}H^E(N)$. Thus, the Hamiltonian constraint is given by

$$\begin{aligned} H_g(N) &= {}^{(\Gamma)}H^E_k(N) + {}^{(\gamma K)}H^E(N) - 2(1+\gamma^2)H^L(N), \\ &= {}^{(\Gamma)}H^E_k(N) + H_0(N). \end{aligned} \tag{6.162}$$

We shall use $N=1$ and the notation $H_g(1) = H_g$ for each term in the constraint. Furthermore, the functional form of the Euclidean term for a flat space ($k=0$) H^E_0 is the same as ${}^{(\gamma K)}H^E$. Indeed, the only term in Eq.(6.162) that does not have the same functional form as in a flat model is ${}^{(\Gamma)}H^E(N)$. Therefore, the flat Hamiltonian constraint H_0 is given by

$$H_0(N) = {}^{(\gamma K)}H^E(N) - 2(1+\gamma^2)H^L(N), \tag{6.163}$$

in eq.(6.162) the term ${}^{(\Gamma)}H^E_k(N) = 0$ when $k=0$, because the spin connection vanishes, then for $k=0$ the gravitational constraint constitutes only the flat Hamiltonian constraint $H_0(N)$. This constraint is studied in Section 6.1. We focus here on the term due to the spin connection ${}^{(\Gamma)}H^E_k(N) = H^\Gamma_{k=-1}$, that in (b,v) variables for $k=-1$ is given by

$$H^\Gamma_{k=-1} = \frac{3(\gamma\sqrt{\Delta}\hbar)^{\frac{1}{3}}V_o^{\frac{2}{3}}}{4(2\pi G)^{\frac{2}{3}}}|v|^{\frac{1}{3}}. \tag{6.164}$$

Thus, the gravitational constraint for $k=-1$ in the symmetry-reduced Ashtekar-Barbero variables can be expressed as

$$H_g^{k=-1} = -\frac{3\hbar|v|}{\gamma\sqrt{\Delta}}\left[\frac{b^2}{4} - V_o^{\frac{2}{3}}\left(\frac{\gamma^2\Delta}{16\pi G\hbar|v|}\right)^{\frac{2}{3}}\right]. \tag{6.165}$$

As for the total Hamiltonian constraint $H_F = H_g^{k=-1} + H_\phi$, where the Hamiltonian part of matter is given (6.5), it yields the classical Friedmann equation (3.29)

$$\begin{aligned} H^2 &= \left(\frac{\dot{v}}{3v}\right)^2 = \left(\frac{\{v, H_F^{k=-1}\}}{3v}\right)^2 \\ &= \frac{8\pi G}{3}\rho + \frac{V_o^{2/3}}{V^{2/3}} = \frac{8\pi G}{3}\rho + \frac{1}{a^2}, \end{aligned} \tag{6.166}$$

where H denotes the Hubble parameter for $k = -1$.
To introduce the quantum description the Hamiltonian part due to spin connection (6.164) can be expressed in flux and holonomy variables. The regularized Hamiltonian term due to the curvature is

$$\begin{aligned} H_{k=-1}^{\Gamma,\bar{\mu}} &= \frac{\mathrm{sgn}(p) V_o^{\frac{2}{3}}}{2\kappa\pi G\gamma\bar{\mu}} \sum_k \mathrm{Tr}\left(\tau_k h_k^{(\bar{\mu})} \left\{h_k^{(\bar{\mu})-1}, V\right\}\right) \\ &= \frac{\hbar(\hbar\gamma\sqrt{\Delta})^{\frac{1}{3}} V_o^{\frac{2}{3}}}{4(2\pi G)^{\frac{2}{3}}} \mathrm{sgn}(v)|v|^{\frac{1}{3}} \sum_k \mathrm{Tr}\left(\tau_k h_k^{(\bar{\mu})} \left\{h_k^{(\bar{\mu})-1}, |v|\right\}\right), \end{aligned} \tag{6.167}$$

where

$$H_{k=-1}^{\Gamma} = \lim_{\bar{\mu}\to 0} H_{k=-1}^{\Gamma,\bar{\mu}}. \tag{6.168}$$

Next the spherical model in LQC is presented in the next section. Then the three models will be given and compared.

6.4 Spherical Universe

Another shape of the Universe is found when the curvature is positive, $k = 1$, this universe describes a closed and spherical form. In LQC these types of models have been studied in [3, 33, 36, 37, 39]. The fiducial metric in 1-form terms ${}^0\omega_a^i$ and vectors ${}^o e_i^a$ is given by

$${}^o q_{ab} = {}^o\omega_a^i \, {}^o\omega_b^j k_{ij}, \tag{6.169}$$

where k_{ij} is the Cartan-Killing metric in $su(2)$. This metric is over a 3-sphere of radius $r_0 = 2$. Additionally, the spacetime manifold $M = \mathbb{R} \times \Sigma$ is formed by the 3d spatial compact manifold Σ, whose volume with respect to this metric is $V_0 = 16\pi^2$ and the scalar curvature is ${}^o R = 3/2$.
Furthermore, since the curvature of the spin connection can be written as ${}^{(\Gamma)}F_{ab}^i = \Omega_{ab}^i$, for a $k = 1$ model, this curvature is non-zero and has the following expression [36, 37, 39]

$${}^{(\Gamma)}F_{ab}^l = \Omega_{ab}^l = -\frac{1}{r_0}\epsilon_{ij}^l \, {}^o\omega_a^i \, {}^o\omega_b^j. \tag{6.170}$$

To obtain the flat case, we can take the limit $r_0 \to \infty$, then r.h.s of eq.(6.170) is zero. The orthogonal Cartan triad ω_a^i in the 3-sphere of radius $r_0 = 2$ obeys

$$\mathrm{d}\omega^k + \frac{1}{2}\epsilon_{ij}^k \omega^i \wedge \omega^j = 0. \tag{6.171}$$

In variables (c, p), we have the physical 3d metric q_{ab} and the extrinsic curvature K_{ab} given by

$$q_{ab} = |p| V_0^{-2/30} q_{ab}, \tag{6.172}$$

$$\gamma K_{ab} = \left(c - \frac{V_0^{1/3}}{2} \right) |p|^{1/2} V_0^{-3/20} q_{ab}. \tag{6.173}$$

The Hamiltonian constraint using the improved canonical pair is read as

$$H_F = -\frac{3\hbar|v|}{\gamma\sqrt{\Delta}} \left[\frac{b^2}{4} + V_0^{2/3} \left(\frac{\gamma^2 \Delta}{16\pi G\hbar|v|} \right)^{2/3} \right] + \frac{p_\phi^2}{4\pi\gamma\ell_p^2\sqrt{\Delta}|v|}. \tag{6.174}$$

The total gravitational constraint H_F is built with the Euclidean part (3.36) and the Lorentzian part (3.37) along with the Hamiltonian part of the matter field (6.5). In (6.162) is expressed in terms of holonomies and fluxes for $k = 1$ as

$$H_{k=1}^{\Gamma,\bar{\mu}} = -\frac{\text{sgn}(p) V_0^{2/3}}{16\pi^2 G\gamma\bar{\mu}} \sum_j \text{Tr} \left(\tau_j h_j^{(\bar{\mu})} \{ h_j^{(\bar{\mu})^{-1}}, V \} \right), \tag{6.175}$$

where the regularized Hamiltonian part due to the curvature $k = 1$ is

$$H_{k=1}^{\Gamma} = \lim_{\bar{\mu} \to 0} H_{k=1}^{\Gamma,\bar{\mu}}. \tag{6.176}$$

6.5 Unified description $k = 0, \pm 1$

In this section, an integrated version of the models is presented for an arbitrary curvature k. The quantum Hamiltonian constraint corresponding to (6.162) is given by

$$\hat{H}_F \psi(v, \phi) = (\hat{H}_g + \hat{H}_\phi)\psi(v, \phi) = 0, \tag{6.177}$$

where the geometric Hamiltonian operator $\hat{H}_g$ takes the following form.

$$\hat{H}_g = \hat{H}_0^E + \hat{H}_k^\Gamma - 2(1 + \gamma^2)\hat{H}^L. \tag{6.178}$$

Note that from the quantum description of this cosmological model there exists an effect due to the curvature. Such an effect is a generalization for an arbitrary k. As discussed as in previous sections, the solution of the Hamiltonian operator does not have an exact solution; for this reason, a simplified form of the Hamiltonian operator is introduced, which includes the effect of the curvature $\hat{\Theta}_g = \hat{\Theta}_0^E - 2(1 + \gamma^2)\hat{\Theta}^L + \hat{\Theta}_k^\Gamma$. Therefore, acting on the basis of $|v\rangle$, we obtain the following expression

$$\begin{aligned} \hat{\Theta}_g |v\rangle &= \frac{3\pi G\gamma^2}{4} v[(v+2)|v+4\rangle - 2v|v\rangle + (v-2)|v-4\rangle] \\ &- \frac{3\pi G(1+\gamma^2)}{16} v[(v+4)|v+8\rangle - 2v|v\rangle + (v-4)|v-8\rangle] \\ &- 3\pi G k\gamma^2 \Delta \frac{V_0^{2/3}}{V^{2/3}} v^2 |v\rangle, \end{aligned} \tag{6.179}$$

where the total simplified operator is given by $\hat{\Theta}_F = \mathbb{I} \otimes \partial_\phi^2 + \hat{\Theta}_g \otimes \mathbb{I}$.
From equation (6.179) using the kinematical states of group averaging, it is possible to obtain the physical states as

$$\psi_f(v,\phi) = \lim_{\alpha_0 \to \infty} \int_{-\alpha_0}^{\alpha_0} \mathrm{d}\alpha e^{i\hat{\Theta}_F} f(v,\phi), \tag{6.180}$$

where $f(v,\phi)$ belongs to $\mathcal{H}_{kin}$. The transition amplitude in the timeless framework is given by the physical inner product as

$$\begin{aligned} A_{tls}(v_f,\phi_f|v_i,\phi_i) &= \langle v_f,\phi_f|v_i,\phi_i|v_f,\phi_f|v_i,\phi_i\rangle_{phy} \\ &= \lim_{\alpha_0\to\infty} \int_{-\alpha_0}^{\alpha_0} \mathrm{d}\alpha \, \langle v_f,\phi_f| \, e^{i\alpha\hat{\Theta}_F} \, |v_i,\phi_i\rangle \, , \end{aligned} \tag{6.181}$$

where $|v_i,\phi_i\rangle$ and $|v_f,\phi_f\rangle$ belong to $\mathcal{H}_{kin}$. Taking into account the path integral method explained in Section 6.1.1 the transition amplitude reads

$$\begin{aligned} A^F_{tls}(v_f,\phi_f|v_i,\phi_i) &= \lim_{N\to\infty} \lim_{\alpha_{N_0},\ldots,\alpha_{1_0}\to\infty} \left(\epsilon \prod_{n=2}^{N} \frac{1}{2\alpha_{n_0}}\right) \int_{-\alpha_{N_0}}^{\alpha_{N_0}} \mathrm{d}\alpha_N \ldots \int_{-\alpha_{1_0}}^{\alpha_{1_0}} \mathrm{d}\alpha_1 \\ \times \int_{\infty}^{\infty} \mathrm{d}\phi_{N-1}\ldots\mathrm{d}\phi_1 &\left(\frac{1}{2\pi\hbar}\right)^N \int_{\infty}^{\infty} \mathrm{d}p_{\phi_{N-1}}\ldots\mathrm{d}p_{\phi_1} \sum_{v_{N-1},\ldots,v_1} \left(\frac{2}{\pi}\right)^N \int_0^{\pi/2} \mathrm{d}b_N\ldots\mathrm{d}b_1 \\ &\times \prod_{n=1}^{N} \exp i\epsilon \left[\frac{p_{\phi_n}}{\hbar}\frac{\phi_n-\phi_{n-1}}{\epsilon} - b_n\frac{v_n-v_{n-1}}{\epsilon}\right. \\ \left. +\alpha_n \left(\frac{p^2_{\phi_n}}{\hbar^2} - 3\pi G\sqrt{v_n v_{n-1}}\frac{v_n+v_{n-1}}{2}\right.\right. &\left.\left.\sin^2(2b_n)[1-(1+\gamma^2)\sin^2(2b_n)] + k\gamma^2\Delta\frac{V_0^{2/3}}{V^{2/3}}\right)\right]. \end{aligned} \tag{6.182}$$

Furthermore, replacing $\sum_{n=1}^{N}\epsilon$ by $\int_0^1 \mathrm{d}\tau$ in the path-integral formulation we get

$$\begin{aligned} A^F_{tls}(v_f,\phi_f|v_i,\phi_i) = \beta \int \mathcal{D}\alpha \int \mathcal{D}\phi \int \mathcal{D}p_\phi \int \mathcal{D}v \int \mathcal{D}b \exp\left\{\frac{i}{\hbar}\int_0^1 \mathrm{d}\tau \left[p_\phi\dot{\phi} - \hbar b\dot{v}\right.\right. \\ \left.\left. +\hbar\alpha\left(\frac{p_\phi^2}{\hbar^2} - 3\pi G v^2\left[\sin^2(2b)(1-(1+\gamma^2)\sin^2(2b)) + k\gamma^2\Delta\frac{V_0^{2/3}}{V^{2/3}}\right]\right)\right]\right\}, \end{aligned} \tag{6.183}$$

where β is a constant, the notation of a dot on a letter means the derivative with respect to the time variable τ. Hence, the effective Hamiltonian constraint $\tilde{C}_{\text{eff}}$ is given by

$$\tilde{C}_{\text{eff}} = \frac{p_\phi^2}{\hbar^2} - 3\pi G v^2\left[\sin^2(2b)(1-(1+\gamma^2)\sin^2(2b)) + k\gamma^2\Delta\frac{V_0^{2/3}}{V^{2/3}}\right]. \tag{6.184}$$

Thus, it is convenient to rewrite it in terms of (6.179) using the constraint is weakly zero. Thus,

$$C_{\text{eff}} = \frac{p_\phi^2}{2V} - \frac{3}{8\pi G\Delta\gamma^2}V\left[\sin^2(2b)(1-(1+\gamma^2)\sin^2(2b)) + k\gamma^2\Delta\frac{V_0^{2/3}}{V^{2/3}}\right]. \tag{6.185}$$

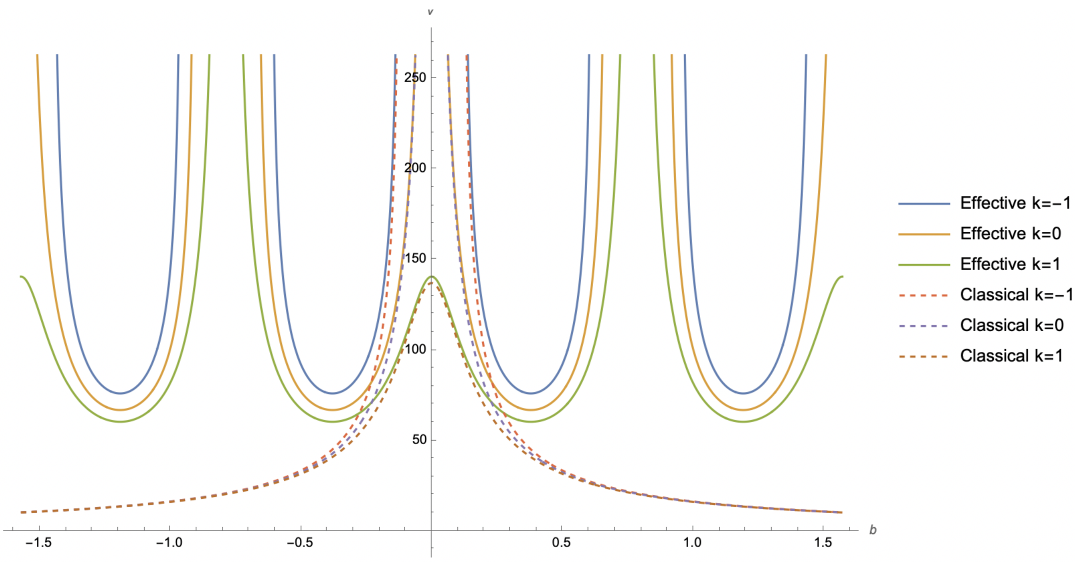

Figure 6.5.1: This plot compares each possible geometry of FLRW universe with $k = -1, 0, 1$, through the relationship between v and b. The total effective Hamiltonian constraint $C_{\text{eff}} = 0$ and natural units are used. Furthermore, we take the values $\gamma = 0.2375$ and $p_\phi = 100$.

Figure 6.5.1 shows the comparison between the different geometries described by each possible value of k. This behavior is obtained with the effective total Hamiltonian constraint $C_{\text{eff}} = 0$. Note that every effective universe replaces the big bang with a quantum bounce, which connects two different universes. Furthermore, the closed universe is a continuous line where the bounce takes a finite volume instead of the open universes given by $k = -1, 0$, which have similar behavior. This plot is consistent with the previous results for open cosmological models that include the Euclidean and Lorentzian terms in the Hamiltonian constraint. The dashed lines represent the classical counterpart defined by the standard Friedmann equation in terms of the variables v and b; this behavior is explained by Eq.(6.12), we note that each classical trajectory in each geometry converges to a line. Moreover, from the effective model, it is possible to obtain the classical dynamic in some limits, which will be discussed in the next section.

The effective model from eq.(6.185), with density energy defined for a curved universe as

$$\rho_k = \frac{3}{8\pi G\gamma^2\Delta}\sin^2(2b)(1-(1+\gamma^2)\sin^2(2b)) + \frac{3}{8\pi G}\frac{k}{a^2}, \tag{6.186}$$

where $\rho_k = p_\phi^2/(2V)$. On the other hand, from the effective Hamilton equation $\dot{v} = \{v, C_{\text{eff}}\}$, we have the modified Friedman equation

$$H_{\text{eff}}^2 = \left(\frac{\dot{v}}{3v}\right)^2 = \frac{1}{\gamma\sqrt{\Delta}}\sin^2(2b)[1-\sin^2(2b)][1-2(1+\gamma^2)\sin^2(2b)]^2, \tag{6.187}$$

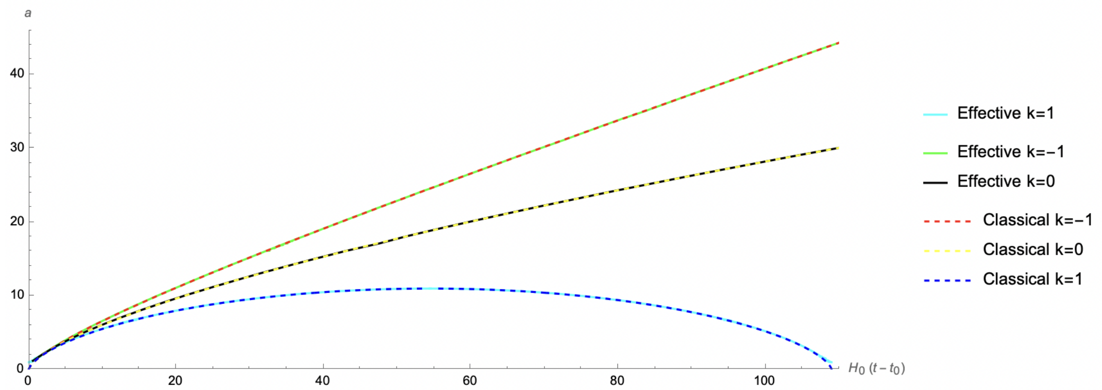

Figure 6.5.2: Each possible geometry of the effective and classical universe ($k = -1, 0, 1$) are compared through the Hubble parameter vs scale factor in Eq.(6.193) at large scales. We take $\gamma = 0.2375$.

where $H_{\text{eff}} = \dfrac{\dot{a}}{a}$ denotes the effective Hubble parameter, and the Raychaudhuri equation is written as

$$\frac{\ddot{a}}{a} = H_{\text{eff}}^2 + \frac{1}{\gamma\sqrt{\Delta}}\dot{b}\left[1 - 2\sin^2(2b) - 2(1+\gamma^2)\sin^2(2b)(3 - 4\sin^2(2b))\right], \quad (6.188)$$

where $\dot{b} = \{b, C_{\text{eff}}\}$. The bounce occurs when $H_{\text{eff}}^2 = 0$, which implies that b_c is at a critical point at

$$b_c = \frac{1}{2}\arcsin\left(\sqrt{\frac{1}{2(1+\gamma^2)}}\right). \quad (6.189)$$

Therefore, the maximum value of the energy density ρ_c when b takes the critical value (6.189)

$$\rho_c = \rho_0 + \frac{3}{8\pi G}\frac{k}{a^2}, \quad (6.190)$$

where ρ_0 takes the value for the energy density of a flat universe such as in eq.(6.89), which is given by

$$\rho_0 = \frac{3}{32\pi G\gamma^2(1+\gamma^2)\Delta}. \quad (6.191)$$

We get two distinct roots b_+ and b_- of the eq.(6.187), which are expressed as

$$\sin^2(2b_\pm) = \frac{1 \pm \sqrt{1 - \dfrac{\rho - \dfrac{3}{8\pi G}\dfrac{k}{a^2}}{\rho_0}}}{2(1+\gamma^2)}. \quad (6.192)$$

For each of these solutions, there exists a different type of classical universe that is connected through a quantum bounce such as is shown in Figure 6.5.3.

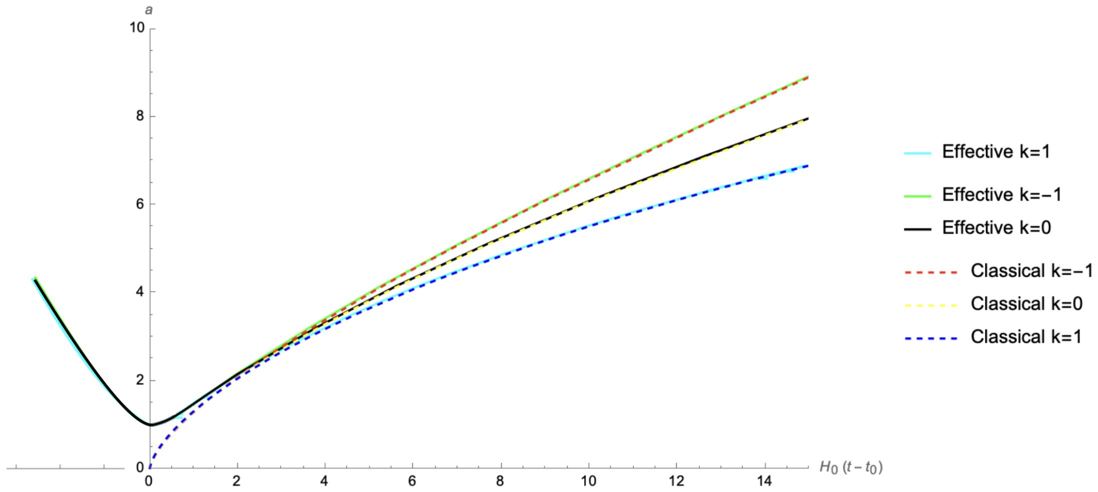

Figure 6.5.3: Each possible geometry of the effective and classical universe ($k = -1, 0, 1$) are compared through the Hubble parameter vs scale factor in Eq.(6.193) and Eq.(6.194) close to quantum bounce. We take $\gamma = 0.2375$.

These classical universes are described by the Hubble parameter, such as

$$H^2_{\text{eff},+} = \frac{8\pi G}{3}\rho_\Lambda\left(1-\frac{\rho-\frac{3}{8\pi G}\frac{k}{a^2}}{\rho_0}\right) \times\left[1+\left(\frac{\rho-\frac{3}{8\pi G}\frac{k}{a^2}}{\rho_0}\right)\frac{1-2\gamma^2+\sqrt{1-\frac{\rho-\frac{3}{8\pi G}\frac{k}{a^2}}{\rho_0}}}{4\gamma^2\left(1+\sqrt{1-\frac{\rho-\frac{3}{8\pi G}\frac{k}{a^2}}{\rho_0}}\right)}\right], \tag{6.193}$$

$$H^2_{\text{eff},-} = \frac{8\pi G}{3}\left(\rho-\frac{3}{8\pi G}\frac{k}{a^2}\right) \times\left(1-\frac{\rho-\frac{3}{8\pi G}\frac{k}{a^2}}{\rho_0}\right)\left[1+\frac{\gamma^2}{1+\gamma^2}\left(\frac{\sqrt{\frac{\rho-\frac{3}{8\pi G}\frac{k}{a^2}}{\rho_0}}}{1+\sqrt{1-\frac{\rho-\frac{3}{8\pi G}\frac{k}{a^2}}{\rho_0}}}\right)^2\right], \tag{6.194}$$

where $H^2_{\text{eff},\pm}$ is the effective Hubble parameter for the corresponding solution $b_\pm$. Furthermore, $\rho_\Lambda = \frac{\Lambda_{\text{eff}}}{8\pi G}$ and Λ_{eff} denote the effective cosmological constant [27–30]

$$\Lambda_{\text{eff}} = \frac{3}{\Delta(1+\gamma^2)^2}. \tag{6.195}$$

As in Section 6.1.1 the corresponding Friedman equation at these asymptotic limits can be written as

$$H_{\text{eff}}^2 = \begin{cases} \dfrac{8\pi G}{3}\rho - \dfrac{k}{a^2}, & \text{for} \quad b = 0, \\ \left(\dfrac{1-5\gamma^2}{1+\gamma^2}\right)\left[\dfrac{8\pi G}{3}\rho - \dfrac{k}{a^2}\right] + \dfrac{\Lambda_{\text{eff}}}{3}, & \text{for} \quad b = \dfrac{1}{2}\arcsin\left(\dfrac{1}{\sqrt{1+\gamma^2}}\right). \end{cases} \tag{6.196}$$

The effective Hubble parameter, which corresponds to the asymptotic limit for $b = 0$, becomes FLRW universe with curvature and coupling to a scalar matter field. On the other hand, the asymptotic limit for $b = b_1 = \frac{1}{2}\arcsin\left(\frac{1}{\sqrt{1+\gamma^2}}\right)$ corresponds to a de Sitter universe with an effective positive cosmological constant and curvature and coupling to a scalar matter field. Both universes are connected by a quantum bounce.

In addition, the asymptotic behavior of the Raychaudhuri equation (6.188) takes the following form

$$\frac{\ddot{a}}{a} = \begin{cases} -\dfrac{4\pi G}{3}(\rho + 3P), & \text{for} \quad b = 0, \\ -\left(\dfrac{1-5\gamma^2}{1+\gamma^2}\right)\left[\dfrac{4\pi G}{3}(\rho + 3P)\right] + \dfrac{\Lambda_{\text{eff}}}{3}, & \text{for} \quad b = b_1, \end{cases} \tag{6.197}$$

where the pressure of the matter is defined as $P = -\dfrac{\partial H_\phi}{\partial V}$. Furthermore, the Ricci scalar is defined as

$$R = 6\left(\left(\frac{\dot{a}}{a}\right)^2 + \frac{\ddot{a}}{a} + \frac{k}{a^2}\right), \tag{6.198}$$

taking into account (6.198) we get the asymptotic limit as

$$R = \begin{cases} -16\pi G\rho, & \text{for} \quad b = 0, \\ -16\pi G\rho\left(\dfrac{1-5\gamma^2}{1+\gamma^2}\right) + 4\Lambda_{\text{eff}} + \dfrac{36\gamma^2}{1+\gamma^2}\dfrac{k}{a^2}, & \text{for} \quad b = b_1, \end{cases} \tag{6.199}$$

where we assume $P = \rho$. Note that the scalar of curvature includes an additional term due to the geometry of the universe given by k.

Figure 6.5.2 and Figure 6.5.3 compare the different geometries of classical behaviour and effective universe built by eq.(6.193) both on large scales and close to the quantum bounce. Note that the effective behavior of hyperbolic, flat, and spherical universes converges rapidly to the classical description of the same geometries. Nevertheless, both descriptions differ for small values of a, where the classical universes approach the Big Bang at $a = 0$, but the effective LQC universes replace the Big Bang singularity by quantum bounce.

Figure 6.5.4 shows the behavior of the flat universe in the branch (6.194) for $k = 0$ for the effective and classical model. The comparison between the effective and classical universe for the open hyperbolic model ($k = -1$) is illustrated in Figure 6.5.5 and Figure 6.5.6 compares the effective and classical branches (6.194) for the closed and spherical model ($k = 1$). For each case ($k = -1, 0, 1$) note that the branch, given by (6.194), comes from the quantum bounce for the effective model

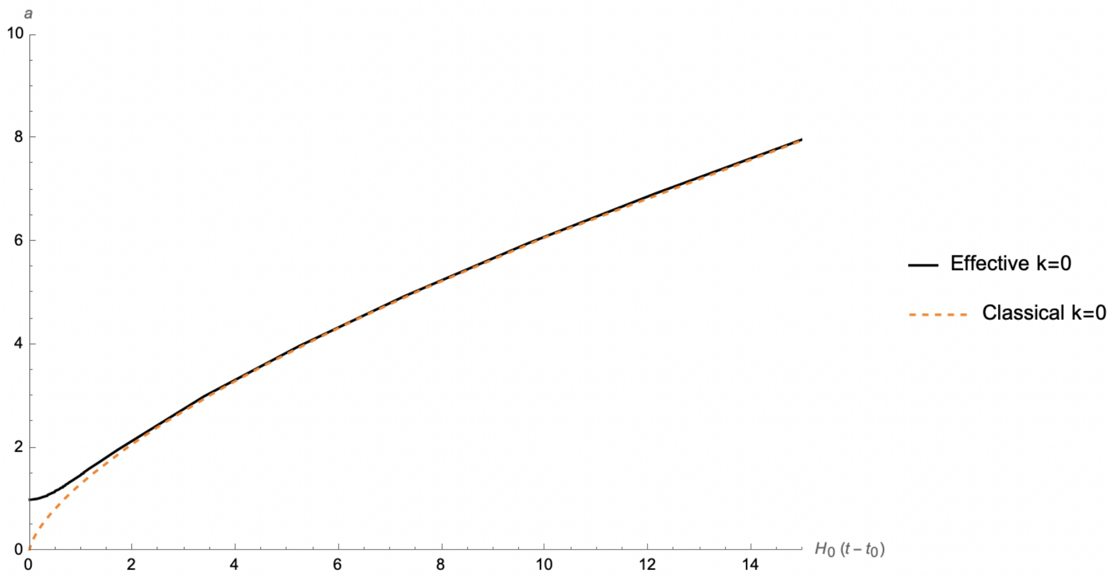

Figure 6.5.4: Comparison of the classical and effective $k = 0$ universe at small scales.

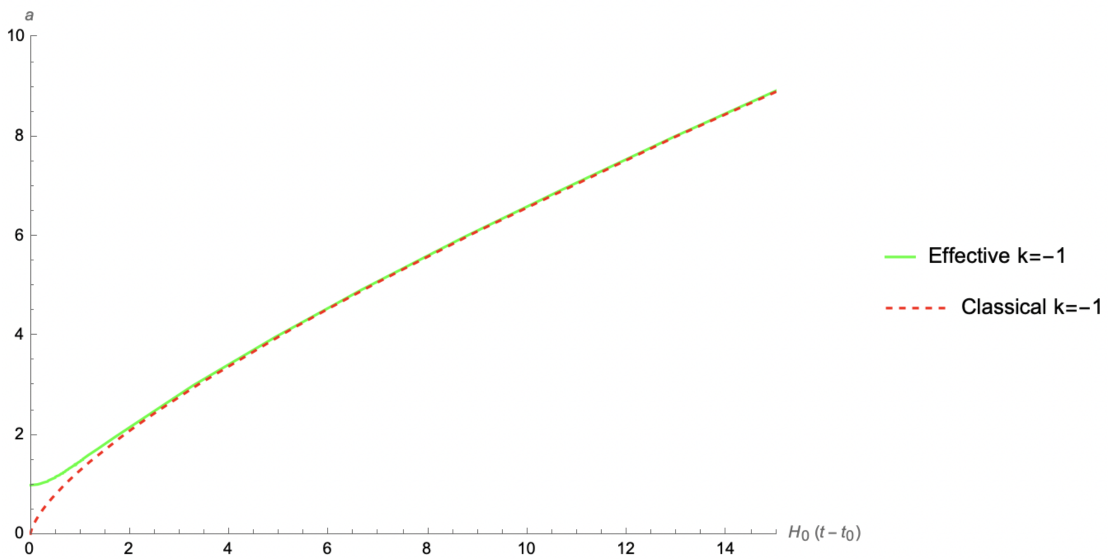

Figure 6.5.5: Comparison of the classical and effective $k = -1$ universe at small scales.

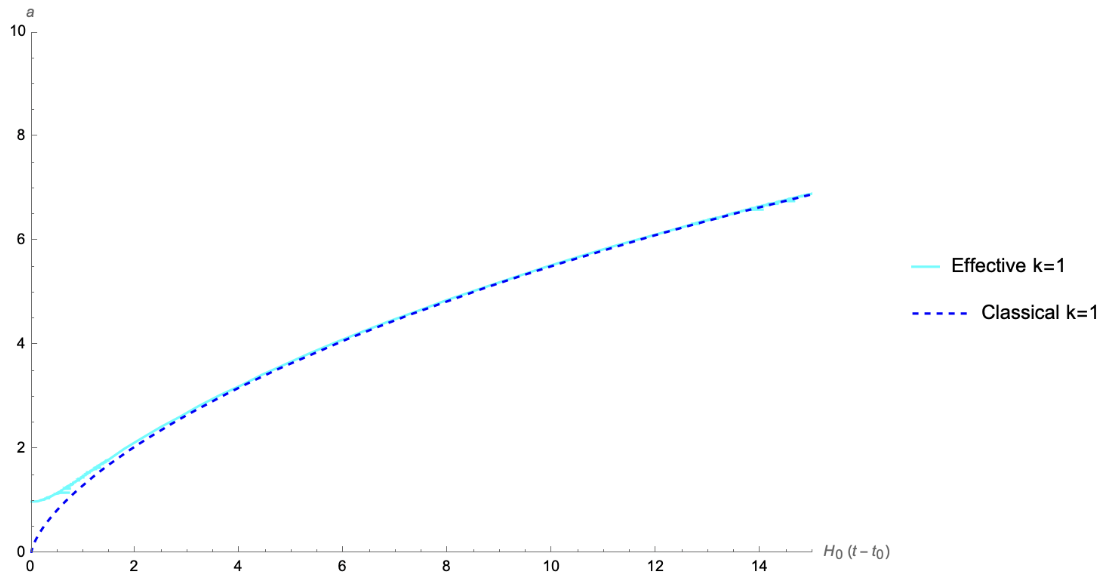

Figure 6.5.6: Comparison of the classical and effective closed universe at small scales.

instead of the big bang singularity, as opposed to the classical model in standard cosmology. The other branch, which is found by the solution (6.193) is connected by the quantum bounce.

These graphics illustrate how in the LQC models as given by the effective solutions, the big bang is replaced by the quantum bounce. This is the main result of the loop quantization. Although this pictorial demonstration is for an effective model, this also comes from the quantum description, because the minimum eigenvalue of the area operator is non-zero. Thus, the discreteness of space-time in this simplified model for each possible geometry solves the classical singularity problem, and the behavior of the evolution of the universe at large scales rapidly converges to the classical behavior. This is consistent with the observations in standard cosmology.

In this Section the general description of the modified Friedmann equation for an arbitrary curvature k was analyzed and some previous results are regained [27, 30, 33–35, 37–39]. Nevertheless, as was discussed previously, the observational value of the cosmological constant differs from 120 orders of magnitude with respect to the theoretical cosmological constant calculated in loop quantum cosmology. The authors in [30] have analyzed a possible solution to this dilemma by introducing a weight parameter between the so-called Euclidean and Lorentzian terms into the Hamiltonian constraint. However, this parameter does not come from the full theory and introduces fine-tuning into this model.

Our interest here was to investigate possible bounds on the weight parameter λ through the unitary evolution. Although the analysis shed light on the possible values for λ it does not fix it.

Furthermore, the inclusion of both Euclidean and Lorentzian terms for open cases were here generalized to the $k = 1$ case. the three possibilities admit a unified effective description consistent with singularity getting replaced by a bounce, although preserving some of the known differences between them.

It remains to see possible restrictions on λ associated with unitary evolution in the $k = \pm 1$ cases.

CHAPTER

SEVEN

CONCLUSIONS

In this final chapter, the main results and conclusions of the thesis are presented. This work was divided into two significant parts which describe important aspects of the quantum nature of matter and spacetime. Moreover, it described some standard and non-standard concepts of general relativity, cosmology, and quantum mechanics, emphasizing ones that are not always exposed in standard textbooks.

As part of the results, a hydrodynamic representation of quantum mechanics was extended to the fermionic case in curved spacetimes. This representation was obtained by applying the Madelung transformation to the Dirac equation in curved spacetimes coupling to an electromagnetic field. Using the Bernoulli equation, which is the first integral of the Euler equation, itself a particular case of the Navier-Stokes equations, together with this description of the fermionic gas, we obtained the energy balance equation. It is possible to compare this representation with previous works concerning classical particles or bosons in curved spacetimes using geometries such as stars, black holes, the early universe, etc.
Although the full equations that describe the hydrodynamic representation of fermions are more complicated than in standard description, the advantage is a closer alignment with an alternative interpretation of QM known as the de Broglie-Bohm interpretation, where the measure problem can be solved in a statistical way. In addition, a non-obvious result found via this representation was the different energy contributions of the fermionic gas.
The difference between the boson and fermionic cases was found in the Bernoulli equation. For bosons, once the Madelung transformation is applied, the KG equation can be separated into real and imaginary parts. In contrast to the fermion case, where the equations of motion do not admit this separation due to the fact that the gamma matrices are a representation of the $SO(1,3)$ group. Moreover, the generalized Madelung transformation used only admits complex parameters to fulfill the Lorentz invariance.
Having explored some aspects of the hydrodynamic representation, we recall that the Dirac equation combines elements from special relativity and quantum mechanics. It was introduced as a relativistic generalization of the Schrödinger equation and solved the problem of negative probability present in the KG equation while naturally giving rise to spin, which is a fundamental property of particles.

Note that in the hydrodynamic representation, the general relativistic Dirac equation introduces an additional contribution due to geometry and spin through the generalized gamma and Pauli matrices. Where the geometry contributions arise from endowing a quantum field with the curvature present in a general metric and, as expected, these contributions are absent in systems without spin, e.g., a scalar field or in flat space-time.
Because no framework is assumed, this hydrodynamic representation is a general description which unfortunately leaves us with an obscured physical interpretation of the quantities obtained. One method to better understand these general results is to solve specific geometric cases or to compare with the bosonic case, which has a better interpretation. However, due to the difficulty to solve the equations of motion, it is necessary to use numerical methods.

Furthermore, this thesis presented relevant aspects of loop quantum cosmology focused on the unitary evolution and curvature of Lorentzian models. The Lorentzian models in LQC using the Thiemann regularization have been important because it is possible to recognize an effect of an emergent or effective cosmological constant. This effect is not found when the Thiemann regularization is not applied, as in the first papers, where only one term was quantized, because classically the Euclidean and Lorentzian terms are proportional in an isotropic and homogeneous universe; this differed from what was done in full theory.
The unitary evolution of the gravitational operator was based on a generalized flat model in LQC, which introduces a weight parameter λ between the Euclidean and Lorentzian terms. This parameter was motivated to solve the discrepancy of 120 orders of magnitude between the observational and effective cosmological constants, as fine tuning. Fortunately, this model could be used to understand and characterize self-adjointness of the gravitational operator and together with the deficiency index methods, its possible extension to the quantum Hamiltonian constraint.
Another result involves the case $\Lambda = 0$ where the explicit cosmological constant vanishes. Here, we found that for $\lambda \leq 0$ the gravitational operator is essentially self-adjoint, which implies that there is only one unique extension. For the case $\lambda > 0$, the operator admits a family of extensions that are related to elements of the group $U(1)$. This is consistent with the LQC models for $\lambda = 1$ [27–29] and $\lambda = -1/\gamma^2$ [24, 25] that have already been studied. Given that many more cases must be considered depending on the value of the weight parameter, the Λ is non-zero calculations were not presented. Nevertheless, we can anticipate intuitively and illustratively that there exist cases where the gravitational operator is effectively self-adjoint and where self-adjoint extensions related to elements of the $U(1)$ and $SU(2)$ groups are admitted due to new boundary conditions. The explicit calculations of this case have been postponed for future work.
To study the self-adjointness of the gravitational operator, we tried different representations, v, b and x, where the representation v introduces a difference equation that is not easy to solve analytically when there are non-constant coefficients. However, it is possible to work with the representation b using a Fourier transformation, which leads to a second-order differential equation equivalent to a KG equation in the representation x. In this representation, there exists a change of variable between $x(b)$, where it would seem that the physical information is

hidden. This is a problem if we include the effect of the self-adjoint extension parameter on the effective dynamics. This was studied using the WDW theory in [26] and was found to be very small. In spite of this, this contribution has never been included in the effective model of LQC to date. We propose, for future work, to find the self-adjoint contributions to the effective model using the path integral method.
Although we studied the self-adjointness character of a generalization of LQC models, another important outcome is the ambiguity in the quantization program regardless of whether the same regularization program is used in this thesis. These ambiguities in LQC have been studied in [27], also in [115] where the authors found a different Hamiltonian operator without this weight parameter that includes both terms but is essentially self-adjoint, that is, using these ambiguities in the regularization program.

Moreover, in this thesis a review of flat and hyperbolic universe in LQC that have been previously studied [27–30, 33–35, 38, 39]. In this work a spherical universe is constructed, and it was possible to generalize it, while obtaining the same functional form, to a flat model plus an extra term that is proportional to the cases $k = -1, 0, 1$. This generalization is analogous to the classical description. In addition, we were able to compare the effective and classical behaviors and, using a figure that better illustrates this comparison, we noted that the description at large scales is identical.
However, close to the classical singularity, both descriptions differ. The classical universes are born from the big bang, while the effective universes from LQC come from a quantum bounce and they converge quickly to the classical behavior. In the LQC description, there exist two branches or universes that are connected by this bounce. This fundamental difference lies in the fact that we have considered the quantum nature of the universe. If LQC is correct, there is a non-zero minimum value for volume which the universe cannot exceed, and therefore the classical singularity is replaced by a quantum bounce.
A natural question to solve in LQC is: In which universe do we live? we have two universes connected by a quantum bounce, our description is invariant under reversal-time. Therefore, a future work to obtain a physical answer to this dilemma could be to explore thermodynamics of LQC, where entropy could give us a time direction, with this we could have information before or after the singularity [116]. This study of entropy would be analogous to calculation of black holes [117–121].
For future work, the self-adjoint character in models with non-zero curvature can be studied. Additionally, the problem of the emergent cosmological constant value persists, as in the flat case. For models with curvature, other descriptions can be analyzed and built using the ambiguities arising when we introduce the quantum description from classical theory. In general, corrections could be added through the inhomogeneities or anisotropies of the cosmological model. Furthermore, more corrections could be introduced having the true LQC or even the cosmological sector of LQG [122, 123], which must have a consistent symmetric reduction in contrast to the classical theory, as we had; however, it is an open problem. We expect the cosmological model to include LQC in some limit, but to find this cosmological sector is work for a slightly more distant future.

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