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Dynamics in Loop Quantum Cosmology

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Resumo

A gravidade quântica surge da necessidade de formular uma teoria de gravidade capaz de fazer previsões físicas em todas as escalas, em particular, nas regiões em que a Relatividade Geral (RG) não o consegue fazer, isto é, em regimes de curvatura muito elevada. É natural pensar que nestes regimes a geometria possa requerer uma descrição quântica e que os efeitos quânticos sejam dominantes, resolvendo assim as singularidades da teoria clássica. Evidentemente, uma teoria de gravidade quântica adequada tem de concordar com a RG também em regimes semiclássicos, isto é, de baixa curvatura.

Uma das teorias mais promissoras de gravidade quântica é a chamada gravidade quântica de *loop* (*Loop Quantum Gravity* – LQG). Mantendo o ponto de vista geométrico da RG, esta abordagem preserva os princípios de covariância geral e independência do *background*. Seguindo o processo de quantização de Dirac, o Hamiltoniano da RG é encontrado como uma combinação linear de quatro constrangimentos locais: três geradores de difeomorfismos espaciais e um constrangimento escalar ou Hamiltoniano, que gera reparametrizações temporais. Os constrangimentos são então promovidos a operadores num espaço de Hilbert cinemático bem definido e encontram-se os estados físicos como aqueles que são aniquilados pelos constrangimentos. Nesta abordagem de LQG canónica, o sistema é descrito em termos de uma conexão SU(2) e a tríade densitizada canonicamente conjugada. Uma das características notáveis deste processo de quantização é que não existe um operador para representar diretamente a conexão, sendo usadas holonomias em torno de um *loop*. Consequentemente, e de forma emergente, a própria geometria é discretizada. A geometria encontra-se codificada em operadores quânticos que representam observáveis físicos e, portanto, resultados físicos são encontrados através dos valores expectáveis destes observáveis sobre estados físicos. Os estados de maior interesse são os semiclássicos, isto é, aqueles que se encontram centrados em trajectórias clássicas em regimes de curvatura baixa, de forma a haver uma concordância entre a teoria clássica e a quântica neste limite. Embora seja uma teoria promissora, não se encontra ainda completa.

Quando o interesse maior recai sobre o Universo primitivo, onde a RG prevê uma singularidade inicial (o *big-bang*), é imperativo considerar uma teoria de gravidade quântica que cure esta singularidade. Seria então necessário desenvolver uma teoria completa de gravidade quântica e extrair as suas consequências cosmológicas. No entanto, esta é uma abordagem extremamente complicada. A alternativa é particularizar à partida a análise para modelos cosmológicos e só depois quantizá-los. Esta abordagem é denominada de cosmologia quântica e tem sido alvo de grande exploração nas últimas décadas. Ao impor homogeneidade já na descrição clássica e só depois quantizar o sistema, reduz-se o número de graus de liberdade a uma quantidade finita, evitando assim algumas das maiores dificuldades de gravidade quântica. No entanto, ao manter a independência do *background*, algumas das questões conceptuais mais atraentes de gravidade quântica podem ser abordadas já neste cenário simplificado. Além de ter o

potencial de oferecer previsões relevantes para cosmologia, permite desenvolver técnicas úteis também para teorias completas de gravidade quântica.

A cosmologia quântica de *loop* (*Loop Quantum Cosmology* – LQC), procura quantizar modelos cosmológicos, de acordo com as prescrições de uma teoria completa de gravidade quântica, LQG. Imitando os procedimentos desenvolvidos para quantizar a RG em LQG canónica e aplicando-os a modelos cosmológicos, não se trata do setor cosmológico de LQG. No entanto, poderá capturar as suas características mais importantes e desenvolver estratégias que serão úteis para a teoria completa.

A dinâmica dos modelos cosmológicos planos Friedmann-Lemaître-Robertson-Walker (FLRW) minimamente acoplados a um campo escalar sem massa tem sido intensivamente estudada no contexto de LQC. Em modelos cosmológicos homgéneos, devido à homogeneidade, apenas sobrevive um constrangimento Hamiltoniano global, gerando reparametrizações temporais. Assim, a coordenada temporal da métrica não é um tempo físico, na medida em que o Hamiltoniano não gera evolução nesta coordenada. Para falar de dinâmica na descrição quântica, é necessário primeiro escolher uma variável como tempo interno, em relação à qual as restantes variáveis do sistema podem ser evoluídas. Na análise deste modelo, apenas se usam duas variáveis: o campo escalar, para representar o sector da matéria, e uma variável relacionada com o factor de escala, descrevendo a geometria. Em LQC é comum escolher o campo escalar como relógio interno, em relação ao qual se evolui o factor de escala. O resultado mais excepcional desta abordagem é a resolução da singularidade do big-bang em termos de um ressalto quântico. Seguindo a prescrição denominada *solvable* LQC (sLQC), é encontrada uma formulação em que o sistema admite solução analítica. Nesta, o valor expectável do observável que representa o volume tem um mínimo positivo e, portanto, o valor expectável da densidade de energia nunca diverge, atingindo um valor máximo finito. Estas quantidades sofrem um ressalto, conectando uma época de contração do Universo com uma de expansão. Este resultado é obtido sem restringir de qualquer forma os estados físicos.

O resultado do ressalto foi encontrado anteriormente recorrendo a tratamentos numéricos, restringindo a análise do valor expectável do operador do volume a estados semiclássiclos. A sua dedução analítica para estados genéricos confere robustez ao resultado. No entanto, nunca foi necessário particularizar a análise na formulação sLQC para estados físicos específicos. Assim, uma dificuldade ignorada até à data é que na realidade não é trivial escrever explicitamente estados físicos no domínio do volume (o principal observável em consideração), na formulação sLQC. Neste trabalho encontramos uma forma de o fazer. Um paralelo com a abordagem de Wheeler-De Witt (WDW) à cosmologia quântica facilita este estudo, na medida em que esta abordagem permite uma formulação semelhante à sLQC de LQC. Mais precisamente, ambas as abordagens (WDW e LQC) partilham o espaço de Hilbert físico nestas formulações. As diferenças entre as duas encontram-se na forma dos operadores que representam os

observáveis. Assim, os estados físicos de ambas vivem no mesmo espaço de Hilbert. Estudando a forma dos estados físicos no domínio do volume da abordagem de WDW, que oferece um cenário mais simplificado, encontramos uma forma de os escrever explicitamente em LQC, colmatando uma lacuna ignorada até agora na literatura.

O estudo de modelos cosmológicos mais realistas requer a introdução de um potencial para o campo escalar. A introdução do potencial origina mais um termo no constrangimento Hamiltoniano. Este termo depende não só do potencial, mas ainda da variável geométrica. Desta forma, em geral, em LQC, o sistema quântico não admite soluções analíticas. Os tratamentos geralmente adotados recorrem a abordagens efectivas ou semiclássicas, introduzindo aproximações, ou a tratamentos numéricos, requerendo frequentemente recursos computacionais elevados. Recentemente, foi proposto na literatura um procedimento para extrair tanto quanto possível as contribuições do potencial para a dinâmica quântica. Este oferece um compromisso entre os dois extremos, recorrendo a aproximações, mas indo além das geralmente adoptadas. O tratamento proposto consiste em considerar em primeiro lugar a dinâmica do caso livre (sem potencial), já devidamente conhecida, passando para uma imagem de interação. Nesta, os valores expectáveis de operadores são obtidos sobre estados do sistema livre, já conhecidos. Desta forma, o principal obstáculo no estudo da dinâmica deste modelo, que se encontrava na integração da evolução dos estados, é evitado. No entanto, a dificuldade transfere-se agora para forma dos operadores na imagem de interação, que inclui operadores de evolução. Estes consistem em integrais de caminho e são, por conseguinte, ainda demasiado complexos para serem calculados. Ao passar para uma nova imagem de interação, as contribuições dominantes do potencial podem ser obtidas, tratando o correspondente operador de evolução de forma perturbativa, mantendo apenas os termos de primeira ordem.

Este método foi proposto para uma forma genérica do potencial, nunca tendo sido aplicado a uma forma específica. Neste trabalho, aplicamo-lo à forma não trivial mais simples possível de um potencial constante. Embora seja um caso simples, é já bastante relevante no contexto de cosmologia, já que é equivalente a um modelo FLRW plano minimamente acoplado a um campo escalar sem potential na presença de uma constante cosmológica. Sendo o potencial constante, o termo correspondente no constrangimento Hamiltoniano é independente do tempo (interno). No entanto, os estados próprios do operador Hamiltoniano não admitem uma forma analiticamente fechada. Este é, portanto, o caso ideal para a primeira aplicação deste procedimento, permitindo algumas simplificações nos cálculos. Neste trabalho aplicamos este procedimento a este modelo, obtendo uma expressão geral para o valor expectável do observável do volume, em primeira ordem no potencial, que pode ser computada, dado um perfil para os estados físicos.

Palavras-chave: Cosmologia quântica, Geometrodinâmica, Cosmologia Quântica de Loop, correcções quânticas, constante cosmológica.

Abstract

The dynamics of a flat Friedmann-Lemaître-Robertson-Walker (FLRW) cosmological model with a massless scalar field has been intensively studied in the context of Loop Quantum Cosmology (LQC), leading to the resolution of the big-bang singularity in terms of a quantum bounce. Following the solvable LQC formulation, in which the cosmological dynamics is driven by a Klein-Gordon equation, this result is found analytically to be valid for a generic physical state. However, the bounce had already been found to occur with numerical treatments, and it was never necessary to write explicitly physical states that belong to the domain of the volume operator in the solvable formulation of LQC. Hitherto, the fact that this is actually not trivial went unnoticed. In this work, we find that a parallel with the Wheeler-De Witt approach is helpful to clarify how to write these states, since the two approaches share the physical Hilbert space in an appropriate formulation. By analysing the form of physical states in the domain of the volume in an analogue Klein-Gordon formulation of the WDW approach, we find a way of writing explicitly physical states in the domain of the volume of the solvable formulation of LQC.

The study of more realistic cosmological models requires the introduction of a non-vanishing potential for the scalar field. Following the LQC approach, this generally implies that there is no analytical solution for the quantum dynamics. A procedure has been proposed to extract as much as possible the contributions of the potential to the quantum dynamics, beyond the approximations usually employed in the literature. The method considers first the well-known dynamics of the free case (with vanishing potential), passing to an interaction picture. The remaining evolution is seen as a kind of geometric interaction and the main contributions can be extracted by passing to a new interaction picture, and treating the corresponding evolution operator in a perturbative manner, keeping only the leading terms. This procedure has been proposed for a generic potential, but never applied to a specific form of it. In this work we apply it to the simplest non-trivial case of a constant potential. This is already a relevant model, as it corresponds to a massless scalar field in the presence of a cosmological constant. The form of the expectation value of the volume observable is found, up to first order in the potential.

Keywords: Quantum cosmology, Geometrodynamics, Loop Quantum Cosmology, quantum corrections, cosmological constant.

Contents

Chapter 1

Introduction

Quantum gravity arises from the need to formulate a theory of gravity that is valid at all scales and capable of making predictions in regimes where General Relativity (GR) breaks down. These are regimes of high curvature, where GR displays singularities. It is natural to think that, in these scenarios, the effects of quantizing the geometry might be important. The geometry of spacetime might require a quantum description, leading to well-defined quantum dynamics.

However, GR is extremely successful away from these singularities. Evidently, any theory of quantum gravity needs to agree with GR in these regimes, while significantly deviating from it close to the singularities. While an effective field theory approach to gravity based on perturbative quantization [1] would, by construction, satisfy the first condition, it cannot provide a proper resolution of this issue, since GR is not perturbatively renormalizable. Hence, we seek a non-perturbative quantum theory for gravity, that agrees with the classical theory far away from the singularities.

Canonical Loop Quantum Gravity (LQG) is precisely an attempt at quantizing GR in a non-perturbative and background independent manner [2–4]. Maintaining the geometrical point of view of GR, it preserves the principles of general covariance and background independence. Following Dirac quantization program for GR, the Hamiltonian is found to be a linear combination of 4 local constraints: 3 generators of spatial diffeomorphisms, and a Scalar or Hamiltonian constraint, that generates time reparametrizations (up to spatial diffeomorphisms). These constraints are then promoted to well-defined operators on a kinematical Hilbert space, and then one looks for the physical states that are annihilated by the constraints. In this canonical LQG approach, the system is described by an SU(2) connection and its canonically conjugate densitized triad. One of the distinguishing features of the theory is that there is no operator directly representing the connection, and holonomies of the connection around a loop are used instead. As consequence, an emergent feature is that the geometry itself turns out to be quantized. Since the geometry is encoded in quantum operators, that represent physical observables, physical results are obtained by computing expectation values of physical observables on physical states, and the relevant

physical states are semiclassical ones, peaked on classical trajectories in low curvature regimes, in order to agree with GR when quantum gravity effects are expected to be small. Even though this is a promising proposal, it is still far from complete.

If we are particularly interested in understanding the physics of the early Universe, where GR predicts an initial singularity (the big-bang), we may take one of two paths. The appropriate one would be to develop a full theory of quantum gravity, and then extract its consequences to the cosmological sector. However, this is too complicated. The alternative is to particularize for cosmological models prior to quantization, which is referred to as quantum cosmology. This approach is based on a huge approximation, by fixing classically most of the diffeomorphism symmetry, with the hope of retaining the most important quantum corrections to the cosmological dynamics. By first imposing homogeneity and only then quantizing the system, we reduce the number of degrees of freedom to a finite quantity, and several difficulties of quantum gravity are thus avoided. Nevertheless, since there is still no background structure (background independence is maintained), most of the conceptual issues of full quantum gravity can be tackled already in this simplified scenario. Also, this allows for some of the mathematical framework to be developed. This way, the goal is to use this setting as a stepping stone, to provide at least some intuition and insight, as well as to develop strategies that can be useful in the full theory. Furthermore, it may already provide relevant predictions in the context of cosmology.

Quantum cosmology was first explored by Wheeler and de Witt in the 70's. In the spirit of quantum mechanics, the geometrodynamical or Wheeler-De Witt (WDW) approach considers a Schrödinger-like representation of the system [5, 6]. However, this approach does not lead to a general resolution of the big-bang singularity, inasmuch as the expectation values of Dirac observables follow the classical trajectory into the big-bang. In this sense, the singularity persists in the WDW approach to quantum cosmology. This led to the exploration of inequivalent quantization procedures. Loop Quantum Cosmology (LQC) is an attempt of quantizing cosmological models, with the guidance of a full theory of quantum gravity, LQG. It mimics the procedures that have been developed for quantizing GR in the canonical LQG approach, applying them to these symmetry reduced models. Since this reduction happens prior to quantization, LQC is not the cosmological sector of the full theory, but it may already capture its crucial features. Furthermore, the development of LQC may establish strategies that can be useful in LQG.

The first endeavors in LQC [7–11] applied the techniques of LQG to the simplest possible case of a flat Friedmann-Lemaître-Robertson-Walker (FLRW) model. The analysis then progressed to the same model minimally coupled to a massless scalar field ϕ, depicting the matter sector [12]. For homogeneous cosmological models, due to homogeneity, only the zero mode of the Hamiltonian constraint survives. If the Hamiltonian vanishes, it does not generate evolution in the time coordinate of the metric. Instead it only generates time reparametrizations. In this sense, this coordinate is not a physical time, as the system

cannot be evolved with respect to it. In the interest of interpreting results in an evolution picture, and speak of quantum dynamics, a variable needs to be chosen as internal time, with respect to which we can evolve the system. In this setting, the variables used to represent the system are the scalar field ϕ, and a variable related to the scale factor a, to describe the geometry. In the LQC approach, it is usual to choose the scalar field ϕ to portrait internal time, and evolve the scale factor a with respect to it. The most attractive result of this approach to this model is that the big-bang singularity is replaced by a quantum bounce, connecting a contracting epoch of the Universe with an expanding one. Numerical simulations of the quantum evolution (in the internal time variable) of the expectation values of observables, such as the volume and the energy density, on semiclassical states reveal that these never diverge. Additionally, the effects of the quantization only become important once the energy density approaches a critical value, below which the dynamics agrees with the classical prediction [12].

However, at this stage there were some important drawbacks in this approach. The critical density at which the bounce occurred was found to be dependent on the momentum of the scalar field [12], and, as result, the effects of quantum geometry could be important even when the energy density was not necessarily high. Thus, the dynamics could deviate significantly from the classical predictions in semiclassical regimes, rendering them physically unsuccessful. The work in [13] pinpointed the source of this problem to a stage in the procedure, where the definition of the Hamiltonian constraint operator relied on fiducial structures instead of physical ones. The introduction of the so-called *improved dynamics* prescription solved this issue, while at the same time maintaining the attractive result of the bounce, by introducing an improved Hamiltonian constraint operator. This way, the LQC approach to the quantization of a flat FLRW model minimally coupled to a massless scalar field resulted in a well-defined and physically successful quantum dynamics. The quantum effects render gravity repulsive when the energy density is of the order of the Planck scale, replacing the big-bang singularity with a quantum bounce. Below the critical energy density (which is now universal) the dynamics agrees with the classical prediction, as required. This prescription proved to be robust, as it was also successful in models with non-zero cosmological constant [13–16], $K = 1$ spatially compact models [17, 18], and Bianchi models [19–22].

One of the concerns at this point was whether this result was particular to semiclassical states alone. The work in [23] settled this question for the case of the simple FLRW model with massless scalar field. It introduced the solvable LQC (sLQC) proposal, where, by interpreting the scalar field as a relational clock already in the classical Hamiltonian, an appropriate change of representation translates the constraint into a Klein-Gordon equation, and the model turns out to be exactly solvable. Its outstanding results are that the bounce is proven to occur for a generic physical state, and that the discreteness of the geometry is fundamental to the occurrence of the bounce. It also showed that the upper bound in the spectrum of the matter energy density, at which the bounce occurs, equals the critical energy density that first resulted

from the numerical simulations.

The determination of predictions of LQC in more realistic models, namely inflationary models, requires the introduction of a potential for the scalar field. As a consequence, generically, the quantum system does not admit analytical solutions. The analysis of the quantum dynamics requires either heavy computational power or the introduction of approximations. The procedure proposed in [24] offers a way of computing the dynamics of LQC for the flat FLRW model in the presence of a scalar field with non-vanishing potential. This analysis offers a compromise between required computational power and the precision of the results. It does not find the exact dynamics, introducing approximations, but goes beyond the semiclassical or effective treatments usually employed in the literature (see e.g. [25, 26]). It takes advantage of the fact that the dynamics of the FLRW model minimally coupled to a massless scalar field is well known. Once the potential is introduced, the extra term that appears in the Hamiltonian constraint is seen as a sort of geometric interaction. By considering first the vanishing potential case and passing to an interaction picture, the expectation values of observables in this picture are applied on the states of the free system. Thus, the main obstacle, which was to integrate the evolution of the states, has been shifted to the computation of the observables in the interaction picture. These include evolution operators, which consist of path-ordered integrals, and are thus still too complicated to be manageable. Then, the main contributions of the potential to the evolution operators can be extracted, by passing to a new interaction picture. Here, the dominant part of the evolution operator can be dealt with perturbatively, keeping only the leading terms. This procedure has been proposed for a generic potential, but never applied to a specific form of it.

The aim of this work is two-fold. Firstly, we will address an issue that has been overlooked hitherto. Because the aforementioned sLQC prescription was developed after the bounce had been found to occur from numerical simulations, it was never necessary to write explicit physical states that belong to the domain of the volume (the main observable under consideration) in the solvable representation of LQC. Thus, the fact that this is actually not trivial has never been noticed. We find that a parallel with the WDW approach is helpful to simplify this task. In this approach, a construction similar to the sLQC can be made [13], where a suitable change of representation leads to a simplification of the Hamiltonian constraint into a Klein-Gordon equation as well. This representation of the WDW approach shares its physical Hilbert space with the solvable formulation of LQC, while their differences lie in the form of the operators that represent observables. We will take advantage of the fact that the WDW approach offers a simpler setting on which to study the form of the physical states in the domain of the volume in the Klein-Gordon representation, to provide a way of writing them in the solvable formulation of LQC.

Then, having a complete understanding at physical level of the solvable formulation of LQC, we can study more realistic models, by introducing a non-vanishing potential for the scalar field. We will intro-

duce the procedure proposed in [24] to extract as much as possible the contributions of the potential to the quantum dynamics of the system, and apply it to the simplest non-trivial case of a constant potential. Even though this is a simple model, it is already relevant for cosmology as it is equivalent to considering the model with a massless scalar field in the presence of a cosmological constant. Since the potential does not depend on the scalar field, many of the computations of the procedure [24] are simplified, and we will find the form of the expectation of the value of the volume, up to first order in the potential.

The structure of this dissertation is the following. In chapter 2, we introduce the Hamiltonian formulation of homogeneous cosmological models suited to the LQC procedure. Then, in chapter 3, we present a detailed analysis of the WDW approach in a way that makes its comparison to LQC simple. In chapter 4, we briefly present the LQC procedure, focusing on its solvable formulation, i.e., the Klein-Gordon representation, along with its main results. We also present a way to write explicit physical states in the domain of the volume in this approach, which has not been established until now. Finally, in chapter 5, we introduce the procedure proposed in [24] to compute the dynamics of LQC for the flat FLRW model in the presence of a scalar field with a generic potential, and apply it to the simple case of a constant potential.

Chapter 2

Hamiltonian formulation of homogeneous cosmological models

In this work, we will restrict the discussion to homogeneous and isotropic cosmological models. The goal of this chapter is to build the Hamiltonian formulation of such systems suited to the quantization procedure of LQC, which mimics the techniques of LQG. This involves choosing suitable variables for the description of a gauge theory: an SU(2) connection and a canonically conjugate densitized triad. Throughout this work, we set the speed of light and the reduced planck constant $\hbar$ equal to 1.

We start by considering a Hamiltonian formulation of GR. The ADM formalism [27] adopts a decomposition of the 4D metric $g_{\mu\nu}$ into three objects: the 3-metric q_{ab} induced in the spatial slices that foliate the manifold, the lapse function N and the shift vector N^a, such that the line element is

$$ds^2 = -\left(N^2 - q_{ab}N^aN^b\right)dt^2 + 2q_{ab}N^a dt dx^b + q_{ab}dx^a dx^b. \tag{2.1}$$

N and N^a are not physical quantities, since they are in fact Lagrange multipliers accompanying the constraints in the action, and the relevant physical information is found in q_{ab} and its canonically conjugated extrinsic curvature K_{ab}.

For a flat FLRW model, various integrals in the Hamiltonian framework diverge, as a consequence of homogeneity, and an infrared regulator needs to be introduced. Thus, we restrict the integrations to a fix finite cell $\mathcal{V}$. Due to homogeneity, the dynamics on $\mathcal{V}$ will reproduce the events of the whole Universe. In fact, the final results will not depend on the choice of this cell. We fix a fiducial Euclidean metric ${}^o q_{ab}$, and denote the volume of the cell $\mathcal{V}$ with respect to this metric by V_o.

In LQG, 3-metrics are replaced by triads [3]. To this end, we define the Euclidean co-triad e^i_a by

$$q_{ab} = e^i_a e^j_b \delta_{ij}, \tag{2.2}$$

where δ_{ij} is the Kronecker delta, and triad e^a_i as its inverse,

$$e^a_i e^j_b = \delta^a_b \delta^j_i. \tag{2.3}$$

Then, we change variables to the Ashtekar-Barbero connection A^i_a, canonically conjugate to the densitized triad E^a_i [28]. The Ashtekar-Barbero connection is formed by the spin connection Γ^i_a compatible with the densitized triad[1], and the extrinsic curvature in triadic form $K^i_a = K_{ab} e^b_j \delta^{ij}$:

$$A^i_a = \Gamma^i_a + \gamma K^i_a. \tag{2.4}$$

Here, γ is an arbitrary real number called the Immirzi parameter [29, 30]. On the other hand, the densitized triad is defined as:

$$E^a_i = \sqrt{q} e^a_i. \tag{2.5}$$

where q is the determinant of the metric q_{ab}. In order to impose homogeneity and isotropy, these variables are parametrized by only one spatially constant parameter for each of them:

$$A^i_a = c(t) V_o^{-1/3} \, {}^o e^i_a, \tag{2.6}$$

$$E^a_i = p(t) V_o^{2/3} \sqrt{{}^o q} \, {}^o e^a_i, \tag{2.7}$$

where ${}^o q$ is the determinant of the fiducial Euclidean metric, with respect to which the fiducial Euclidean co triad ${}^o e^i_a$ is defined. The variable $p(t)$ is related to the scale factor $a(t)$ through:

$$a(t) = \sqrt{|p(t)|} V_o^{-1/3}. \tag{2.8}$$

Furthermore, the sign of $p(t)$ represents the relative orientations of the physical triad and the fiducial triad. The variable $c(t)$, on the other hand, is related to the momentum of the scale factor da/dt:

$$c(t) = \gamma V_o^{-1/3} \frac{da}{dt}. \tag{2.9}$$

This way, the gravitational degrees of freedom are encoded in the canonically conjugate variables $c \equiv c(t)$ and $p \equiv p(t)$ with Poisson brackets [11]:

$$\{c, p\} = \frac{8\pi G \gamma}{3}. \tag{2.10}$$

[1] I.e., it verifies $\nabla_b E^a_i + \epsilon_{ijk} \Gamma^j_b E^{ak} = 0$, where ∇_b is the usual spatial covariant derivative and ϵ_{ijk} the totally antisymmetric symbol.

As in LQG, in LQC there is no operator corresponding to the connection itself, and we take holonomies of the connection and fluxes of the densitized triad as variables instead [11, 31–34]. The fluxes are simply proportional to p. Objects that are defined classically in terms of the connection, on the other hand, could be obtained by considering holonomies of the connection around a loop and taking the limit where the area of the loop shrinks to zero. However, this limit is not defined in the cosmological setting. Thus, instead of taking the limit where the area is zero, we take the limit where it is the non-vanishing minimum eigenvalue of the area operator. In an initial LQC treatment, this minimum area was calculated using the fiducial structure, which resulted in some unwanted features that rendered the quantum dynamics unsuccessful. Namely, it was found that the quantum effects of the geometry could be important even when the energy density was not high, thus deviating significantly from the classical predictions in semi-classical regimes. The so-called *improved dynamics* prescription introduced in [23] solved this issue, by defining this area with respect to the physical geometry instead. Thus, the basic holonomies are taken along straight lines and in the fundamental representation of SU(2), with a length such that the square formed by them has a physical area equal to Δ, the non-vanishing minimum allowed by LQG[2][35, 36].

To simplify calculations, we perform another change of variables to a new canonical set, such that the holonomies simply produce a constant shift in the new geometric variable v, which replaces p [13]:

$$v = \text{sign}(p)\frac{|p|^{3/2}}{2\pi G\gamma\sqrt{\Delta}}, \tag{2.11}$$

$$b = \sqrt{\frac{\Delta}{|p|}}c, \tag{2.12}$$

with $\{b, v\} = 2$.

To summarize, we started with a description of the spacetime based on the scale factor and its momentum, and changed variables to the canonical pair v and b:

$$|v| = \frac{V}{2\pi G\gamma\sqrt{\Delta}} \equiv \frac{a^3 V_o}{2\pi G\gamma\sqrt{\Delta}}, \tag{2.13}$$

$$b = \gamma\sqrt{\Delta}H = \gamma\sqrt{\Delta}\frac{1}{a}\frac{da}{dt}, \tag{2.14}$$

where t is the proper time and $H = \frac{1}{a}\frac{da}{dt}$ is the Hubble parameter. This way, the physical volume of the cell $\mathcal{V}$ is given by:

[2] i.e., the smallest non-zero eigenvalue of the area operator in LQG, for spins equal to $1/2$ (i.e., the fundamental representation).

$$V = 2\pi G\gamma\sqrt{\Delta}|v|. \tag{2.15}$$

Additionally, we are going to consider as matter content a homogeneous massless scalar field ϕ and its momentum π_ϕ, which form a canonical pair with Poisson brackets $\{\phi, \pi_\phi\} = 1$.

This is the simplest possible cosmological model with non-trivial dynamics. Even so, it already contains enough features to display interesting consequences coming from LQC.

As discussed in the introduction, in GR, the Hamiltonian of the system is found to be a linear combination of constraints, and so it vanishes [37]. In our case, due to homogeneity, the only constraint left is a global Hamiltonian one, namely the zero mode of the full Hamiltonian constraint, which generates time reparametrizations [13]:

$$\pi_\phi^2 - \frac{3}{4\pi G\gamma^2}\Omega_0^2 = 0, \tag{2.16}$$

where we used $\Omega_0 = 2\pi G\gamma bv$. Thus, the time coordinate of the metric is not a physical time, since the Hamiltonian does not generate evolution in it. If we want to speak of dynamics in an evolution picture at the quantum level, we first need to address this concept of evolution. We need to elect a variable to portrait the role of internal time, with respect to which we evolve the remaining variables of the system. In this setting, we only work with two variables: v and ϕ. It seems more intuitive to evolve v (which is essentially the volume), with respect to ϕ, as is in fact common in LQC for this model [13, 38], so we choose the scalar field ϕ as internal time.

The next step is to promote this constraint (2.16) to a well-defined operator on a kinematical Hilbert space. The total kinematical Hibert space will be given by two sectors: one for geometry and another for matter. The quantum representation of the geometrical sector is where LQC distinguishes itself from other quantum cosmology procedures, such as the Wheeler-De Witt approach [13, 38].

Chapter 3

The Wheeler-De Witt approach

To maintain as much as possible GR's key principles while having in mind a canonical approach for quantization, we have taken as a starting point the Hamiltonian formulation of it described in chapter 2. The next step is to adopt a quantum representation of the system, in order to promote the constraint (2.16) to a well-defined operator on a kinematical Hilbert space. Having standard quantum mechanics in mind, the most intuitive path is to consider a Schrödinger-like representation of the system. In fact, in the 70's, the Wheeler-de Witt (WDW), or geometrodynamical, approach considered such a representation of the scale factor and its conjugate momentum.

With this approach, one finds that the initial (big-bang) singularity is not generically cured, as the expectation values of Dirac observables, such as the energy density, still diverge at this point. This led to the need to explore other inequivalent quantization procedures, such as the one we are interested in, Loop Quantum Cosmology (LQC) [13].

Nevertheless, the study of the WDW approach is of interest in the context of LQC. For a flat FLRW model, a suitable change of variables leads to a simplification of the Hamiltonian constraint, turning it into a Klein-Gordon equation. A similar construction is also possible in LQC, and leads to a solvable formulation of the quantum dynamics of this simple model. These two approaches share the physical Hilbert space of their respective Klein-Gordon formulations, while the differences are found on the representations of physical observables. The WDW approach offers a simpler setting to analyse the physical Hilbert space and physical states, along with their transformation from the original representation to the Klein-Gordon one, and so this analysis will prove useful for LQC.

Thus, in this chapter we analyse in detail the physical Hilbert space and physical states in the WDW theory and track its transformation through the different representations that lead to the Klein-Gordon formulation of the system. This will allow us to explicitly construct physical states (and in particular semiclassical ones) in the Klein-Gordon representation, both in the WDW approach and in LQC.

3.1 Kinematical vs Physical Hilbert space

Having a representation of the system based on the canonically conjugate variables v and b, we promote the Hamiltonian constraint (2.16) to an operator on a kinematical Hilbert space (by promoting v, b, ϕ and π_ϕ to operators $\hat{v}$, $\hat{b}$, $\hat{\phi}$ and $\hat{\pi_\phi}$, respectively, and looking for representations of the canonical commutation relations $[\hat{b}, \hat{v}] = 2i$, $[\hat{\phi}, \hat{\pi}_\phi] = i$) and find the physicals states as the ones that are annihilated by the constraint. Focusing on the geometric sector, we will start from the v-representation, where $\hat{v}$ is diagonal, and study carefully the procedure to pass to the y-representation, where the constraint is simplified to a Klein-Gordon equation. This consists on first building the kinematical and physical Hilbert spaces (by defining the kinematical/ physical states and inner product) in the v-representation, then passing to the b-representation and finally, through a change of the geometric variable from b to $y(b)$, passing to the y-representation. By keeping track of the maps between these representations, we find the relation between the profiles that define a state in the y and v-representations.

3.1.1 v-representation

In this section, we will review the work presented in [13]. In this representation, the quantum counterpart of the Hamiltonian constraint (2.16) is given by:

$$\underline{\hat{C}} = -\partial_\phi^2 - \underline{\hat{\Theta}}, \tag{3.1}$$

where we use underlines when referring to operators/ states of the WDW approach, that are not the same as in the LQC approach. The geometric part of the constraint is:

$$\underline{\hat{\Theta}} = \underline{\hat{\Omega}}^2 = \frac{3}{4\pi G}\,\underline{\hat{\Omega}}_0^2, \tag{3.2}$$

$$\underline{\hat{\Omega}} = -i\sqrt{12\pi G}\,:v\partial_v: \tag{3.3}$$

where $:v\partial_v:$ represents the symmetric ordering of $v\partial_v$. We will use here the convenient symmetric ordering

$$:v\partial_v: \;= \frac{v\partial_v + \partial_v v}{2}, \tag{3.4}$$

which leads to:

$$\underline{\hat{\Omega}} = -i\sqrt{12\pi G}\left(v\partial_v + \frac{1}{2}\right). \tag{3.5}$$

The operator $\hat{\underline{\Omega}}$ is (essentially) self-adjoint in the domain $\mathcal{D}_v$ of the Schwartz space of rapidly decreasing functions dense in $L^2(\mathbb{R}, dv)$, with absolutely continuous and non-degenerate spectrum $\sigma(\hat{\underline{\Omega}}) = \mathbb{R}$. Its generalized eigenfunctions $\underline{e}_k(v)$ with eigenvalue $\omega = \sqrt{12\pi G}k$ are:

$$\underline{e}_k(v) = \frac{1}{\sqrt{2\pi|v|}} e^{ik\ln(v)}, \tag{3.6}$$

normalized such that $\langle \underline{e}_k, \underline{e}_{k'} \rangle = \delta(k - k')$, where $\langle\ ,\ \rangle$ is the inner product in $L^2(\mathbb{R}, dv)$, and $\delta(k - k')$ is the Dirac delta. This way, these eigenfunctions provide a basis for $L^2(\mathbb{R}, dv)$.

The operator $\hat{\underline{\Theta}}$ is (essentially) self-adjoint in $\mathcal{D}_v$, with absolutely continuous and double degenerate spectrum $\sigma(\hat{\underline{\Theta}}) = \mathbb{R}^+$. For each eigenvalue $\omega^2 = 12\pi G k^2$, there are two eigenfucntions: $\underline{e}_k(v)$ and its complex conjugate $\bar{\underline{e}}_k(v)$.

Finally, the operator $-\partial_\phi^2$ is (essentially) self-adjoint in the domain $\mathcal{D}_\phi$ of the Schwartz space of rapidly decreasing functions dense in $L^2(\mathbb{R}, d\phi)$, with absolutely continuous double degenerate spectrum $\sigma(-\partial_\phi^2) = \mathbb{R}^+$. Its generalized eigenfunctions of eigenvalue λ^2 are the plane waves $e^{\pm i\lambda\phi}$, which then provide a basis for $L^2(\mathbb{R}, d\phi)$.

Thus, the constraint operator $\hat{\underline{C}}$ is defined in a dense domain $\mathcal{D} \equiv \mathcal{D}_v \otimes \mathcal{D}_\phi \subset L^2(\mathbb{R}, dv) \otimes L^2(\mathbb{R}, d\phi) \equiv \mathcal{H}_{kin}$, where $\mathcal{H}_{kin}$ is the kinematical Hilbert space. Each of the operators act as the identity in the sector where they do not have a dependence.

Physical states

Physical states $\underline{\psi}$ are the ones that are annihilated by the constraint: $\hat{\underline{C}}\underline{\psi} = 0$. These have to be normalizable. Generally, the solutions of the constraint are not normalizable in the kinematical Hilbert space, unless 0 is in the *discrete* spectrum of the constraint operator. However, $\hat{\underline{C}}$ has *continuous* spectrum, so states $\underline{\psi}$ are not normalizable in $\mathcal{H}_{kin}$. We need to regard them as elements of a bigger space, specifically the topological dual $\mathcal{D}^*$ of the domain:

$$\mathcal{D} \subset \mathcal{H}_{kin} \subset \mathcal{D}^* \equiv \mathcal{D}_v^* \otimes \mathcal{D}_\phi^*. \tag{3.7}$$

This way, we find that the general states $\underline{\psi}(v, \phi) \in \mathcal{D}^*$ are given by:

$$\begin{aligned}\underline{\psi}(v,\phi) = \int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} d\lambda \Big(& \tilde{\underline{\psi}}_{++}(k,\lambda)\underline{e}_k(v)e^{i\lambda\phi} + \tilde{\underline{\psi}}_{+-}(k,\lambda)\underline{e}_k(v)e^{-i\lambda\phi} \\ & + \tilde{\underline{\psi}}_{-+}(k,\lambda)\bar{\underline{e}}_k(v)e^{i\lambda\phi} + \tilde{\underline{\psi}}_{--}(k,\lambda)\bar{\underline{e}}_k(v)e^{-i\lambda\phi} \Big),\end{aligned} \tag{3.8}$$

We simply require $\underline{\psi}(v, \phi) < \infty$ for $\underline{\psi}(v, \phi)$ to belong to $\mathcal{D}^*$. This way, imposing the constraint:

$$-\partial_\phi^2 \underline{\psi}(v,\phi) = \hat{\underline{\Theta}}\underline{\psi}(v,\phi), \tag{3.9}$$

we find $\lambda^2 = \omega^2$. Redefining $\omega(k)$ as:

$$\omega(k) = \sqrt{12\pi G}|k| > 0, \tag{3.10}$$

the physical states are generally given by:

$$\underline{\psi}(v,\phi) = \int_{-\infty}^{+\infty} dk \left[\tilde{\underline{\psi}}_+(k)\underline{e}_k(v)e^{i\omega(k)\phi} + \tilde{\underline{\psi}}_-(k)\bar{\underline{e}}_k(v)e^{-i\omega(k)\phi}\right]. \tag{3.11}$$

Furthermore, they can be separated in positive and negative frequency sectors:

$$\underline{\psi}_+(v,\phi) = \int_{-\infty}^{+\infty} dk\tilde{\underline{\psi}}_+(k)\underline{e}_k(v)e^{i\omega(k)\phi}, \tag{3.12}$$

$$\underline{\psi}_-(v,\phi) = \int_{-\infty}^{+\infty} dk\tilde{\underline{\psi}}_-(k)\underline{\bar{e}}_k(v)e^{-i\omega(k)\phi}, \tag{3.13}$$

respectively, such that the positive frequency sector corresponds to taking $\tilde{\underline{\psi}}_-(k) = 0$ and the negative frequency sector to taking $\tilde{\underline{\psi}}_+(k) = 0$. As we will see later, the complete set of commuting observables preserves the space of positive/ negative frequencies so that they are superselected, and we can focus our analysis on only one of them.

Evolution picture

As has been mentioned, to deal with the fact that the time variable of the metric does not appear in this description of spacetime, we choose the scalar field ϕ as internal time, with respect to which we evolve the remaining variables of the system, in this particular case v. We can thus deparametrize the system and write a Schrödinger evolution equation:

$$-i\partial_\phi \underline{\psi}(v,\phi) = \hat{\mathcal{H}}\underline{\psi}(v,\phi), \tag{3.14}$$

where $\hat{\mathcal{H}}$ is the physical Hamiltonian, in the sense that it generates time evolution (in the internal time variable ϕ). $\hat{\mathcal{H}}$ is given by $\sqrt{\underline{\hat{\Theta}}}$ for the positive frequency sector and by $-\sqrt{\underline{\hat{\Theta}}}$ for the negative frequency sector:

$$-i\partial_\phi \underline{\psi}_\pm(v,\phi) = \pm\sqrt{\hat{\underline{\Theta}}}\underline{\psi}_\pm(v,\phi). \tag{3.15}$$

Thus, physical states can be found by evolving an initial datum (at initial 'time' $\phi = \phi_o$) with the

evolution generated by $\hat{\mathcal{H}}$:

$$\underline{\psi}_{\pm}(v,\phi) = e^{\pm i\sqrt{\underline{\hat{\Theta}}}(\phi-\phi_o)}\underline{\psi}_{\pm}(v,\phi_o). \tag{3.16}$$

Choosing ϕ as internal time, we can say that, if the profiles $\underline{\tilde{\psi}}_{\pm}(k)$ of (3.12) and (3.13) have support only for $k > 0$, the solution is incoming (or contracting), whereas if they only have support for $k < 0$, we have an outgoing (expanding) solution [13].

Physical observables and physical inner-product

Finally, we have to endow the space of physical states with a Hilbert space structure, specifically, by finding a complete set of commuting observables along with a physical inner product, i.e., an inner product that makes them self-adjoint.

This complete set of commuting observables consists of $\hat{\pi}_\phi = -i\partial_\phi$ and $|\hat{v}|_\phi$ [13]. π_ϕ is already a Dirac observable in the classical theory, given that it is a constant of motion. This way, its quantum counterpart commutes with the constraint. On the other hand, $|v|$ is not a constant of motion in the classical theory, but it is monotonic in ϕ, and so it is in fact a Dirac observable for any fixed ϕ. The action of its quantum counterpart on an initial datum is given by:

$$|\hat{v}|_\phi\underline{\psi}(v,\phi_o) = |v|\underline{\psi}(v,\phi_o). \tag{3.17}$$

This way, we can separate the physical states in positive and negative frequency sectors, act on an initial datum (at $\phi = \phi_o$) with $|\hat{v}|_\phi$, and then evolve it through (3.16), which yields:

$$|\hat{v}|_\phi\underline{\psi}(v,\phi) = e^{i\sqrt{\underline{\hat{\Theta}}}(\phi-\phi_o)}|v|\underline{\psi}_{+}(v,\phi_o) + e^{-i\sqrt{\underline{\hat{\Theta}}}(\phi-\phi_o)}|v|\underline{\psi}_{-}(v,\phi_o). \tag{3.18}$$

Since both these operators preserve the positive and negative frequency spaces, there is a superselection of the two sectors, and we can restrict our analysis to one of them. We will choose to focus on the positive frequency sector.

Finally, the physical inner-product that makes these operators self-adjoint is:

$$\left(\underline{\psi}_1, \underline{\psi}_2\right) = \int_{\phi=\phi_o} dv\ \underline{\bar{\psi}}_1(v,\phi)\underline{\psi}_2(v,\phi), \tag{3.19}$$

which is independent of the value of ϕ, and so we evaluate it at, e.g., ϕ_o. This way, the norm of a physical state is

$$
\begin{aligned}
||\underline{\psi}||^2 &= \int_{-\infty}^{+\infty} dv |\underline{\psi}(v,\phi)|^2 \\
&= \int_{-\infty}^{+\infty} dk |\underline{\tilde{\psi}}_+(k)|^2.
\end{aligned}
\tag{3.20}
$$

The physical states of positive frequency are defined by the physical profiles $\underline{\tilde{\psi}}_+(k)$, normalizable in the physical Hilbert space $\mathcal{H}_{phys} = L^2(\mathbb{R}, dk)$, so that the norm of a physical state is finite.

Semiclassical states: Gaussian profiles

In this description, we have made no restrictions to the physical states so far. However, in the interest of agreeing with GR in the classical regime (low curvature), we are particularly interested in semiclassical states. These are states that are peaked in classical trajectories for large volumes, such that the dispersions of physical observables remain bounded, and can be defined by choosing an appropriate profile $\underline{\tilde{\psi}}_+(k)$. A profile that peaks the states in a certain k^* of the classical trajectory is adequate, and the most obvious formulation of such a function is a Gaussian.

Focusing on the positive frequency sector, from now on, we can write the physical states as:

$$
\underline{\psi}(v,\phi) = e^{i\sqrt{\underline{\Theta}}(\phi-\phi_o)}\underline{\psi}(v,\phi_o). \tag{3.21}
$$

We can choose the initial datum $\underline{\psi}(v,\phi_o)$ as one that is peaked on a classical trajectory. To this end, we will define a profile peaked on $v^* \gg 1$ and $\pi_\phi^* \gg 1$ (in natural units $c = G = 1$ and also $\hbar = 1$) at ϕ_o [13]:

$$
\underline{\psi}(v,\phi_o) = \int_{-\infty}^{+\infty} dk\ \underline{\tilde{\psi}}_+(k)\underline{e}_k(v)e^{i\omega(k)(\phi_o-\phi^*)}, \tag{3.22}
$$

with

$$
\underline{\tilde{\psi}}_+(k) = N(\sigma)e^{-\frac{(k-k^*)^2}{2\sigma^2}}, \qquad k^* = -\frac{\pi_\phi^*}{\sqrt{12\pi G\hbar^2}}, \qquad \phi^* = -\frac{\ln|v^*|}{\sqrt{12\pi G}} + \phi_o. \tag{3.23}
$$

We choose $N(\sigma) = \frac{1}{\sqrt{2\sigma\sqrt{\pi}}}e^{-\frac{1}{8\sigma^2}}$, so that

$$
\begin{aligned}
\left(\underline{\psi}, \hat{V}|_\phi\underline{\psi}\right) &= 2\pi G\gamma\sqrt{\Delta}\left(\underline{\psi}|\hat{v}|_\phi\underline{\psi}\right) \\
&= 2\pi G\gamma\sqrt{\Delta}|v^*|e^{\sqrt{12\pi G}(\phi-\phi_o)} \\
&= 2\pi G\gamma\sqrt{\Delta}\, e^{\sqrt{12\pi G}(\phi-\phi^*)},
\end{aligned}
\tag{3.24}
$$

i.e., under evolution, the state remains peaked on the classical trajectory [13]:

$$\phi = \frac{1}{\sqrt{12\pi G}} \ln \frac{|v|}{|v^*|} + \phi_o. \tag{3.25}$$

We obtain, in this description, an expanding evolution (3.24). The semiclassical state follows the classical trajectory, contracting into the big-bang in the backwards evolution. If we had chosen to work with positive k^* (negative π_ϕ^*), we would have obtained a contracting evolution and the semiclassical state would follow the classical trajectory into a big-crunch in the forward evolution. Furthermore, the expectation value of the dispersion of the volume observable is found to be bounded, and we conclude that the states remain semiclassical throughout the evolution [13].

3.1.2 Klein-Gordon formulation

Now that the physical Hilbert space, physical states and inner-product are well defined in the v-representation, we will find the appropriate changes of representations that simplify the form of the constraint to a Klein-Gordon equation, building a map between the initial and final representations. This correspondence was developed in [23] at the kinematic level. In this section, we will review this procedure. However, the map at the physical level is not available in the literature yet, and is one of the novelties of this work, which will be presented in section 3.1.3. This way, we will be able to take a profile $\tilde{\underline{\psi}}_+(k)$ defining a physical state $\underline{\psi}(v,\phi)$ in the v-representation and obtain the corresponding physical state in the Klein-Gordon representation.

The fact that changing representations cannot affect the physics is translated to the invariance of expectation values between representations. Hence, we will check that the physical inner product agrees when performing such a change.

b-representation

First, we need to change from the v-representation to the b-representation, through a Fourier transformation. We want to map $\underline{\psi}(v,\phi) \in L^2(\mathbb{R}, dv)$ to $\tilde{\underline{\psi}}(b,\phi) \in L^2(\mathbb{R}, db)$. Since $\{b, v\} = 2$, Dirac's rule gives $\left[\hat{b}, \hat{v}\right] = 2i$ and so, given the action of the operators $\hat{v}$ and $\hat{b}$ in the v-representation:

$$\hat{v}\, \underline{\psi}(v,\phi) = v\, \underline{\psi}(v,\phi), \tag{3.26}$$

$$\hat{b}\, \underline{\psi}(v,\phi) = 2i\partial_v\, \underline{\psi}(v,\phi), \tag{3.27}$$

we find the corresponding actions in the b-representation to be:

$$\hat{v}\,\underline{\tilde{\psi}}(b,\phi) = -2i\partial_b\,\underline{\tilde{\psi}}(b,\phi), \tag{3.28}$$

$$\hat{b}\,\underline{\tilde{\psi}}(b,\phi) = b\,\underline{\tilde{\psi}}(b,\phi). \tag{3.29}$$

The states $\underline{\psi}(v,\phi)$ and $\underline{\tilde{\psi}}(b,\phi)$ are thus related through the Fourier transformation:

$$\underline{\tilde{\psi}}(b,\phi) = \frac{1}{\sqrt{4\pi}}\int_{-\infty}^{+\infty} dv e^{\frac{i}{2}vb}\underline{\psi}(v,\phi), \tag{3.30}$$

$$\underline{\psi}(v,\phi) = \frac{1}{\sqrt{4\pi}}\int_{-\infty}^{+\infty} db e^{-\frac{i}{2}vb}\underline{\tilde{\psi}}(b,\phi). \tag{3.31}$$

This way, $v\partial_v$ transforms to $(-1-b\partial_b)$ and the operator $\underline{\hat{\Omega}}$ becomes:

$$\underline{\hat{\Omega}} = i\sqrt{12\pi G}(b\partial_b + \frac{1}{2}), \tag{3.32}$$

defined in the Fourier transform of $\mathcal{D}_v$, namely $\tilde{\mathcal{D}}_v \subset L^2(\mathbb{R}, db)$. The physical inner product:

$$\begin{aligned}\left(\underline{\psi}_1,\ \underline{\psi}_2\right) &= \int_{-\infty}^{+\infty} dv\ \overline{\underline{\psi}}_1(v,\phi)\underline{\psi}_2(v,\phi)\\ &= \int_{-\infty}^{+\infty} db\ \overline{\underline{\tilde{\psi}}}_1(b,\phi)\underline{\tilde{\psi}}_2(b,\phi)\end{aligned} \tag{3.33}$$

agrees, as it has to.

Rescaling

Keeping in mind that our goal is to change variable to one that transforms the constraint into a Klein-Gordon equation, we will now perform another change of representation, in order to obtain $\underline{\hat{\Theta}} = -\sqrt{12\pi G}\,(b\partial_b)^2$. This can be accomplished by rescaling the states:

$$\underline{\tilde{\psi}}(b,\phi) = \frac{1}{\sqrt{|b|}}\underline{\varphi}(b,\phi), \tag{3.34}$$

with $\underline{\varphi}(b,\phi) \in L^2(\mathbb{R}, \frac{1}{|b|}db)$. This way, the constraint now reads

$$\partial_\phi^2\underline{\varphi}(b,\phi) = 12\pi G(b\partial_b)^2\underline{\varphi}(b,\phi), \tag{3.35}$$

and the physical inner product:

$$\begin{aligned}\left(\underline{\psi}_1,\,\underline{\psi}_2\right) &= \int_{-\infty}^{+\infty} db\,\overline{\underline{\tilde{\psi}}}_1(b,\phi)\underline{\tilde{\psi}}_2(b,\phi) \\ &= \int_{-\infty}^{+\infty} \frac{1}{|b|} db\,\overline{\underline{\varphi}}_1(b,\phi)\underline{\varphi}_2(b,\phi).\end{aligned} \tag{3.36}$$

y-representation

Now, we can make another change of representation, by changing from b to the related variable y [23]:

$$y = \frac{1}{\sqrt{12\pi G}} \ln\frac{|b|}{b_o}, \tag{3.37}$$

$$|b| = b_o e^{\sqrt{12\pi G}y}, \tag{3.38}$$

where we take b_o to be a positive constant. In the b-representation, this constant played no role, hence, in this representation, physical results cannot depend on it. In fact, different choices for the value of b_o correspond to unitarily equivalent theories [23]. For convenience, we choose $b_o = 2$.

In this representation, $\underline{\varphi}(y,\phi) = \underline{\varphi}(2e^{\sqrt{12\pi G}y},\phi) \in L^2(\mathbb{R}, \frac{1}{|b(y)|}db(y)) = L^2(\mathbb{R}, \sqrt{12\pi G}\,dy)$, and the inner product reads:

$$\begin{aligned}\left(\underline{\psi}_1,\,\underline{\psi}_2\right) &= \int_{-\infty}^{+\infty} \frac{1}{|b|} db\,\overline{\underline{\varphi}}_1(b,\phi)\underline{\varphi}_2(b,\phi) \\ &= \int_{-\infty}^{+\infty} \sqrt{12\pi G}\,dy\,\overline{\underline{\varphi}}_1(y,\phi)\underline{\varphi}_2(y,\phi).\end{aligned} \tag{3.39}$$

Physical states

With this change of variables, the constraint gets transformed to a Klein-Gordon equation:

$$\partial_\phi^2\underline{\chi}(y,\phi) = \partial_y^2\underline{\chi}(y,\phi). \tag{3.40}$$

The precise relation between the physical profiles $\underline{\chi}(y,\phi)$ and $\underline{\varphi}(y,\phi)$ will be made clear in section 3.1.3, which I emphasize is one of the novelties of this work. The solution to the Klein-Gordon equation can be split into left and right-moving modes $\underline{\chi}_L(\phi+y)$ and $\underline{\chi}_R(\phi-y)$, respectively [23]. Focusing again on positive frequency solutions only:

$$\underline{\chi}(y,\phi) = \underline{\chi}_L(\phi+y) + \underline{\chi}_R(\phi-y), \tag{3.41}$$

$$\underline{\chi}_L(\phi+y) = \frac{1}{\sqrt{2\pi}}\int_0^{+\infty} d\tilde{\omega} e^{i\tilde{\omega}(\phi+y)} e^{-i\tilde{\omega}\phi_o} \underline{\tilde{\chi}}(-\tilde{\omega}), \tag{3.42}$$

$$\underline{\chi}_R(\phi-y) = \frac{1}{\sqrt{2\pi}}\int_0^{+\infty} d\tilde{\omega} e^{i\tilde{\omega}(\phi-y)} e^{-i\tilde{\omega}\phi_o} \underline{\tilde{\chi}}(\tilde{\omega}), \tag{3.43}$$

where the factor $e^{-i\tilde{\omega}\phi_o}$ was introduced for convenience, to match initial data with the previous formulation. This way,

$$\underline{\chi}(y,\phi_o) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} d\tilde{\omega} e^{-i\tilde{\omega}y} \underline{\tilde{\chi}}(\tilde{\omega}). \tag{3.44}$$

Defining $y_\pm = \phi \pm y$, notice that $\underline{\chi}_{L/R}(y_\pm)$ can be any function which Fourier transform is supported on the positive real line.

Physical inner product

The physical inner product in this representation is the Klein-Gordon product [23], namely:

$$\begin{aligned}\left(\underline{\chi}_1, \underline{\chi}_2\right)_{phys} &= 2\int_{-\infty}^{+\infty} d\tilde{\omega}|\tilde{\omega}|\overline{\underline{\tilde{\chi}}_1}(\tilde{\omega})\underline{\tilde{\chi}}_2(\tilde{\omega}) \\ &= 2\int_{-\infty}^{+\infty} dy\, \overline{\underline{\chi}_1}(y,\phi_o)\, |i\partial_y|\, \underline{\chi}_2(y,\phi_o),\end{aligned} \tag{3.45}$$

where $i\partial_y$ is a positive definite self-adjoint operator on right-moving modes and a negative definite self-adjoint operator on left-moving modes. Furthermore, the Klein-Gordon inner-product is independent of the value of ϕ, and we have particularized it to, e.g., $\phi = \phi_o$.

Since the left and right-moving sectors of this physical Hilbert space are mutually orthogonal [23], we can focus our analysis on the left-moving modes:

$$\left(\underline{\chi}_1, \underline{\chi}_2\right)_{phys_L} = -2i\int_{-\infty}^{+\infty} dy\, \overline{\underline{\chi}_{1_L}}(y,\phi_o)\partial_y \underline{\chi}_{2_L}(y,\phi_o), \tag{3.46}$$

keeping in mind that the analysis for the right-moving modes is analogous (with a plus sign in the inner product), and that the expectation value of an observable is given by the sum of the expectation value on the left and right sectors.

Volume observable

Focusing on left-moving modes (3.42), with the Klein-Gordon product (3.45), the expectation value of the volume observable is found to be:

$$\left(\underline{\chi}, \hat{V}|_{\phi}\underline{\chi}\right)_{phys_L} = V_o\, e^{\sqrt{12\pi G}\,\phi}, \tag{3.47}$$

$$V_o \equiv 2\pi G\gamma\sqrt{\Delta}\, v_o, \tag{3.48}$$

$$v_o \equiv \frac{1}{\sqrt{12\pi G}} \int_{-\infty}^{+\infty} dy_+ \left|\frac{d\underline{\chi}_L(y_+)}{dy_+}\right|^2 e^{-\sqrt{12\pi G}\, y_+}, \tag{3.49}$$

for all physical states. Furthermore, we now find that, for a state $\underline{\chi}_L(y_+)$ to belong to the domain of the volume, it has to be such that (3.49) is well defined (i.e., the integral converges). Recall that it also needs to have Fourier transform with support on the positive real line to be well-defined as an element of the Hilbert space (see (3.42)). Then, the choice of such a function is quite complicated. The solution we propose to provide explicit physical states that belong to the domain of the volume in this Klein-Gordon formulation is to find the map between the v-representation and this one.

3.1.3 Relation between formulations

In the original v-representation, a Gaussian profile $\underline{\tilde{\psi}}(k)$ for the physical states peaked in a classical trajectory leads to an expanding evolution for the expectation value of the volume observable (3.24). In the Klein-Gordon representation, we find the same type of behaviour for the expectation value of the volume (3.47), without specifying the profile $\underline{\chi}_L$. However, it is not trivial to explicitly construct a physical state in the domain of the volume. The profile $\underline{\chi}_L$ needs to be chosen such that its Fourier transform has support on the positive real line and the integral in (3.49) converges. Thus, in this section, we will build a clear dictionary at the physical level between the v and y-representations, in order to determine the $\underline{\chi}_L$ that corresponds to a given $\underline{\tilde{\psi}}(k)$. Then, in particular, by choosing a Gaussian profile for $\underline{\tilde{\psi}}(k)$ as in (3.23), we will obtain a well defined v_o and physical states peaked on a classical trajectory also in the y-representation.

Given a profile

$$\underline{\tilde{\psi}}(k) \in L^2(\mathbb{R}, dk), \tag{3.50}$$

in v-representation, and choosing an initial data as in (3.22), this corresponds to:

$$\underline{\psi}(v,\phi) = \int_{-\infty}^{+\infty} dk\, \underline{\tilde{\psi}}(k)\underline{e}_k(v)e^{i\omega(k)(\phi-\phi^*)} \in L^2(\mathbb{R}, dv). \tag{3.51}$$

Through (3.30), we change from the v-representation to the b-representation and obtain:

$$\begin{aligned}\underline{\tilde{\psi}}(b,\phi) &= \frac{1}{\sqrt{4\pi}}\int_{-\infty}^{+\infty} dk\ \underline{\tilde{\psi}}(k) e^{i\omega(k)(\phi-\phi^*)} \int_{-\infty}^{+\infty} dv e^{\frac{i}{2}vb} \frac{1}{\sqrt{2\pi|v|}} e^{i\ k\ln|v|} \\ &= \frac{1}{\pi\sqrt{b}}\int_{-\infty}^{+\infty} dk\ \underline{\tilde{\psi}}(k) \left|\frac{2}{b}\right|^{i\ k} \cos\left(\frac{1+2ik}{4}\pi\right)\ \Gamma\left(\frac{1}{2}+ik\right) e^{i\omega(k)(\phi-\phi^*)} \in L^2(\mathbb{R}, db).\end{aligned} \tag{3.52}$$

Then, we perform the rescaling (3.34):

$$\underline{\varphi}(b,\phi) = \sqrt{|b|}\underline{\tilde{\psi}}(b,\phi) \in L^2(\mathbb{R}, \frac{1}{|b|}db), \tag{3.53}$$

and change variable from b to y through (3.38):

$$\underline{\varphi}(y,\phi) = \underline{\varphi}(b(y),\phi) \in L^2(\mathbb{R}, \sqrt{12\pi G}\, dy). \tag{3.54}$$

As pointed out before, these still are not the states $\underline{\chi}(y,\phi)$. The states $\underline{\varphi}(y,\phi)$ live in a Hilbert space with inner product (3.39) while $\underline{\chi}(y,\phi)$ live in a space with the Klein-Gordon product (3.45). We need to perform first another change of representation from $L^2(\mathbb{R}, \sqrt{12\pi G}dy)$ to $L^2(\mathbb{R}, dy)$, which corresponds to the rescaling:

$$\begin{aligned}\underline{\tilde{\chi}}(y,\phi) &= (12\pi G)^{1/4}\, \underline{\varphi}(y,\phi) \\ &= \frac{(12\pi G)^{1/4}}{\pi}\int_{-\infty}^{+\infty} dk\ \underline{\tilde{\psi}}(k) e^{-i\sqrt{12\pi G}ky} \cos\left(\frac{1+2ik}{4}\pi\right)\ \Gamma\left(\frac{1}{2}+ik\right) e^{i\omega(k)(\phi-\phi^*)}.\end{aligned} \tag{3.55}$$

These states can be split into right and left moving modes $\underline{\tilde{\chi}}(y,\phi) = \underline{\tilde{\chi}}_L(y_+) + \underline{\tilde{\chi}}_R(y_-)$ with $y_\pm = \phi \pm y$:

$$\underline{\tilde{\chi}}_{L/R}(y_\pm) = \frac{(12\pi G)^{1/4}}{\pi}\int_0^{+\infty} dk\ \underline{\tilde{\psi}}(\mp k) \cos\left(\frac{1\mp 2ik}{4}\pi\right)\ \Gamma\left(\frac{1}{2}\mp ik\right) e^{i\omega(k)(y_\pm-\phi^*)}. \tag{3.56}$$

Focusing on left-moving modes, we take another Fourier transform:

$$\underline{\tilde{\chi}}_L(\tilde{\omega},\phi) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dy e^{-i\tilde{\omega}y} \underline{\tilde{\chi}}_L(y_+) \in L^2(\mathbb{R}, d\tilde{\omega}), \tag{3.57}$$

and another rescaling

$$\underline{\chi}_L(\tilde{\omega},\phi) = \frac{1}{\sqrt{2|\tilde{\omega}|}}\underline{\tilde{\chi}}_L(\tilde{\omega},\phi) \in L^2(\mathbb{R}, 2|\tilde{\omega}|d\tilde{\omega}), \tag{3.58}$$

which is finally transformed to:

$$\underline{\chi}_L(y_+) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} d\tilde{\omega} e^{i\tilde{\omega}y} \underline{\chi}_L(\tilde{\omega}, \phi). \tag{3.59}$$

Putting everything together, we find that the left moving modes of the physical states of the Klein-Gordon representation are given by:

$$\underline{\chi}_L(y_+) = \frac{1}{\sqrt{2\pi}} \int_0^{+\infty} \frac{dk}{\sqrt{k}} \underline{\tilde{\psi}}(-k) \cos\left(\frac{1-2ik}{4}\pi\right) \Gamma\left(\frac{1}{2} - ik\right) e^{i\sqrt{12\pi G}k(y_+ - \phi^*)}. \tag{3.60}$$

In summary, in the Klein-Gordon representation, the physical states $\underline{\chi}(y, \phi)$ can be split in left and right-moving modes:

$$\underline{\chi}_{L/R}(y_\pm) = \frac{1}{\sqrt{2\pi}} \int_0^{+\infty} dk \underline{\tilde{\chi}}_\pm(k) e^{i\sqrt{12\pi G}k(y_\pm - \phi^*)}, \tag{3.61}$$

respectively, whose Fourier transform $\underline{\tilde{\chi}}_\pm(k)$ have support on the positive real line. These Fourier transforms are the profiles that define the physical state, and are related to the profile $\underline{\tilde{\psi}}(k)$ defining (3.51) by:

$$\underline{\tilde{\chi}}_\pm(k) = \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{k}} \underline{\tilde{\psi}}(\mp k) \cos\left(\frac{1 \mp 2ik}{4}\pi\right) \Gamma\left(\frac{1}{2} \mp ik\right). \tag{3.62}$$

Now, it is possible to compute the expectation value of the volume from (3.47), given a profile $\underline{\tilde{\psi}}(k)$. For the gaussian profile (3.23), in order for the expectation value of the volume to agree in both representations (3.24) and (3.47), we find that[1] $2v_o = e^{-\sqrt{12\pi G}\phi^*}$. Without loss of generality, we can choose $\phi^* = 0$, so that $v_o = 1/2$, independently of the parameters of the profile.

3.2 Summary

In this chapter, we have shown that, in the WDW approach, the expectation value of the volume for semiclassical states (3.24) follows the classical trajectory into the big-bang located at $\phi \to -\infty$. We can also find the expectation value of the observable that represents the matter energy density. Classically, this is given by $\rho|_\phi = \pi_\phi^2/(2V|_\phi^2)$ and so the corresponding operator is written as [23]:

$$\hat{\rho}|_\phi = \frac{1}{2}\hat{A}|_\phi^2 \,, \qquad \hat{A}|_\phi = \hat{V}|_\phi^{-1/2} \hat{\pi}_\phi \hat{V}|_\phi^{-1/2}. \tag{3.63}$$

Thus, since the expectation value of $\hat{V}|_\phi$ vanishes at the big-bang, the expectation value of the energy

[1] Note that the total expectation value is the sum of the expectation values on the right and left sectors. Furthermore, the expectation value on the right sector is found to be the same as for the left sector. Hence, the expectation value of the volume on left-moving modes is $1/2$ of the total expectation value

density diverges and, in this sense, the big-bang singularity is not resolved.

However, the analysis carried out in this chapter will be relevant also in the context of LQC. These two approaches (WDW and LQC) share the physical Hilbert space in their Klein-Gordon formulation. Thus, the states $\underline{\chi}(y,\phi)$ of the WDW approach and the corresponding $\chi(y,\phi)$ of LQC live in the same Hilbert space, and the difference between the two approaches in this representation lies in the form of the operators that represent observables. A well defined $\underline{\chi}(y,\phi)$ is therefore also a suitable physical state $\chi(y,\phi)$ of LQC. Furthermore, writing explicitly the physical states that live in the domain of the volume operator is not trivial in the Klein-Gordon representation of either approach. Their Fourier transform has support only on the positive real line and the integral in (3.49) has to converge. By doing this analysis, we managed to write explicitly the physical states in the Klein-Gordon representation in terms of profiles $\underline{\tilde{\psi}}_+(k) \in L^2(\mathbb{R}, dk)$. This way, we can simply choose any profile $\underline{\tilde{\psi}}_+(k) \in L^2(\mathbb{R}, dk)$, and find the corresponding physical state in the Klein-Gordon formulation through (3.61) and (3.62). More importantly, this clarifies the mathematical conditions for semiclassicality in the Klein-Gordon representation. In the v-representation, a semiclassical state $\underline{\psi}(v,\phi)$ is simply defined by any physical profile $\underline{\tilde{\psi}}_+(k)$ peaked on a classical trajectory with bounded dispersions, whereas the choice of such a state in the Klein-Gordon representation is not clear by itself, but it is made clear with this mapping.

The dictionary between the v and y representations of the WDW approach is not the same as the one between the equivalent v and x representations of LQC, which is more complicated to obtain. Nevertheless, since the physical Hilbert space in the Klein-Gordon representations of both approaches is the same, we can use for the states $\chi(x,\phi)$ of LQC the same well defined states $\underline{\chi}(y,\phi)$ of the WDW approach, even if the corresponding profile $\psi(v,\phi)$ in the v representation of LQC is not the same as $\underline{\psi}(v,\phi)$ of the WDW approach. We will use this in the next chapter.

Chapter 4

Homogeneous and isotropic Loop Quantum Cosmology

In the WDW approach, as shown in the previous chapter, the expectation value of the matter energy density still diverges at the big-bang, and so this singularity is not generically cured. This leads to the need to explore other inequivalent quantization procedures, such as LQC.

In LQG, the phase space is described in terms of suitable variables for a gauge theory: an SU(2) connection and its canonically conjugate densitized triad [3]. The quantum configuration space is then constructed from holonomies of the connection along discrete edges, leading to a discretization of the geometry. LQC consists of the application of similar methods to cosmological models. For a flat FLRW model with a massless scalar field, similarly to the WDW approach, a change of representation leads to a transformation of the Hamiltonian constraint into a Klein-Gordon equation. This is usually called the solvable formulation of LQC (or solvable LQC – sLQC) as it provides an analytical solution of the physical states. The key result of this approach is that, as a consequence of the discretization of the geometry, the expectation value of the volume observable is found to have a minimum positive value and the energy density a maximum finite value. These quantities undergo a bounce, connecting a contracting epoch of the Universe with an expanding one. Hence, the big-bang singularity is resolved and replaced with a quantum bounce. Furthermore, this result is not restricted to any particular form of the physical states. In this chapter, we will briefly review the quantization procedure for this simple model and analyse its key results.

We will also address an issue that has been overlooked hitherto. Because the solvable formulation was obtained only after the bounce had been found to occur in the original v-representation, by resorting to heavy numerical computations [13], the analytical solutions of the solvable formulation were never expressed for any specific physical state. Thus, the fact that it is highly non trivial to write an explicit state in the domain of the volume operator in this formulation went unnoticed. We will provide a way

of dealing with this issue, by taking advantage the of the fact that the physical Hilbert space of the Klein-Gordon formulation is shared by LQC and the WDW approach.

Finally, the occurrance of a bounce is not particular to this simple model. For example, it has been shown numerically [16] that in the presence of a cosmological constant the bounce still occurs. The study of more realistic models requires the introduction of a potential for the scalar field, which generally means that there is no analytical solution. The usual approach in the literature is to employ semiclassical or effective treatments, where additional quantum corrections are considered negligible. As a consequence, different formalisms and prescriptions in quantum cosmology cannot be suitably discriminated. Therefore, it is important to explore procedures that go beyond the usual treatments.

In [24], a mathematical procedure is proposed to deal with the inclusion of a generic potential for the scalar field, and extract the dominant contributions to the quantum dynamics. The treatment is based on the solvable formulation of the case with vanishing potential, and so it is a natural continuation of this chapter. In the next chapter, we explore this procedure and apply it to a constant potential.

4.1 Kinematics an physical Hilbert space in v-representation

In chapter 2, we have introduced the Hamiltonian formulation of the cosmological model of interest, and found that the Hamiltonian of the system is simply the Hamiltonian constraint (2.16). We then promoted the constraint to an operator, in chapter 3, using the Schrödinger-like representation of the system following the WDW approach. We will now adopt a different representation of the system, following the LQC approach.

LQC mimics the procedures of LQG, where there is no operator to directly represent b. Instead, there is one to represent the holonomies $\widehat{e^{i\lambda b/2}}$. Denoting the quantum states as $|v\rangle$, the kinematical Hilbert space of the geometrical sector, $\mathcal{H}_{grav}$, has the basic algebra:

$$\widehat{e^{\frac{i\lambda b}{2}}}|v\rangle = |v+\lambda\rangle, \tag{4.1}$$

$$\hat{v}|v\rangle = v|v\rangle, \tag{4.2}$$

such that the Dirac rule $\left[\widehat{e^{i\lambda b/2}}, \hat{v}\right] = i\{\widehat{e^{i\lambda b/2}}, v\}$ is satisfied. Remarkably, the inner product is discrete, given by the Kronecker delta (instead of the Dirac delta, as in the WDW approach):

$$\langle v|v'\rangle = \delta_{v,v'}, \tag{4.3}$$

which is a consequence of the fact that in this representation there is no infinitesimal generator $\hat{b}$ of trans-

lations in v, but only finite translations $\widehat{e^{i\lambda b/2}}$ are well defined. Thus, the basis states $|v\rangle$ are normalizable and provide an orthonormal basis. If λ is any real parameter, the resulting geometric sector of the kinematical hilbert space is the Bohr compactification of the real line, which is non-separable. However, the improved dynamics prescription [23] fixes $\lambda = 1$ and no other values for λ are considered.

Explicitly, the quantum counterpart of the Hamiltonian constraint is now given by:

$$\hat{C} = -\partial_\phi^2 - \hat{\Theta}, \tag{4.4}$$

The geometric part of the constraint is given by $\hat{\Theta} = \frac{3}{4\pi G\gamma^2}\hat{\Omega}_0^2$, and $\hat{\Omega}$ is found to be [39]:

$$\hat{\Omega}_0 = \frac{1}{2\sqrt{\Delta}}\hat{V}^{1/2}\left[\widehat{\text{sign}(v)}\,\widehat{\sin b} + \widehat{\sin b}\,\widehat{\text{sign}(v)}\right]\hat{V}^{1/2}. \tag{4.5}$$

where $\widehat{\sin b} = \left(\widehat{e^{ib}} - \widehat{e^{-ib}}\right)/(2i)$. Then, the operator $\hat{\Theta}$ is a difference operator of step 4, densely defined in the semilattices $\mathcal{L}_\varepsilon^\pm$:

$$\mathcal{L}_\varepsilon^\pm = \{v = \pm(\varepsilon + 4n)\,,\ n \in \mathbb{N}\}, \qquad \varepsilon \in (0, 4], \tag{4.6}$$

such that it is essentially self-adjoint in the Hilbert spaces $\mathcal{H}_\varepsilon^\pm$, the closure of $\mathcal{L}_\varepsilon^\pm$ with respect to the inner product (4.3).

Its generalized eigenfunctions $e_k(v)$ verify a recurrence relation and do not admit a closed form. In the limit of large v, they tend to a real linear combination of the two corresponding eigenfunctions of the WDW approach for the same eigenvalue. In other words, they behave like standing waves with both outgoing and incoming components, which then do not decouple unlike in the WDW approach [39].

For the matter field, a standard Schrödinger-like representation is adopted, like in the WDW approach, where $\hat{\phi}$ acts by multiplication and $\hat{\pi}_\phi = -i\partial_\phi$ as derivative. These operators are defined on the Hilbert space $L^2(\mathbb{R}, d\phi)$, with the domain $\mathcal{D}_\phi$ of the Schwartz space of rapidly decreasing functions, dense in $L^2(\mathbb{R}, d\phi)$.

The total kinematical Hilbert space is found to be $\mathcal{H}_{kin} = \mathcal{H}_\varepsilon^\pm \otimes L^2(\mathbb{R}, d\phi)$. Hence, as in the WDW approach, each of the operators act as the identity in the sector where they do not have a dependence.

With an analysis analogously to that exposed in section 3.1.1 for the WDW approach, we find that the physical states are given by:

$$\psi(v, \phi) = \int_{-\infty}^{+\infty} dk\; e_k(v)\left[\tilde{\psi}_+(k)e^{i\omega(k)\phi} + \tilde{\psi}_-(k)e^{-i\omega(k)\phi}\right]. \tag{4.7}$$

Note that, because the eigenfucntions $e_k(v)$ do not admit a closed form, this is a formal expression for the physical states. Here, as in the WDW approach, the physical Hilbert state is $\mathcal{H}_{phys} = L^2(\mathbb{R}, dk) \ni$

$\tilde{\psi}_{\pm}(k)$. Thus, $\tilde{\psi}_{\pm}(k)$ provide again superselected positive and negative frequency sectors, in the same way as in the WDW approach.

4.2 Solvable LQC

For the case of a flat FLRW model with a massless scalar field, there is a specially useful representation to work with, which allows for the constraint to be solved analytically. This is obtained by following the solvable LQC (sLQC) prescription [23]. The procedure is similar to that exposed in section 3.1.2. Firstly, we change from the v-representation to the b-representation. This time, the Fourier transform will not be the same as in the WDW approach, since now the kinematical Hilbert space is no longer $L^2(\mathbb{R}, dv)$. Instead, we need to perform a *discrete* Fourier transform. For this purpose, we need to define $\hat{\Theta}$ in a lattice supported over the whole real line, symmetrically spread around $v = 0$:

$$\mathcal{L} = \{v = 4n,\ n \in \mathbb{Z}\}, \tag{4.8}$$

so that $\mathcal{L} = \left(\mathcal{L}_4^+ \cup \mathcal{L}_4^- \cup |0\rangle\right)$[1]. This way, the Hilbert space under consideration $\mathcal{H}_{grav}$ is the closure of $\mathcal{L}$ with respect to the inner-product (4.3). Given that the states $\psi(v, \phi)$ are symmetric under the change from v to $-v$, as consequence of the fact that a change in the orientation of the triad does not have physical meaning, the operator $\hat{\Theta}$ is still essentially self-adjoint in this domain, with non-degenerate spectrum.

Then, the wave functions $\psi(v, \phi)$ and $\tilde{\psi}(b, \phi)$ of the v and b-representations are related by:

$$\tilde{\psi}(b, \phi) = \sum_{v \in \mathcal{L}} e^{\frac{ibv}{2}} \psi(v, \phi), \tag{4.9}$$

$$\psi(v, \phi) = \frac{1}{\pi} \int_0^{\pi} db\, e^{-\frac{ibv}{2}} \tilde{\psi}(b, \phi). \tag{4.10}$$

Notice that this Fourier transform maps $\mathcal{H}_{grav}$ to $L^2([0, \pi], db)$ (with periodic boundary conditions), i.e., since v is supported on a lattice of equidistant points over the real line, b is now an angle. Then, we introduce a scaling $\chi = \psi/(\pi v)$ and finally we implement a change of variable:

$$x = \frac{1}{\sqrt{12\pi G}} \ln\left[\tan\left(\frac{b}{2}\right)\right], \tag{4.11}$$

analogous to the change of variable from b to y in the WDW approach. The constraint in the x-representation is simplified to:

[1] We define the states $\psi(v, \phi)$ to vanish at $v = 0$

$$\hat{\pi}_\phi^2 - \hat{\pi}_x^2 = 0, \tag{4.12}$$

where $\hat{\pi}_\phi = -i\partial_\phi$ and $\hat{\pi}_x = -i\partial_x$ are the two momentum operators. This is precisely a Klein-Gordon equation, making the quantum dynamics easily integrated. $\hat{\pi}_\phi$ and $\hat{\pi}_x$ are Dirac observables, preserved by the dynamics, and we take the operator $\hat{\pi}_\phi$ to be positive (to remove double counting of solutions, given the time-reversal invariance). The operator $\hat{x}$ satisfies:

$$\hat{x} = \hat{x}_0 + (\phi - \phi_0)\text{sign}(\hat{\pi}_x). \tag{4.13}$$

Here, $\hat{x}_0$ is the operator $\hat{x}$ in the section where the configuration of the scalar field is ϕ_0, which can be seen as the initial section of the evolution. Physical states are found to have the form [13]:

$$\chi(x, \phi) = \frac{1}{\sqrt{2}} \left[\chi(x_+) - \chi(x_-)\right]. \tag{4.14}$$

Here, $x_\pm = \phi \pm x$ correspond to the left and right moving modes, respectively, and χ is any function with Fourier transform supported on the positive real line. Notice that, while in the WDW approach, the left and right sectors are completely independent, in LQC they are not. The fundamental reason is that in the WDW approach outgoing and incoming solutions are independent, while in LQC both contributions are present [39]. Using only, e.g., left moving modes, the inner product on physical states is given by:

$$\begin{aligned}(\chi_1, \chi_2)_L &= -2i \int_{\mathbb{R}} dx \overline{\chi_1}(x_+) \partial_x \chi_2(x_+) \\ &= 2i \int_{\mathbb{R}} dx \left(\partial_x \overline{\chi_1}(x_+)\right) \chi_2(x_+),\end{aligned} \tag{4.15}$$

while on right-moving modes

$$\begin{aligned}(\chi_1, \chi_2)_R &= 2i \int_{\mathbb{R}} dx \overline{\chi_1}(x_-) \partial_x \chi_2(x_-) \\ &= -2i \int_{\mathbb{R}} dx \left(\partial_x \overline{\chi_1}(x_-)\right) \chi_2(x_-),\end{aligned} \tag{4.16}$$

such that the total inner product is

$$(\chi_1, \chi_2) = \frac{1}{2} \left[(\chi_1, \chi_2)_L - (\chi_1, \chi_2)_R\right]. \tag{4.17}$$

Taking $\hat{P}_R$ and $\hat{P}_L$ to be projectors on the right and left-moving modes, it is shown [23] that:

$$\hat{v} = \frac{1}{\sqrt{3\pi G}} \sum_{j=R,L} \hat{P}_j \cosh\left(\sqrt{12\pi G}\hat{x}\right) \hat{\pi}_x \hat{P}_j. \tag{4.18}$$

Hence, having the physical volume represented by the operator $\hat{V} = 2\pi G\gamma\sqrt{\Delta}|\hat{v}|$, we find that the

expectation value of the volume can be written as:

$$\langle \hat{V}|_\phi \rangle = \left(\chi, \hat{V}|_\phi \chi\right) = 2\pi G\gamma\sqrt{\Delta}\,(\chi, |\hat{v}|_\phi \chi)\,. \tag{4.19}$$

Recalling that $\hat{\pi}_x$ is positive (negative) on the sector of left (right)-moving modes[2], we conclude that $\langle \hat{V}|_\phi \rangle = \langle \hat{V}|_\phi \rangle_L$, and finally:

$$\begin{aligned} \langle \hat{V}|_\phi \rangle &= \frac{4\pi G\gamma\sqrt{\Delta}}{\sqrt{3\pi G}} \int_{-\infty}^{\infty} dx_+ \left|\frac{d\chi(x_+)}{dx_+}\right|^2 \cosh(\sqrt{12\pi G}x) \\ &= V_+ e^{\sqrt{12\pi G}\phi} + V_- e^{-\sqrt{12\pi G}\phi}, \end{aligned} \tag{4.20}$$

with

$$V_\pm = \frac{2\pi G\gamma\sqrt{\Delta}}{\sqrt{3\pi G}} \int_{-\infty}^{\infty} dx_+ \left|\frac{d\chi(x_+)}{dx_+}\right|^2 e^{\mp\sqrt{12\pi G}x_+}. \tag{4.21}$$

Note that this imposes a strong condition on $\chi(x_+)$: it has to be such that the integrals in (4.21) converge, for $\chi(x, \phi)$ to live in the domain of the volume. This issue will be addressed later.

It is straightforward to find analytically that there is a minimum V_B for the physical volume,

$$V_B = 2\frac{\sqrt{V_+ V_-}}{\|\chi\|^2}, \tag{4.22}$$

at the bounce point ϕ_B,

$$\phi_B = \frac{1}{\sqrt{12\pi G}} \ln\left(\frac{V_-}{V_+}\right). \tag{4.23}$$

One can also easily find that the internal-time evolution of the volume is exactly symmetric around the bounce point for all states, by writing $\langle \hat{V}|_\phi \rangle$ as:

$$\langle \hat{V}|_\phi \rangle = V_B \cosh\left[\sqrt{12\pi G}(\phi - \phi_B)\right]. \tag{4.24}$$

Finally, we can obtain the expectation value of the observable that represents the matter energy density. Classically, this is given by $\rho|_\phi = \pi_\phi^2/(2V|_\phi^2)$ and so the corresponding operator is written as:

$$\hat{\rho}|_\phi = \frac{1}{2}\hat{A}|_\phi^2\,, \qquad \hat{A}|_\phi = \hat{V}|_\phi^{-1/2}\hat{\pi}_\phi\hat{V}|_\phi^{-1/2}. \tag{4.25}$$

By computing the spectrum of $\hat{A}|_\phi$, one finds that $\hat{\rho}|_\phi$ is bounded from above by:

$$\rho_{sup} = \frac{3}{8\pi G\Delta\gamma^2}. \tag{4.26}$$

[2]Which implies that $|\hat{\pi}_x|\chi(x_\pm) = \pm\hat{\pi}_x\chi(x_\pm)$.

Note that there is no implicit dependence of ρ_{sup} on the choice of the finite cell $\mathcal{V}$, proving that, indeed, due to homogeneity, the analysis of this cell represents the dynamics of the whole Universe. Moreover, remarkably, ρ_{sup} is universal, namely independent on the state. This is a special feature of the improved dynamics prescription, which makes it a physically successful quantization choice.

Finally, for large values of ϕ, and thus for large volumes, $V(\phi)$ is proportional to the classical solutions of the model $e^{\sqrt{12\pi G}|\phi|}$, agreeing with GR when the curvature is small.

The fact that these results have been derived in a purely analytical manner is a powerful feature, since it does not restrict their validity to any specific type of sates. Nevertheless, it is important to recognise that the choice of a specific function $\chi(x_+)$ that defines the physical states in the domain of the volume is not trivial. Its Fourier transform is supported on the positive real line and it has to be such that the integrals in (4.21) converge. To date, this issue has been overlooked, due to the fact that the bounce had been shown to occur already in the v-representation, with numerical treatments [13]. Thus, when the analytical formulation was derived, there was no need to define explicit physical states. In the next chapter, we will rely on the solvable formulation to explore the effects on the dynamics of including a potential for the scalar field. To obtain results for specific forms of the potential, and compare to other results obtained numerically in the literature, a specific state has to be defined, and this issue needs to be addressed.

To this end, it is useful to compare this formulation with the Klein-Gordon representation of the WDW approach. The integrals in (3.49) and (4.21) have the same structure. The functions $\underline{\chi}_L(y_+)$ of (3.49) play the same role as $\chi(x_\pm)$ in (4.21). This way, we can choose $\chi(x_+)$ to be the same as $\underline{\chi}_L(y_+)$ for a given profile $\underline{\tilde{\psi}}_+(k) \in L^2(\mathbb{R}, dk)$. This will not correspond to the same profile in the v-representation in the LQC approach, because the map from v to y of the WDW is not the same as the map from v to x in LQC. However, we know that this makes the integral in (4.21) converge and is therefore a suitable choice for $\chi(x_\pm)$.

This analysis already showcases the most important results of LQC. As mentioned in the beginning of this chapter, these are not particular to the simplest case of a flat FLRW model with a massless scalar field. In the next chapter we will introduce a non-vanishing potential for the scalar field, thus enabling the study of more interesting models.

Chapter 5

Dealing with a potential in Loop Quantum Cosmology

The next step towards the study of more realistic models is the introduction of a non-vanishing potential for the scalar field $W(\phi)$. In this case, the form of the classical constraint is found to be [24]:

$$\pi_\phi^2 - \frac{3}{4\pi G\gamma^2}\Omega_0^2 + 8\pi^2 G^2 \Delta\gamma^2 v^2 W(\phi) = 0. \tag{5.1}$$

Consequently, as long as the potential is not constant, as we will see, the resulting Hamiltonian becomes time dependent (in the internal time variable ϕ), and the system does not admit an analytical solution. Furthermore, the term in $W(\phi)$ also depends on the geometrical variable v, and so, even if the potential is constant (eliminating the time dependence in the Hamiltonian), the eigenfunctions of the Hamiltonian do not admit an analytically closed form. It is necessary either heavy computational power, and to generate the eigenfunctions numerically (as in [16] for constant potential), or the use of approximations.

The usual procedure in the literature is to adopt effective or semiclassical treatments that consider further quantum corrections negligible. This way, different prescriptions within quantum cosmology cannot be properly discriminated. One possible avenue for the discrimination of distinct procedures is through the quantum corrections to the power spectrum of primordial fluctuations. The treatment proposed in [24] to extract as much as possible the contributions of the potential to the quantum dynamics was motivated by this problem. A compromise between required computational power and the precision of the final results is offered, by introducing approximations but going beyond the semiclassical or effective treatments usually employed in the literature. We will apply this method for the case of constant potential, but in the following we will first introduce the proposal for a generic form of the potential.

5.1 Generic potential

For this analysis, it is helpful to define the operator $\hat{B} = \sqrt{4\pi G/3}\gamma\hat{V}|\hat{\Omega}_0|^{-1}\hat{V}$. The loop quantization provides the operator $\hat{\Omega}_0^2$, acting on states $|v\rangle$, as a difference operator of step 4. To preserve the lattices of step 4, we define the quantum counterpart of Ω_0 by doubling the length of the holonomies. Namely, for this operator, replacing the canonical set $\{v, b/2\}$ with a new one $\{v/2, b\}$:

$$\hat{\Lambda}_0 = 2\pi G\gamma\frac{\hat{v}}{2}\widehat{\sin(2b)} = 2\pi G\gamma\hat{v}\,\widehat{\cos b}\,\widehat{\sin b}. \tag{5.2}$$

After a careful calculation in the x-representation, one finds [24]:

$$\hat{\Lambda}_0 = -\sqrt{\frac{4\pi G\gamma^2}{3}}\tanh\left(\sqrt{12\pi G}\hat{x}\right)\hat{\pi}_x, \tag{5.3}$$

$$\hat{B} = \frac{4\pi G\Delta\gamma^2}{3}\cosh^2\left(\sqrt{12\pi G}\hat{x}\right)|\hat{\pi}_x|. \tag{5.4}$$

Notice that, in sLQC, the quantum evolution of these operators is that dictated by the evolution of $\hat{x}$ given in (4.13), having $\hat{\pi}_x$ constant.

Now, we have the necessary tools to proceed with the analysis. The goal of this procedure is to be able to compute expectation values of operators over the FLRW geometry. The main obstacle is to compute the quantum evolution of FLRW states. In order to do this, we will take advantage of the fact that the free dynamics (with vanishing potential) is known and easily dealt with (see chapter 4). Setting $W = 0$, we would obtain the trajectory (4.13) and an analytical expression for the physical states (4.14) along with the inner product (4.15). We can first take the generator of the FLRW dynamics, extract its free geometric part (for $W = 0$) and use it to pass to an interaction picture.

Allowing for a non vanishing potential, the constraint is given by (5.1). We can write the quantum counterpart as:

$$\hat{C} = \hat{\pi}_\phi^2 - \hat{\mathcal{H}}_0^{(2)}, \tag{5.5}$$

$$\hat{\mathcal{H}}_0^{(2)} = \hat{\pi}_x^2 - 2W(\hat{\phi})\hat{V}^2. \tag{5.6}$$

Interpreting ϕ as time, the quantum Hamiltonian is $\hat{\mathcal{H}}_0 = \hat{\pi}_\phi = -i\partial_\phi$. Using the Hamiltonian constraint (5.5), and considering only positive frequency solutions, we have that $\hat{\mathcal{H}}_0$ is the positive square root of $\hat{\mathcal{H}}_0^{(2)}$, and can be seen as a modification of the evolution generator along ϕ of the homogeneous system with massless scalar field.

Now, we write the physical states as:

$$\chi(x,\phi) = \hat{U}(x,\phi)\chi_0(x), \tag{5.7}$$

where χ_0 is the initial FLRW state at a value ϕ_0 for the homogeneous scalar field, and $\hat{U}$ is the evolution operator given by:

$$\hat{U}(x,\phi) = \mathcal{P}\left[e^{-i\int_{\phi_0}^{\phi} d\tilde{\phi}\hat{\mathcal{H}}_0(x,\tilde{\phi})}\right], \tag{5.8}$$

where $\mathcal{P}$ denotes time ordering (with respect to ϕ). This way, expectation values are taken on the state χ of the FLRW geometry, with the inner product of sLQC (4.15). For a non constant scalar field potential $W(\phi)$, the dynamics is not solvable, since it requires the integration of the evolution of χ provided by $\hat{\mathcal{H}}_0$. Even in numerical computations complications arise [40]. To deal with this, we can first extract the dynamics of the free case, corresponding to vanishing potential. Treating the remaining evolution as a kind of geometric interaction, we can pass to an interaction picture.

Firstly, we define the operator $\hat{\mathcal{H}}_0$ for vanishing potential (free dynamics) as:

$$\hat{\mathcal{H}}_0^{(F)} = \sqrt{\frac{3}{4\pi G\gamma^2}}|\hat{\Omega}_0|. \tag{5.9}$$

In particular for sLQC, $\hat{\mathcal{H}}_0^{(F)} = |\hat{\pi}_x|$. Then, the states in the interaction picture are written as:

$$\chi_I(x,\phi) = e^{i\hat{\mathcal{H}}_0^{(F)}(\phi-\phi_0)}\chi(x,\phi), \tag{5.10}$$

which from equation (5.7) becomes:

$$\chi_I(x,\phi) = e^{i\hat{\mathcal{H}}_0^{(F)}(\phi-\phi_0)}\mathcal{P}\left[e^{-i\int_{\phi_0}^{\phi} d\tilde{\phi}\hat{\mathcal{H}}_0(x,\tilde{\phi})}\right]\chi_0(x) = \hat{U}_I(x,\phi)\chi_0(x), \tag{5.11}$$

$$\hat{U}_I(x,\phi) = \mathcal{P}\left[e^{-i\int_{\phi_0}^{\phi} d\tilde{\phi}\hat{\mathcal{H}}_{1I}(x,\tilde{\phi})}\right]. \tag{5.12}$$

Here, $\hat{\mathcal{H}}_1 = \hat{\mathcal{H}}_0 - \hat{\mathcal{H}}_0^{(F)}$. Any operator $\hat{O}$ in the Schrödinger-like picture has a corresponding operator $\hat{O}_I$ in the interaction picture:

$$\hat{O}_I = e^{i\hat{\mathcal{H}}_0^{(F)}(\phi-\phi_o)}\hat{O}e^{-i\hat{\mathcal{H}}_0^{(F)}(\phi-\phi_o)}, \tag{5.13}$$

and in total we find:

$$\langle\hat{O}(\phi)\rangle_\chi = \langle\hat{O}_I(\phi)\rangle_{\chi_I} = \langle\hat{U}_I(\phi)^\dagger\hat{O}_I(\phi)\hat{U}_I(\phi)\rangle_{\chi_0}, \tag{5.14}$$

where the dagger denotes the adjoint. Since the integration of the dynamics of the free case can be performed analytically in the sLQC prescription, the form of the FLRW geometry operators in the interaction picture is easy to obtain. In fact, it simply corresponds to the substitution of their dependence on $\hat{x}$ by the same dependence on the evolved operator, according to (4.13):

$$\hat{x} \to \hat{x}(\phi) = \hat{x} + (\phi - \phi_0)\text{sign}(\hat{\pi}_x). \tag{5.15}$$

Thus, the dynamical evolution of the expectation values reduces to the computation of the path-ordered integral of (5.12). This computation is still too difficult and, at this point, one may treat the evolution semiclassically. However, since we want to go further in the analysis, we will extract the dominant contributions of the potential in the quantum evolution. assuming we can regard the potential as a perturbation of the free case., i.e., $8\pi^2 G^2 \Delta\gamma^2 v^2 W(\phi) \ll 3\Omega_0^2/(4\pi G\gamma^2)$.

The operator $\hat{\mathcal{H}}_{1I}$ is the counterpart of $\hat{\mathcal{H}}_1$ in the interaction picture, and is thus obtained from $\hat{\mathcal{H}}_1$ with the replacement (5.15). Up to first order terms in the potential, $\hat{\mathcal{H}}_1$ can be represented in the approximate form [24]:

$$\hat{\mathcal{H}}_1 \approx \hat{\mathcal{H}}_2 = -W(\phi)\hat{B}. \tag{5.16}$$

Generally, we can write

$$\hat{\mathcal{H}}_{1I} = \hat{\mathcal{H}}_{2I} + \hat{\mathcal{H}}_{3I}, \tag{5.17}$$

where $\hat{\mathcal{H}}_{2I}$ is $\hat{\mathcal{H}}_2$ in the interaction picture, and $\hat{\mathcal{H}}_{3I}$ is the remaining part of $\hat{\mathcal{H}}_{1I}$, at least of second order in the potential. This way, the dominant contribution of the potential to the generator of the evolution in the interaction picture is found, for sLQC, from (5.16) with the substitution (5.15) in the expression of $\hat{B}$ given in (5.4). The dynamics generated by $\hat{\mathcal{H}}_{2I}$ can be obtained by passing to a new interaction picture J. In this sense, we introduce:

$$\hat{U}_{2I} = \mathcal{P}\left[e^{-i\int_{\phi_0}^{\phi} d\tilde{\phi}\hat{\mathcal{H}}_{2I}(\tilde{\phi})}\right], \tag{5.18}$$

and find that for any operator $\hat{O}_I$ in the initial interaction picture, the corresponding operator in the new interaction picture is given by:

$$\hat{O}_J = \hat{U}_{2I}^{\dagger}\hat{O}_I\hat{U}_{2I}. \tag{5.19}$$

Finally, the expectation value of this operator can be found by:

$$\langle \hat{O}(\phi)\rangle_\chi = \langle \hat{O}_I(\phi)\rangle_{\chi_I} = \langle \hat{U}_J^\dagger \hat{O}_J \hat{U}_J\rangle_{\chi_0}, \tag{5.20}$$

$$\hat{U}_J = \mathcal{P}\left[\exp\left(-i\int_{\phi_0}^{\phi} d\tilde{\phi}\hat{\mathcal{H}}_{3J}(\tilde{\phi})\right)\right]. \tag{5.21}$$

Now, the remaining obstacle is the integration of the evolution generated by $\hat{\mathcal{H}}_{2I}$ and $\hat{\mathcal{H}}_{3I}$. Up to this point, no approximations have been introduced and the treatment has been exact. At this stage, however, we need to renounce to an exact treatment. We will first consider that the evolution generated by $\hat{\mathcal{H}}_3$ can be ignored. This way, $\hat{U}_J \approx \mathbb{1}$ and

$$\langle \hat{O}(\phi)\rangle_\chi \approx \langle \hat{O}_J\rangle_{\chi_0}. \tag{5.22}$$

Since the form of $\hat{O}_I$ and χ_o are known, the only obstacle left is the computation of $\hat{U}_{2I}$. To that end, we will truncate the series expansion of $\hat{U}_{2I}$ in terms of path ordered integrals of powers of $\hat{\mathcal{H}}_{2I}$, in order to compute $\hat{O}_J$ up to a certain order of the potential:

$$\hat{U}_{2I} = \mathbb{1} - i\int_{\phi_0}^{\phi} d\tilde{\phi}\hat{\mathcal{H}}_{2I}(\tilde{\phi}) + \mathcal{O}(W^2). \tag{5.23}$$

Keeping the linear contributions of the potential in the operator $\hat{O}_J$ and using the relation (5.16), we find [24]:

$$\hat{O}_J \approx \hat{O}_I + i\left[\hat{O}_I, \int_{\phi_0}^{\phi} d\tilde{\phi}W(\tilde{\phi})\hat{B}_I(\tilde{\phi})\right]. \tag{5.24}$$

The relative order of the terms neglected in $\hat{U}_{2I}$, with respect to the conserved ones is found to be [24]:

$$R_B = \sqrt{G}\gamma(\phi-\phi_0)W\frac{V_I^2}{|\Omega_0|}, \tag{5.25}$$

where Ω_0 is a constant of motion for the vanishing potential case and it is assumed that the change of WV_I^2 is negligible. This way, the truncation is valid if $R_B \ll 1$.

Finally, it is necessary to determine when the remaining dynamics needs to be accounted for. It is found [24] that the first contribution in powers of the potential in $\hat{U}_J$ are of the order of $R_B^2 r_B$, where

$$r_B = \frac{\sqrt{G}\gamma}{|\Omega_0(\phi-\phi_0)|}. \tag{5.26}$$

Then, the remaining dynamics, generated by $\hat{U}_J$, can only be ignored if $R_B^2 r_B \ll 1$. Furthermore, if the first contributions of the potential in $\hat{U}_J$ (of order $R_B^2 r_B$) are larger than the first terms neglected

in $\hat{U}_{2I}$ (of order R_B^2), then the remnant of the evolution cannot be ignored either. Hence, recalling that $R_B \ll 1$ for the truncation of $\hat{U}_{2I}$ to be valid, the dynamics generated by $\hat{U}_J$ can be ignored if $r_B < 1$.

In the case where $\hat{U}_J$ needs to be considered, an effective approximation is required, since its quantum evolution is too complicated to be manageable. By effective approximation, one means that the considered state of the FLRW geometry needs to be peaked around an effective trajectory of the evolution generated by $\hat{\mathcal{H}}_{3J}$. In this work, we will not concern ourselves with these details yet, as we will first consider situations where the dynamics generated by $\hat{U}_J$ are negligible, i.e., where $r_B < 1$ and $R_B \ll 1$.

Under these conditions, given the inner-product of sLQC (4.15), one simply needs to compute (5.24) to find the expectation value of an observable, since now $\langle \hat{O} \rangle_\chi \approx \langle \hat{O}_J \rangle_{\chi_0}$. For this calculation, it is of course necessary to particularize the discussion to a specific form of the potential.

5.2 Constant Potential

To apply this procedure to a specific potential, we choose to start with the simplest non trivial case of a constant potential. Even though this is a simple case, it is already very relevant for cosmology, as it is equivalent to considering a massless scalar field in the presence of a cosmological constant, by taking $W = \Lambda/(8\pi G)$ [16].

In this situation, taking ϕ as relational clock, we will still get a time-independent Hamiltonian. However, its eigenfunctions do not admit an analytical closed form. Hence, this is a suitable model for the first application of the procedure outlined above. Alternatively, one could numerically try to diagonalize the Hamiltonian of the system. Its eigenfunctions would have to be generated numerically, requiring heavy computational power, as has been performed in [16].

For constant potential, the computation of (5.24) is quite simplified. It is simply necessary to compute the integral $\int_{\phi_0}^{\phi} d\tilde{\phi} \hat{B}_I(\tilde{\phi})$. This calculation is carried out in Appendix A.1, which yields an expression for any operator $\hat{O}_J$, to first order in the constant potential. This expression, together with the inner product (4.15) of sLQC allows us to compute expectation values $\langle \hat{O}_J \rangle_\chi$ of certain operators.

We are interested in tracking the expectation value of the volume observable. We find that, in the (x, ϕ) representation (where x and ϕ act by multiplication), $\hat{V}_J$ can be written as (see Appendix A.2 for further details of this calculation):

$$\hat{V}_J = \frac{2\pi G\gamma\sqrt{\Delta}}{\sqrt{3\pi G}} E(x,\phi)\hat{\pi}_x, \tag{5.27}$$

where we define $E(x, \phi)$ in equation (A.11) of the Appendix A.2.

Taking the inner-product of sLQC (4.15), the expectation value of $\hat{V}_J$ on left-moving modes is found to be:

$$\begin{aligned}\langle\hat{V}_J\rangle_L &= 2i\int_{\mathbb{R}} dx\,(\partial_x\overline{\chi}(x_+)|_{\phi_o})\,\hat{V}_J\chi(x_+)|_{\phi_o}\\ &= \frac{4\pi G\gamma\sqrt{\Delta}}{\sqrt{3\pi G}}\int_{\mathbb{R}} dx\,|\partial_x\chi(x_+)|_{\phi_o}|^2\,E(x,\phi),\end{aligned} \tag{5.28}$$

where the states $\chi(x_+)$ are evaluated at $\phi = \phi_o$ before being acted on by the operators. A careful calculation with a suitable change of variable in the integration variable leads to (see Appendix A.2):

$$\begin{aligned}\langle\hat{V}_J\rangle &= V_+e^{\sqrt{12\pi G}\phi}\left[1+W\sqrt{3\pi G}\frac{2\pi G\Delta\gamma^2}{3}\left(\frac{3}{2\sqrt{12\pi G}}+2(\phi-\phi_o)\right)\right]\\ &+ V_-e^{-\sqrt{12\pi G}\phi}\left[1+W\sqrt{3\pi G}\frac{2\pi G\Delta\gamma^2}{3}\left(\frac{3}{2\sqrt{12\pi G}}-2(\phi-\phi_o)\right)\right]\\ &+ W\frac{\pi G\Delta\gamma^2}{6}\Big[e^{3\sqrt{12\pi G}\phi}\left(V_{3+}-3V_+e^{-2\sqrt{12\pi G}\phi_o}\right)+e^{-3\sqrt{12\pi G}\phi}\left(V_{3-}-3V_-e^{+2\sqrt{12\pi G}\phi_o}\right)\\ &- e^{5\sqrt{12\pi G}\phi}\,V_{3+}e^{-2\sqrt{12\pi G}\phi_o}-e^{-5\sqrt{12\pi G}\phi}\,V_{3-}e^{+2\sqrt{12\pi G}\phi_o}\Big],\end{aligned} \tag{5.29}$$

with $V_\pm$ given in (4.21), and $V_{3\pm}$ defined as:

$$V_{3\pm} = \frac{2\pi G\gamma\sqrt{\Delta}}{\sqrt{3\pi G}}\int_{-\infty}^{\infty} dx_+\left|\frac{d\chi(x_+)}{dx_+}\right|^2 e^{\mp 3\sqrt{12\pi G}x_+}. \tag{5.30}$$

An inspection of the $W = 0$ case reveals that this agrees with the expectation value of $\hat{V}$ of sLQC, as it has to.

Ultimately, to evaluate it for specific states, the profile $\chi(x_+)$ has to be chosen. Recall that these have Fourier transform with support on the positive real line, i.e., they can be written as:

$$\chi(x_+) = \int_0^{+\infty} dk\tilde{\chi}(k)e^{ikx_+}. \tag{5.31}$$

Thus, the states will be defined by $\tilde{\chi}(k)$. As previously discussed, this has to be such that the integrals (4.21) and (5.30) converge. To find such a function is not trivial, and so we choose to use the same profile $\underset{\pm}{\tilde{\chi}}(k)$ (3.62) with a suitable profile for $\underset{+}{\tilde{\psi}}(k)$, as in the WDW approach. The Gaussian profile (3.23) would be an appropriate choice, although others can be considered, such that the final form of $\tilde{\chi}(k)$ is simplified. Specifically, it would be convenient to choose a profile such that the integrals in $V_\pm$ and $V_{3\pm}$ can be solved analytically.

All that there is left to do upon defining this profile is to actually compute the expectation value of the volume operator, tracking its evolution in ϕ. With this method, this is achieved with minimum computation power. The only possibly numerical integrations are the values of $V_\pm$ and $V_{3\pm}$. Notice that these are independent of ϕ, and therefore only need to be computed once, for a given profile. In fact, these values of $V_\pm$ do not even need to be computed, as they can be set by the normalization of $\tilde{\chi}(k)$.

Then, it is straightforward to evaluate (5.29) for different moments in time ϕ.

Finally, the results can be compared with the ones obtained in [16] for the same model. That work required a functional analysis of the Hamiltonian constraint operator, which involves the consideration of self-adjoint extensions. Furthermore, the eigenfunctions of the Hamiltonian had be generated numerically, requiring heavy computational power. Our method avoids such an analysis, which can be quite complicated for more general potentials. Hopefully, we will reveal that the difference between these methods is negligible, or at least that the qualitative nature of the two is the same, thus demonstrating the power of this procedure to obtain accurate results while being computationally inexpensive, and without the need of very complicated functional analysis.

This treatment can be extended to second order in the potential and, if necessary, we can consider the evolution generated by $\hat{U}_J$ with an effective approximation. Ultimately, having proven the robustness of this procedure, we intend to apply it to a more interesting model with non constant potential.

Chapter 6

Conclusions

In this work, we first studied the WDW approach to quantum cosmology for a flat FLRW model coupled to a massless scalar field. Even though this approach does not cure the big-bang singularity, in the sense that Dirac observables still diverge in some instant of the evolution, it provides a simpler setting to clarify some procedures that are analogous in the approach we are interested in, LQC. We managed to establish the map between the original formulation and the Klein-Gordon representation of the WDW approach, by finding the precise relation between the physical profiles of the two. This map, that had not been explicitly established before at the physical level, allows one to write the same physical state in both formulations. More importantly, it allows one to write a semiclassical state in the Klein-Gordon formulation, by first defining a semiclassical profile in the original formulation, where the notion of semiclassicality is clear. This was not addressed before, and has become clarified with this study.

Next, we focused our attention on the LQC approach, which has the appealing outcome of solving the big-bang singularity, by replacing it with a quantum bounce. It also admits a Klein-Gordon formulation, which allows for analytical solutions to be found. However, the result of the quantum bounce was already found in the original representation, by means of numerical computations. Thus, when the Klein-Gordon formulation was first studied, there was no need to build explicit physical states, since it was proven analytically that the bounce occurs for any physical profile. It turns out that it is not trivial to find physical states in the domain of the volume, our main physical observable, in this representation, but the previous analysis of the WDW approach offers a simple way of doing so. The two approaches share the physical Hilbert space of their respective Klein-Gordon formulations. By taking a semiclassical profile of the original formulation in the WDW approach, we find a well defined physical profile in the domain of the volume in its Klein-Gordon formulation. The same profile will define a state in the domain of the volume also in the Klein-Gordon formulation of LQC. This way we tackled an issue that had not been noticed before and provided a way of defining specific physical states in the domain of the volume in the Klein-Gordon formulation of LQC.

Having a full understanding at the physical level of the solvable formulation of LQC, we then progressed to the study of more realistic models, by introducing a potential for the scalar field. With this intent, we exposed a treatment that aims at extracting the main contributions of the potential to the quantum dynamics, by taking advantage of the fact that the dynamics of the free case is known. This procedure had been proposed in [24], but never applied to a specific form of the potential. Thus, we employed it to the simplest non trivial form possible, a constant potential. A final expression for the expectation value of the volume observable was obtained up to first order in the potential. This allows us to track this quantity, given a specific physical profile.

We intend to complete this analysis by providing a suitable physical profile, and comparing the results of this method with other results in the literature. Finally, the same procedure can be applied to more interesting forms of the potential, such as a mass term, which is a common model for inflation.

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Appendix A

Auxiliary computations for constant potential

In this appendix we will provide some more details regarding the calculations of the constant potential case.

A.1 Form of an operator in the interaction picture J

Writing $\hat{\mathcal{H}}_{2I} = -W\hat{B}_I(\phi)$, we find from (5.23):

$$\hat{U}_{2I} = \mathbb{1} + iW\int_{\phi_0}^{\phi} d\tilde{\phi}\hat{B}_I(\tilde{\phi}) + \mathcal{O}(W^2). \tag{A.1}$$

And so, up to first order in W:

$$\hat{O}_J \approx \hat{O}_I + iW\left[\hat{O}_I, \int_{\phi_0}^{\phi} d\tilde{\phi}\hat{B}_I(\tilde{\phi})\right]. \tag{A.2}$$

Thus, it is only necessary to calculate the integral $\int_{\phi_0}^{\phi} d\tilde{\phi}\hat{B}_I(\tilde{\phi})$, which is accomplished using

$$\hat{B}_I(\phi) = \frac{4\pi G\Delta\gamma^2}{3}\cosh[2\sqrt{3\pi G}\hat{x}(\phi)]|\hat{\pi}_x|. \tag{A.3}$$

This calculations involves a subtlety explained in Appendix A.3. We find that:

$$\int_{\phi_0}^{\phi} d\tilde{\phi}\hat{B}_I(\tilde{\phi}) = \frac{2\pi G\Delta\gamma^2}{3}\left[F(\phi) - F(\phi_0)\right]\hat{\pi}_x, \tag{A.4}$$

where we define

$$F(\phi) := \frac{1}{4\sqrt{3\pi G}}\sinh[4\sqrt{3\pi G}\hat{x}(\phi)] + \phi\text{sign}(\hat{\pi}_x). \tag{A.5}$$

A.2 Calculation of the expectation value of the volume to first order

From the procedures exposed in chapter 5, we find that the expectation value of the volume observable is written as:

$$\langle \hat{V}(\phi) \rangle_{\chi_L} \approx \langle \hat{V}_J \rangle_{\chi 0_L} = 2i \int_{-\infty}^{+\infty} dx \, (\partial_x \overline{\chi}(x_+)|_{\phi_o}) \, \hat{V}_J \chi(x_+)|_{\phi_o}. \tag{A.6}$$

From the previous calculations of this Appendix, $\hat{V}_J$ is found to be, up to first order in the potential:

$$\hat{V}_J \approx \hat{V}_I + iW \frac{2\pi G \Delta \gamma^2}{3} \left[\hat{V}_I \left(F(\phi) - F(\phi_o) \right) \hat{\pi}_x - \left(F(\phi) - F(\phi_o) \right) \hat{\pi}_x \hat{V}_I \right], \tag{A.7}$$

where

$$\hat{V}_I = \frac{2\pi G \gamma \sqrt{\Delta}}{\sqrt{3\pi G}} \left| \cosh(\sqrt{12\pi G} x(\phi)) \hat{\pi}_x \right|. \tag{A.8}$$

Recall that, in this formulation, we have defined the states as divided in the left and right-moving components in such a way that the total expectation value of an observable is given by (4.17). As explained below equation (4.19), this implies that $\langle \hat{V}_J \rangle = \langle \hat{V}_J \rangle_L$. Thus, we can focus on left-moving modes, and $\hat{V}_I$ can be written as:

$$\hat{V}_I = \frac{2\pi G \gamma \sqrt{\Delta}}{\sqrt{3\pi G}} \cosh(\sqrt{12\pi G} x(\phi)) \hat{\pi}_x. \tag{A.9}$$

Some careful mathematical manipulations lead to

$$\hat{V}_J = \frac{2\pi G \gamma \sqrt{\Delta}}{\sqrt{3\pi G}} E(x, \phi) \hat{\pi}_x, \tag{A.10}$$

where we define:

$$\begin{aligned} E(x,\phi) := \cosh\left(\sqrt{12\pi G} x(\phi)\right) - W \frac{2\pi G \Delta \gamma^2}{3} \Bigg\{ \sqrt{12\pi G} \left[F(\phi) - F(\phi_o) \right] \sinh\left(\sqrt{12\pi G} x(\phi)\right) \\ - \cosh\left(\sqrt{12\pi G} x(\phi)\right) \left[\cosh\left(2\sqrt{12\pi G} x(\phi)\right) - \cosh\left(2\sqrt{12\pi G} x\right) \right] \Bigg\}. \end{aligned} \tag{A.11}$$

Before proceeding, it is worth it to inspect the form of $\langle \hat{V}_J \rangle$ so far:

$$\langle \hat{V}_J \rangle = \frac{4\pi G \gamma \sqrt{\Delta}}{\sqrt{3\pi G}} \int_{-\infty}^{+\infty} dx \, |\partial_x \chi(x_+)|_{\phi_o}|^2 \, E(x, \phi). \tag{A.12}$$

An appropriate change of the integration variable will simplify its comparison to the free case. To this end, let us inspect the $W = 0$ case:

$$\begin{aligned}\langle\hat{V}_J\rangle|_{W=0} &= \frac{4\pi G\gamma\sqrt{\Delta}}{\sqrt{3\pi G}}\int_{-\infty}^{+\infty} dx\,|\partial_x\chi(x_+)|_{\phi_o}|^2\cosh\left(\sqrt{12\pi G}x(\phi)\right)\\ &= \frac{4\pi G\gamma\sqrt{\Delta}}{\sqrt{3\pi G}}\int_{-\infty}^{+\infty} d(x(\phi))\left|\partial_{x(\phi)}\chi(x(\phi)-\phi+2\phi_o)\right|^2\cosh\left(\sqrt{12\pi G}x(\phi)\right),\end{aligned} \tag{A.13}$$

At first sight, it is not obvious that this agrees with (4.20). To make it clear, we point out that, from (5.7), using only left-moving modes,

$$\begin{aligned}\chi(x+) &= \hat{U}(x,\phi)\chi(x+)|_{\phi_o}\\ &= \hat{U}(x,\phi)\int_0^{+\infty} dk\tilde{\chi}(k)e^{ik(x+\phi_o)}.\end{aligned} \tag{A.14}$$

For $W=0$, $\hat{U}(x,\phi)|_{W=0} = e^{-i|\hat{\pi}_x|(\phi-\phi_o)}$, and hence we find

$$\chi(x+)|_{W=0} = \int_0^{+\infty} dk\tilde{\chi}(k)e^{-ik(\phi+\phi_o)}e^{ik(x+\phi_o)} = \chi(x-\phi+2\phi_o), \tag{A.15}$$

which shows that (A.13) agrees with (4.20). Furthermore, we now see that changing the integration variable from x to $x(\phi)$ simplifies this comparison. Then, another change of variable from $x(\phi)$ to $\tilde{x}_+ = x(\phi)+\phi$ will allow us to write the result in terms of the $V_\pm$ and similar functions. Thus, we obtain

$$\begin{aligned}\langle\hat{V}_J\rangle &= V_+e^{\sqrt{12\pi G}\phi}\left[1+W\sqrt{3\pi G}\frac{2\pi G\Delta\gamma^2}{3}\left(\frac{3}{2\sqrt{12\pi G}}+2(\phi-\phi_o)\right)\right]\\ &+ V_-e^{-\sqrt{12\pi G}\phi}\left[1+W\sqrt{3\pi G}\frac{2\pi G\Delta\gamma^2}{3}\left(\frac{3}{2\sqrt{12\pi G}}-2(\phi-\phi_o)\right)\right]\\ &+ W\frac{\pi G\Delta\gamma^2}{6}\left[e^{3\sqrt{12\pi G}\phi}\left(V_{3+}-3V_+e^{-2\sqrt{12\pi G}\phi_o}\right)+e^{-3\sqrt{12\pi G}\phi}\left(V_{3-}-3V_-e^{+2\sqrt{12\pi G}\phi_o}\right)\right.\\ &\left.- e^{5\sqrt{12\pi G}\phi}\,V_{3+}e^{-2\sqrt{12\pi G}\phi_o}-e^{-5\sqrt{12\pi G}\phi}\,V_{3-}e^{+2\sqrt{12\pi G}\phi_o}\right],\end{aligned} \tag{A.16}$$

with $V_\pm$ and and $V_{3\pm}$ given in (4.21) and (5.30), respectively.

A.3 Commutation subtlety

In these calculations, it was necessary to compute $\partial_\phi e^{\hat{x}(\phi)}$, where $\hat{x}(\phi) = \hat{x}_0 + (\phi-\phi_0)\text{sign}(\hat{\pi}_x)$. This calculation is quite subtle.

Note that, even though classically $\partial_\phi e^{x(\phi)} = \text{sign}(\pi_x)e^{x(\phi)}$, in the quantum model we have:

$$\partial_\phi e^{\hat{x}(\phi)} = \text{sign}(\hat{\pi}_x)\left[\mathbb{1} + \frac{\text{sign}(\hat{\pi}_x)\hat{x}_0\text{sign}(\hat{\pi}_x) + \hat{x}_0}{2} + (\phi-\phi_0)\text{sign}(\hat{\pi}_x) + ...\right], \quad \text{(A.17)}$$

$$\text{sign}(\hat{\pi}_x)e^{\hat{x}(\phi)} = \text{sign}(\hat{\pi}_x)\left[\mathbb{1} + \hat{x}_0 + (\phi-\phi_0)\text{sign}(\hat{\pi}_x) + ...\right], \quad \text{(A.18)}$$

where we have used:

$$\begin{aligned} e^{\hat{x}(\phi)} &= \sum_n \frac{\hat{x}^n}{n!} \\ &= \mathbb{1} + \hat{x}_0 + (\phi-\phi_0)\text{sign}(\hat{\pi}_x) + \frac{1}{2}\Big[\hat{x}_0^2 + \hat{x}_0(\phi-\phi_0)\text{sign}(\hat{\pi}_x) + \\ &\quad + (\phi-\phi_0)\text{sign}(\hat{\pi}_x)\hat{x}_0 + (\phi-\phi_0)^2\Big] + ... \end{aligned} \quad \text{(A.19)}$$

Note that (A.17) is different from (A.18) because $\text{sign}(\hat{\pi}_x)$ and $\hat{x}_0$ do not generally commute and so:

$$\text{sign}(\hat{\pi}_x)\hat{x}_0\text{sign}(\hat{\pi}_x) \neq \hat{x}_0\,(\text{sign}(\hat{\pi}_x))^2 = \hat{x}_0. \quad \text{(A.20)}$$

However, in the expressions where they appear, they are accompanied by $\hat{\pi}_x$ on either side, and in practice we can replace $\text{sign}(\hat{\pi}_x)\hat{x}_0\text{sign}(\hat{\pi}_x)$ by $\hat{x}_0$.

This is more easily seen in the representation where $\hat{\pi}_x$ acts by multiplication, having therefore $\hat{x} = i\partial_{\hat{\pi}_x}$. We find that $[\hat{x}, \text{sign}(\hat{\pi}_x)] = i\delta(\hat{\pi}_x)$. On the other hand, if $\hat{\pi}_x$ is present, defining $\text{sign}(0)$ to be zero:

$$\delta(\hat{\pi}_x)\hat{\pi}_x = 0, \quad \text{(A.21)}$$

$$\delta(\hat{\pi}_x)\text{sign}(\hat{\pi}_x) = 0. \quad \text{(A.22)}$$

Then, $\hat{\pi}_x[\hat{x}, \text{sign}(\hat{\pi}_x)] = 0 = [\hat{x}, \text{sign}(\hat{\pi}_x)]\hat{\pi}_x$. Thus, $\hat{\pi}_x\text{sign}(\hat{\pi}_x)\hat{x}_0\text{sign}(\hat{\pi}_x) = \hat{\pi}_x\hat{x}_0$ and so $\hat{\pi}_x\partial_\phi e^{\hat{x}(\phi)} = \hat{\pi}_x\text{sign}(\hat{\pi}_x)e^{\hat{x}(\phi)}$.