# Hamiltonian corrections in Loop Quantum Cosmology

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# Hamiltonian corrections in Loop Quantum Cosmology


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*A mi familia y, en especial, a mi abuelo...*

# Abstract

Recently, there has been a growing interest in examining the mathematical ambiguities in the formalism of Loop Quantum Cosmology with the objective of seeking alternatives that also result in viable physical pictures and compare their respective physical predictions. In this way, we would be able to discern whether the remarkable results of standard Loop Quantum Cosmology (such as the singularity resolution) are robust. In this Master's Thesis, I will focus on two sources of ambiguities: the regularisation of the Hamiltonian constraint and the choice of a quantisation prescription.

On the one hand, the regularisation procedure is relevant to this discussion because the one employed in standard Loop Quantum Cosmology has fundamental differences with respect to the one employed in full Loop Quantum Gravity. Thus, the doors are open to constructing formalisms which actually follow more closely the precepts of Loop Quantum Gravity as far as the regularisation of the Hamiltonian constraint is concerned. Dapor and Liegener proposed such a modified Hamiltonian constraint, obtained by adopting without any substantial modification the regularisation procedure of the full theory.

On the other hand, the selection of a quantisation prescription (that is, a factor ordering rule) is important inasmuch as the same classical regularised Hamiltonian, when quantised adopting different quantisation prescriptions, leads to quantum theories that are not totally equivalent (although the differences in the physical predictions due to this choice are expected to be slight). In the community of Loop Quantum Cosmology, two prescriptions are predominant. For this thesis, I will adopt the Martín-Benito–Mena Marugán–Olmedo (MMO) prescription, which is characterised by resulting in a quantum theory with very attractive features at least in the standard approach. Hence, with the work presented in this text, I aim to fill a gap that existed in the literature by determining whether these nice features remain present under the modification proposed by Dapor and Liegener.

Since the MMO prescription is inspired by the treatment of anisotropic spacetimes, I deal in parallel with both isotropic and anisotropic, flat, homogeneous cosmologies. I begin by introducing some preliminary concepts of Loop Quantum Gravity with the objective of motivating the treatment of cosmological spacetimes in the rest of the thesis. After this introduction, I review the classical and quantum kinematical aspects of the isotropic and anisotropic cosmologies under consideration. Next, I proceed to the regularisation using holonomy variables of the Hamiltonian constraint; first according to the standard method, and then considering the modified one instead. After the Hamiltonian is regularised via the modified procedure, I quantise it by adopting the MMO prescription in the isotropic scenario. After examining its action on the Hilbert space of the system, I conclude that this prescription still displays the attractive features that characterise it in the standard approach: a) the singularity is decoupled at the kinematical level, b) the action of the quantum modified Hamiltonian defines superselection sectors that are simpler than those found adopting other prescriptions, and c) it is possible to find the exact form of the eigenfunctions of the quantum Hamiltonian. Finally, to complete the description of this alternative formalism, I perform a numerical analysis of its effective cosmological dynamics and compare it with the effective dynamics of standard Loop Quantum Cosmology and General Relativity, concluding that, whereas the Big Bang singularity is still replaced by a quantum bounce, the bouncing mechanism is qualitatively different from the one found in standard Loop Quantum Cosmology.



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# Contents

# 1 Introduction

Modern theoretical physics lies on two fundamental pillars: General Relativity (GR) and Quantum Mechanics (QM). The former describes the classical motion of matter in the presence of gravitational fields, in a purely geometric framework. At the same time, this theory explains how matter alters the geometry of space and time, giving rise to these gravitational effects in the first place. GR is characterised by providing a covariant description of the aforementioned phenomena, that is, a description which is independent of the choice of coordinate system [1, 2, 3]. On the other hand, QM is the paradigm governing the physics of the microscopic world, where the classical laws no longer hold. Instead of being based on the notion of spacetime trajectories, QM relies on a probabilistic description of Nature where physical observables have an intrinsic uncertainty. Within this theory, the probability distribution of physical observables is determined by the state of the system and its time evolution is given by the Schrödinger equation (which preserves the probabilistic character of the quantum states) [4, 5].

Physical predictions of both GR and QM have been tested with extremely high precision in their respective regimes of application. Furthermore, the partial combination of both formalisms when physical systems are described by relativistic quantum fields (which receives the name of Quantum Field Theory or QFT, for short) has led to numerous predictions that have been experimentally confirmed as well. These fields describe *quantum* material excitations (or particles) propagating on a *classical* (spacetime) background. QFT has proven to be extremely successful and is at the core of, e.g., the Standard Model of Particle Physics, one of the biggest achievements of the history of science. In this scenario, elementary particles and their fundamental interactions (excluding gravitation) are described: physical events take place in a flat spacetime, which is not affected by the physics itself.

Beyond the aforementioned success of the quantisation of relativistic fields in flat geometries, there exists a theoretical formulation of Quantum Field Theory in Curved Spacetime [6, 7]. In this formulation, the inclusion of gravitational effects is realised in the form of considering a *classical* curved spacetime as the background of the field theory. Several theoretical predictions exist at this point (such as the Hawking radiation [8], the Unruh effect [9, 10] or the particle production in nonstationary backgrounds [11, 12]) but they remain to be confirmed experimentally. These effects typically arise due to the fact that the generalisation of QFT to curved backgrounds is far from immediate. Indeed, the consideration of a general spacetime leads to an ambiguity in the choice of quantum representation of the classical algebra of canonical variables. In the context of a standard Fock quantisation, this means that there is not a preferred choice of creation and annihilation operators. In turn, this implies that the definition of the vacuum of the theory (i.e., the state annihilated by all the annihilation operators) is not unique: in general, there is an infinite number of *a priori* equally valid vacua. In standard QM (where the number of degrees of freedom is finite), all the possible quantum representations are ensured to be unitarily equivalent by the Stone-von Neumann Theorem [13] (provided that certain reasonable continuity conditions are met). Nevertheless, when the number of degrees of freedom is infinite (as occurs in QFT), the theorem no longer holds and, in general, the quantisation is not unique. In Minkowski spacetime, there is a preferred vacuum (and, thus, a preferred notion of particle) owing to the fact that only one vacuum is invariant under the Poincaré group (that is, the isometry group of Minkowski spacetime). Similar physical criteria can be used to select preferred quantisations when the background admits a series of isometries, e.g., in stationary spacetimes, in which the imposition that the quantum theory respects the time-translational symmetries of the classical spacetime essentially selects a single possible vacuum, as in the case of Minkowski space.

Nevertheless, such a selection cannot be performed when considering quantum fields propagating in more general spacetimes (which, for instance, are not stationary). Many processes of physical interest are described by spacetimes that fall into this category, from the gravitational collapse of a star to the cosmological evolution of the Universe itself. Indeed, no continuous time symmetry exists in these cases and, as a consequence, the quantum theory cannot be restricted by the means mentioned in the previous paragraph. The gravity of the consequences of this nonstationarity is twofold if we realise that the quantum representations of the classical (anti)commutation relations need not be unitarily equivalent among themselves at different times. Therefore, the standard probabilistic interpretation may not be respected and the theoretical robustness of all the predictions based on the quantum evolution of the states is compromised. An extensive number of studies carried out during the past decade appear to point towards an intimate relation between these two problems (nonuniqueness of the quantisation and nonunitarity of the evolution). Indeed, it has been shown that, for (free) scalar and fermionic fields in a variety of cosmological scenarios, the unitarity of the quantum dynamics guarantees the uniqueness of the Fock representation of the classical (anti)commutation relations (provided that the symmetries of the field equations are imposed at the quantum level). For this reason, the possibility of implementing the quantum Heisenberg dynamics by a unitary operator has recently been proposed as a criterion for the selection of a unique equivalence class of quantisations (for some examples, see Refs. [14, 15, 16, 17]).

Once we have reached this point of the discussion, it is important to remark that QFT and GR appear to be, in general, in tension with each other. Indeed, it seems strange to consider matter of a quantum nature living in a classical spacetime, since the Einstein equations state that matter affects the classical curvature of the spacetime. Thus, some serious conceptual problems emerge when we try to formulate the effect of quantum matter fields on the background spacetime, especially if such matter is in a state with large quantum fluctuations. Therefore, it seems rather convincing that, if there exist physical scenarios where it is valid to consider quantum fields in classical spacetimes (as suggested by experimental evidence), other regimes may exist where the quantum nature of both matter and spacetime must be taken into account to capture the real physics. Then, the classical Einstein equations could be understood as a certain limit of the full theory of quantum gravity that would govern such physical regimes. In addition, knowing the full theory would allow us to alleviate the conflicts that appear when accommodating QFT in the intermediate stages between the fully classical and the fully quantum. Apart from this fundamental motivation (based on the consistency between the two fundamental cornerstones of modern theoretical physics), other reasons push the scientific community to seek a theory of quantum gravity. For instance, GR predicts the presence of spacetime singularities, where some physical observables diverge and the theory breaks down, no longer being predictive [2]. Indeed, some of these singularities appear to exist in scenarios of physical interest, such as the formation of black holes at the end of the life of massive stars and the Big Bang singularity in the primeval Universe. For this reason, there is a widespread hope that quantum effects may resolve the singularities of the classical theory, allowing for the extraction of robust physical predictions in the regions nearby.

In the past fifty years, several attempts to formulate a quantum theory of gravity have been made. Among these, Loop Quantum Gravity (LQG) is a formally robust attempt to quantise gravity following the theoretical precepts of GR [18, 19, 20, 21]. LQG is a nonperturbative quantisation of GR in 3+1 dimensions, independent of any spacetime background structure. Unlike other preexisting canonical approaches to Quantum Gravity (such as the Wheeler-DeWitt theory [22]), it relies on the use of techniques extracted from Yang-Mills gauge theories. In its canonical formulation, the basic variables are holonomies of the Ashtekar-Barbero connection along loops and fluxes of the densitised triad across surfaces. A key feature of the LQG programme is that it employs a quantum representation which is not unitarily equivalent to the Fock representation of ordinary QFT, but it is instead compatible with the background independence characteristic of GR. Besides, it attempts to respect the general covariance of the classical theory at the quantum level. In order to do so, the constraints that generate the spacetime diffeomorphisms (regarded as a fundamental symmetry of the theory) are imposed at the quantum level, following Dirac's formalism for the quantisation of constrained systems [23]. Indeed, classical GR is a completely constrained system, meaning that its total Hamiltonian is purely a(n integrated) linear combination of four constraints: the three *spatial diffeomorphism* constraints and the *scalar* or *Hamiltonian* constraint (which generates time reparametrisations up to spatial diffeomorphisms). Apart from these four constraints, the Gauss constraint (which encodes the information about an SU(2) symmetry introduced in the triadic formulation of GR that LQG is based upon) also plays an important role. In summary, in LQG the geometric degrees of freedom in vacuum are described by pairs of canonical variables given by the components of the densitised triad and the gauge connection. Their respective fluxes across surfaces and holonomies along loops form an algebra under Poisson brackets, which one seeks to represent quantum mechanically on a Hilbert space. This Hilbert space is called the *kinematical* Hilbert space of the theory and the quantum (operator) constraints are imposed on it, requiring that they annihilate the physical states.

The foundations of LQG have undergone an exhaustive examination for the past decades. Notwithstanding the fact that the quantisation programme has not yet been completed in general scenarios, it can be done in systems with a large number of symmetries: the so-called symmetry reduced sectors. These have been studied thoroughly, in addition to perturbations around them, driving LQG closer to making robust physical predictions that can be falsified by observations [24, 25, 26, 27, 28, 29]. Notably, the techniques of LQG have succeeded in achieving a complete and consistent quantisation of cosmological spacetimes. This conjunction of LQG and cosmology led to the birth of a new field of research named Loop Quantum Cosmology (LQC) [30, 31, 32, 33], that has experienced a rapid evolution in the past years. Indeed, there exists a large number of studies in a variety of scenarios. See, for example, Refs. [34, 35, 36, 32, 37, 38, 39, 40] for homogeneous and isotropic models such as Friedmann-Lemaître-Robertson-Walker (FLRW) spacetimes. For works concerning anisotropic Bianchi cosmologies, one can consult Refs. [41, 42, 43, 44, 45, 46, 47]. Analyses of inhomogeneous cosmologies have been carried out as well. Examples of this last class can be found in Refs. [48, 49, 50, 51], where Gowdy spacetimes are treated.

In LQC, the Big Bang singularity is found to be resolved, which is counted among the most outstanding results in the field. Instead of collapsing, the Universe undergoes a regular quantum bounce when the energy density becomes comparable with the Planck density. The (spacetime) curvature turns out to decrease quickly before and after the bounce. Therefore, just a few Planck times after or before the bounce, GR is fit to describe the cosmological dynamics with a very good accuracy. For this reason, it is often said that two *classical* universes (the prebounce one, that contracts; and the postbounce one, that expands) are linked together by the bounce. Moreover, semiclassical states at large volumes have been found to stay peaked across the bounce region [52] and the quantum evolution of their peaks is well approximated by an effective dynamics [36]. In this sense, the bounce is referred to as being *deterministic*. The disappearance of the classical singularity by virtue of the effects of quantum geometry not only has been found in general homogeneous cosmologies (both isotropic and anisotropic [31, 53, 54, 55, 56]), but also has been confirmed in inhomogeneous scenarios [57]. In fact, a variety of results suggests that all strong singularities are resolved in LQC (at the very least in systems with a large number of symmetries [58]).

The regularisation and quantum representation of the Hamiltonian constraint in LQG is, as of today, an open problem. A number of strategies were introduced by Thiemann within the framework of LQG, which serve to regularise the Hamiltonian. Later on, LQC fell heir to these strategies. Nonetheless, the regularisation procedure involves certain ambiguities [59, 60, 61], which were originally resolved by appealing to some apparently natural physical criteria. However, a new tendency has arisen recently: other options that result in viable physical pictures are being examined by comparing their physical predictions. This exercise is particularly interesting when it comes to alternatives that lie closer to full LQG, in that their regularisation procedure follows more faithfully the strategy of the full theory. These cases have sparked the curiosity of the scientific community lately, resulting in an extensive analysis of the cosmological dynamics and the singularity resolution in these modified alternatives, in order to seek quantitative and/or qualitative differences with respect to the standard LQC picture.

One is led to expect the existence of alternatives that are closer to full LQG because the regularisation procedure in LQG and the one that has been commonly employed in LQC have fundamental differences. These lie in the treatment of the two pieces that compose the gravitational Hamiltonian constraint in GR: the so-called Euclidean and the Lorentzian parts. In LQG, each of them requires a separate quantisation strategy. The regularisation procedure usually employed in LQC, however, relies on the fact that the Euclidean and Lorentzian parts are proportional when the spatial sections of the spacetime under consideration are flat. For this reason, the Hamiltonian constraint has predominantly been quantised as being proportional to the Euclidean part alone. As of yet, we do not fully comprehend the details of how LQG and LQC are related to each other (see Refs. [62, 63]). Therefore, the cosmological dynamics resulting from the standard approach to LQC is not ensured to capture the full cosmological dynamics in LQG, even at leading order. Hence, it seems reasonable to analyse suitable alternative approaches to LQC that are closer to LQG with the objective of shedding light on whether the classical singularity is also resolved by a quantum bounce in the full theory.

Yang, Ding, and Ma first addressed this matter in Ref. [64] by explicitly constructing a different Hamiltonian for LQC using a regularisation procedure similar to that in LQG. Whereas the standard Hamiltonian constraint yields a second-order difference equation, this alternative Hamiltonian results in a fourth-order one by cause of the Euclidean and Lorentzian parts being quantised separately. Moreover, the authors found that the modified Hamiltonian led to a bounce mechanism with the standard features described above: no qualitative differences were noticed.

Dapor and Liegener considered, in a more recent work [65], a nongraph-changing regularisation scheme [66] within the framework of LQG. Computing the expected value of the resulting Hamiltonian constraint on complexifier coherent states (representing homogeneous and isotropic spacetimes), they recovered an effective Hamiltonian identical (at leading order in a semiclassical expansion) to the one found in Ref. [64]. This regularisation procedure (that was originally conceived in the context of LQG) was applied, without any modification, to LQC in a later work [67]; resulting in the same effective Hamiltonian found in the previous investigations [64, 65][1]. Although an examination of the quantum dynamics revealed that the initial singularity was resolved in this formalism, the bouncing picture underwent a qualitative modification: while it still involved a large classical universe, a de Sitter epoch with an emergent Planckian cosmological constant appeared as well[2]. Therefore, unlike in Ref. [64], the bounce was asymmetric: it either joins a de Sitter contracting solution and a classical expanding universe or the other way around. In a follow-up publication [69], where the whole detailed analysis underlying Ref. [67] was presented, the authors have partially filled a gap in the understanding of the spectral analysis of the modified Hamiltonian operator. In particular, they have shown that it admits a family of self-adjoint extensions (although this proof relies on the choice of a very particular superselection sector, as I will briefly comment in Sec. 7.4).

Moreover; some months ago Li, Singh, and Wang studied in a systematic way the effective cosmological dynamics that resulted from this alternative Hamiltonian [70], to which I will refer as the *modified Hamiltonian* for the rest of this thesis. Using numerical and analytical techniques, they considered massless and massive scalar fields as the matter content of a flat FLRW cosmology. They realised that, while one set of Hamilton's equations is sufficient to compute the evolution of the Universe, *two* different sets of Friedmann-Raychaudhuri equations are needed for the same purpose: both descriptions are not related by a one-to-one correspondence. This resolves the tension between the previous works concerning the symmetric or asymmetric nature of the bounce. Indeed, considering only one set of equations, the bounce appears to be symmetric, but this conclusion is proven to be physically inconsistent in Ref. [70], where it is shown that the bounce must be asymmetric, as suggested in Refs. [65, 67]. The main interest of this alternative formalism is that this asymmetry may give rise to phenomenological consequences that differ from those arising from the standard LQC formalism. In a following article [71], the same authors broadened their analysis by considering yet another alternative Hamiltonian, arriving at a formalism that they designated as mLQC-II. Moreover, a further study and comparison of the alternative effective dynamics for various inflationary potentials allowed to conclude that both mLQC-I and mLQC-II display a nonsingular inflationary era. In a very recent work [72], the authors have established a series of dynamical features that appear to be shared by the three formalisms of LQC that they discussed in previous papers. Furthermore, they compute the probability that the Universe undergoes inflation, finding a large one in the three scenarios.

Efforts have also been made in the direction of extracting physical predictions for observables in cosmology which are sensitive to this quantisation ambiguity. In this respect, Agullo used the modified Hamiltonian constraint to obtain the scalar power spectrum and compared it with the one that had been computed in standard LQC [73].

Some other aspects of the alternative formalisms have been explored in very recent publications. For instance, Liegener and Singh have argued that the bounce needs to be asymmetric, employing for the first time a gauge invariant treatment of the singularity resolution [74]. In this sense, the symmetric bounces obtained in the standard approach to LQC appear to be an artefact of the gauge fixing in the fluxes of the densitised triad. On the other hand; Yang, Zhang, and Ma have proposed a procedure to obtain yet another modification of the Hamiltonian constraint [75]. This procedure is based on a regularisation of the Euclidean and Lorentzian parts of the Hamiltonian by expressing them in terms of the Chern-Simons action defined on the spatial sections. The resulting model (which appears to yield the cor-

[1]This alternative Hamiltonian constraint results in a formalism of LQC sometimes referred to as mLQC-I in the literature.

[2]An emergent cosmological constant had already been encountered in the inner region of black holes [68].

rect classical limit) is nonsingular, since the Big Bang is also replaced by a quantum bounce that is asymmetric.

The main original contribution of this thesis is the construction of a new formalism of LQC. To achieve this purpose, I will quantise the modified Hamiltonian constraint by selecting the MMO quantisation prescription (put forward by Martín-Benito, Mena Marugán, and Olmedo in Ref. [37]), instead of the one proposed in Ref. [36]. The result of this construction will be presented throughout the following sections and was first published in Ref. [76]. The MMO prescription differs from other existing prescriptions in that it incorporates in isotropic LQC a symmetrisation of the Hamiltonian that is natural in anisotropic scenarios such as Bianchi I cosmologies (from which the proposers of the prescription drew inspiration). This symmetrisation, which comprises a special treatment of the signs of the components of the triad, gives rise to some attractive features after the quantisation of the theory. One of these features is the decoupling of the (quantum analogue of the classically) singular state at the kinematical level. Moreover, in the quantum theory, the MMO prescription results in superselection rules that pick superselection sectors which are much simpler than the ones found when using other prescriptions. In standard LQC, these simpler superselection sectors make it possible to explicitly find a closed expression for the generalised eigenfunctions of the Hamiltonian constraint operator, which is exceptionally efficient computationally speaking. This efficiency permits the construction of the eigenfunctions in a more rapid and precise way. All these defining characteristics are regarded as strengths of the MMO prescription. Hence, it seems natural to wonder whether these strengths prevail when the MMO prescription is adopted for the representation of the modified Hamiltonian instead.

The rest of this thesis is organised as follows. I will start with a brief account of the notation and conventions that I will be using throughout this text. I will devote the next section (Sec. 2) to the discussion of the classical and quantum Hamiltonian formalisms for constrained systems. In Sec. 3, I will introduce some preliminary concepts and techniques employed in LQG, which serve to motivate the treatment of cosmological spacetimes in the rest of the thesis. In Sec. 4, we review the kinematical aspects of the loop quantisation of FLRW and Bianchi I cosmologies, whose study is motivated by the fact that we want to identify a symmetrisation structure that is clear in anisotropic scenarios. In Sec. 5, I illustrate the regularisation of the Hamiltonian constraint according to the standard scheme. In Sec. 6, I regularise the Lorentzian part of the Hamiltonian constraint separately and compute the modified gravitational Hamiltonian in FLRW and Bianchi I cosmologies. Once the full Hamiltonian is regularised in a manner that does not rely on the spatial flatness and homogeneity of the cosmological models that I am considering, I proceed to quantise it in Sec. 7. In this section, I compute the action of the Hamiltonian constraint operator on an orthonormal basis of the kinematical Hilbert space and identify the superselection sectors defined by its action. Additionally, I discuss the form of its generalised eigenfunctions and how they can be computed by finding a closed analytical expression for them. Finally, in Sec. 8, I study analytically and numerically the effective dynamics arising from standard and modified LQC, and compare the results with the ones obtained in classical GR. In Sec. 9, I conclude by summarising the main ideas covered in this work.

# Notation and conventions

Throughout this Master's Thesis, I will use Greek letters $(\mu, \nu, \rho, \sigma ...)$ for *spacetime* indices. Therefore, they take values from 0 to 3. Additionally, since we will be working with objects defined in spacelike sections of the spacetime manifold, I will use Latin letters from the beginning of the alphabet $(a, b, c, d...)$ to denote *spatial* indices. Finally, Latin letters from the middle of the alphabet $(i, j, k, l...)$ will play the role of internal indices, associated with an SU(2) freedom. Both spatial and SU(2) indices will take values from 1 to 3.

I will use Einstein's summation convention (unless I explicitly state the contrary) whereby a sum must be understood over every pair of repeated indices as long as one is upstairs and the other is downstairs.

The complete symmetrisation of a number of indices will be indicated using parentheses and vertical lines to separate the indices affected by the symmetrisation from those who are not. For instance, $(\mu| \dots |\nu)$ means that the indices $\mu$ and $\nu$ are symmetrised, whereas the ones between them are left unchanged. A similar notation is used with the antisymmetrisation of indices, but I employ square brackets instead. Note that, in my convention, the appropriate combinatory factor is included in the definition. For example, with two indices,

$$T_{(\mu\nu)} := \frac{1}{2}(T_{\mu\nu} + T_{\nu\mu}), \tag{1}$$

$$T_{[\mu\nu]} := \frac{1}{2}(T_{\mu\nu} - T_{\nu\mu}). \tag{2}$$

$\delta_{ab}$ and $\epsilon_{ijk}$ (with the indices properly placed) denote the Kronecker delta and the Levi-Civita symbol, respectively, defined by

$$\delta_{ab} = \begin{cases} 1 & a = b \\ 0 & a \neq b \end{cases} \tag{3}$$

$$\epsilon_{ijk} = \epsilon_{[ijk]}, \quad \epsilon_{123} = 1. \tag{4}$$

Finally, the content of this thesis is written in units where $\hbar = c = 1$, and using the metric signature composed of mostly plus signs: $(-, +, +, +)$.

# 2 Hamiltonian formalism of constrained systems

As I mentioned in Sec. 1, canonical LQG is a quantisation programme which starts from the Hamiltonian formulation of classical GR. Since the classical theory is invariant under general coordinate transformations, we must answer the questions of how to deal with systems with symmetries and how to construct a Hamiltonian formulation of GR when the time should be treated on the same footing as the rest of the coordinates.

The symmetries of a system result, as I commented above, in constraints. To illustrate this idea in a straightforward way, let us consider a simple two-dimensional system described by a Lagrangian which is invariant under rotations,

$$L = \frac{1}{2}(\dot{r}^2 + r^2\dot{\phi}^2) - V(r). \tag{5}$$

Since the angular coordinate $\phi$ is cyclic, its equation of motion reads

$$\frac{\partial L}{\partial \phi} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\phi}} = 0 \Rightarrow r^2\dot{\phi} = l, \tag{6}$$

where $l$ (which is essentially the angular momentum) is a constant. Therefore, the existence of a symmetry implies the conservation of a quantity which is a function of the generalised coordinates and velocities. Hence, the dynamical variables that describe the system cannot vary arbitrarily: they are bound to vary in such a way that the conservation law is always satisfied. In this sense, a system with symmetries is a *constrained* one.

In view of this simple example, it seems natural to adopt a formalism which is appropriate for the treatment of constrained systems. Next, I will discuss the basics of the Hamiltonian formulation of theories with constraints, following Dirac [23, 78].

## 2.1 Classical theory

Consider a dynamical system with $N$ independent constraints of the form $\chi_n = 0$ (with $n = 1, \ldots, N$), where $\chi_n$ are functions of the dynamical variables. These receive the name of *primary constraints*. It should be noted that, in constrained systems, the Hamiltonian is not uniquely determined. Indeed, if $H$ is a Hamiltonian that describes the dynamics of the system, a Hamiltonian obtained from this one by summing an arbitrary linear combination of the constraints is equally valid. As a result, the evolution of a dynamical function $f$ can be written as $\dot{f} = \{f, H_T\}$, where $\{\cdot\,,\cdot\}$ denotes the Poisson bracket, $H_T = H + u^n\chi_n$ is the total Hamiltonian of the system and $u^n$ are $N$ unknown coefficients. By virtue of the standard properties of the Poisson bracket, this expression can be rewritten as

$$\dot{f} = \{f, H\} + \{f, u^n\chi_n\} = \{f, H\} + u^n\{f, \chi_n\} + \{f, u^n\}\chi_n. \tag{7}$$

The third term is not defined, given that the Poisson bracket is only defined for functions of the dynamical variables. However, the ill-defined bracket is multiplied by a quantity that vanishes identically for all $n$: the primary constraints. As a result, $\dot{f}$ is well-defined. We have to remark, though, that the Poisson bracket has to be computed *before* imposing the constraints, since both processes do not commute in general. For this reason, we will declare the following notation: we will use the symbol $\approx$ in *weak* identities (that is, identities that only hold once the constraints are imposed) instead of the standard $=$, which we will reserve for the *strong* ones. Hence, we write $\chi_n \approx 0$ and express the evolution of a dynamical variable as

$$\dot{f} \approx \{f, H_T\}. \tag{8}$$

This notion of evolution can be applied on the constraints themselves to obtain consistency equations (the constraints must remain satisfied under time evolution):

$$\dot{\chi}_m \approx \{\chi_m, H\} + u^n\{\chi_m, \chi_n\} \approx 0, \qquad m = 1, \ldots, N. \tag{9}$$

We then have $N$ consistency conditions and we can encounter three distinct situations:

i) The consistency conditions are trivially satisfied.

ii) The consistency conditions involve the dynamical variables, resulting in new constraints called *secondary* (as long as they are independent from the primary ones)[3].

iii) The consistency conditions involve the unknown coefficients $u^n$.

In the first scenario, the primary constraints are robust under evolution. In the second scenario, however, we obtain $K$ new constraints $\{\xi_k\}_{k=1,\ldots,K}$, whose consistency under evolution must be checked as we did for the primary constraints

$$\dot{\xi}_k \approx \{\xi_k, H\} + u^n\{\xi_k, \chi_n\} \approx 0, \qquad k = 1, \ldots, K. \tag{10}$$

Again, these consistency checks can result in the three different cases listed above. After exhausting all the possible consistency conditions, we will end up with $P$ additional constraints $\{\varrho_p\}_{p=1,\ldots,P}$ and a series of conditions that the coefficients $u^n$ must satisfy.

In general, the additional constraints need to be treated on the same footing as the primary ones, so it is useful to express all the constraints in a tuple $\{\phi_j\}_{j=1,\ldots,J}$ such that the $N$ first constraints are the primary ones and the rest are the additional (secondary) constraints:

$$\phi_j \approx 0 \quad (j = 1, \ldots, N + P = J): \quad \begin{cases} \phi_n = \chi_n \approx 0 & n = 1, \ldots, N. \\ \phi_p = \varrho_p \approx 0 & p = N + 1, \ldots, N + P. \end{cases} \tag{11}$$

Finally, the conditions on the coefficients $u^n$ (where $n = 1, \ldots, N$) can be written as

$$\{\phi_j, H\} + u^n\{\phi_j, \phi_n\} \approx 0, \tag{12}$$

as long as they do not reduce to one of the constraints. These conditions can be regarded as a set of inhomogeneous linear equations where the coefficients $u^n$ are the unknowns. Provided that the equations of motion are consistent, we must be able to find a solution to these equations $u^n = U^n(\zeta)$ (where $\zeta$ compactly refers to all the dynamical variables of the system under consideration) [23]. Nevertheless, this solution is *not* unique. Indeed, it is easy to see that $U^n + V^n$ is also a solution if $V^n\{\phi_j, \phi_n\} = 0$. In fact, the most general solution can be constructed out of all the independent solutions of $V^n\{\phi_j, \phi_n\} = 0$. Let $A$ be the number of independent solutions, $\{V^n_a\}_{a=1,\ldots,A}$. Then,

$$u^n = U^n(\zeta) + v^a V^n_a(\zeta) \tag{13}$$

is the most general solution, where $v^a$ are arbitrary coefficients. Finally, we can write the total Hamiltonian as

$$H_T = H + U^m\phi_m + v^a V^m_a \phi_m = H' + v^a\phi_a, \tag{14}$$

where

$$H' = H + U^m\phi_m, \tag{15}$$

$$\phi_a = V^m_a \phi_m. \tag{16}$$

[3]Notice that there is no fundamental difference between primary and secondary constraints: which is which merely depends on the Lagrangian we start with.

In the light of this result, we conclude that the total physical Hamiltonian of a constrained system involves $A$ arbitrary coefficients $v^a$, which are not fixed even when we have satisfied all the requirements of our dynamical theory. For this reason, the dynamical variables at a certain time $t$ cannot be uniquely determined by their initial values at $t_0$. This is a reflection of the fact that we are working in a frame where there is an ambiguity, intimately related with the freedom of fixing a gauge.

To close this discussion about constrained Hamiltonian systems, I will introduce two concepts which will be useful to illustrate the procedure by which these systems are quantised (often referred to as *quantisation à la Dirac*). A dynamical function $R$ is said to be *first-class* if it commutes with all the constraints under Poisson brackets

$$\{R, \phi_j\} \approx 0, \quad j = 1, \ldots, J. \tag{17}$$

It is only necessary that they weakly commute, which is a more relaxed condition. If this does not occur, the dynamical variable is said to be *second-class*.

It should be noted that both $H'$ and $v^a\phi_a$ (defined above) are first-class. Indeed, using the properties of the Poisson bracket,

$$\{H', \phi_j\} = \{H + U^m\phi_m, \phi_j\} = \{H, \phi_j\} + U^m\{\phi_m, \phi_j\} + \{U^m, \phi_j\}\phi_m \approx 0, \tag{18}$$

which follows from the fact that $U^m$ is a solution of Eq. (12) and $\phi_m \approx 0$. Similarly,

$$\begin{aligned}\{v^a\phi_a, \phi_j\} &= v^a\{\phi_a, \phi_j\} + \{v^a, \phi_j\}\phi_a \approx v^a\{\phi_a, \phi_j\} \\ &= v^a\{V_a^m\phi_m, \phi_j\} = v^a V_a^m\{\phi_m, \phi_j\} + v^a\{V_a^m, \phi_j\}\phi_m \approx 0,\end{aligned} \tag{19}$$

where I have used the fact that $\phi_a \approx 0$ (it is a linear combination of constraints) and that, by definition, $V_a^m\{\phi_m, \phi_j\} = 0$ for all $j$ (recall that this is what enabled us to find the most general solution to Eq. (12) in the first place).

Since the $\phi^a$ are linear combinations of primary constraints, they also are primary. Furthermore, given that $V_a^m$ are all the independent solutions of $V^m\{\phi_m, \phi_j\} = 0$, $\{\phi_a\}_{a=1,\ldots,A}$ is the set of *all* the primary constraints which are also first-class.

Before discussing the quantum theory, let us examine the role of the first-class constraints as generators of transformations. Let $f$ be a dynamical variable whose value at an initial time $t = 0$ is $f_0$. Then, its value at an infinitesimal time $\delta t$ is given by

$$f(\delta t) \approx f_0 + \dot{f}\delta t \approx f_0 + \delta t\{f, H_T\} = f_0 + \delta t\left(\{f, H'\} + \{f, v^a\phi_a\}\right). \tag{20}$$

Notice the appearance of the arbitrary coefficients $v^a$ in the expression above. This results in the fact that the value of the dynamical variable $f$ at time $\delta t$ is not uniquely determined by its initial value at $t = 0$, as we mentioned before. These coefficients are arbitrary and at our disposal, so we could choose a different set of them, $v'^a$. If we did so, the value of $f$ at $\delta t$ would differ. The difference would only involve the third term of the previous expression and would read

$$\Delta f(\delta t) \approx \delta t\{f, (v'^a - v^a)\phi_a\} \equiv \{f, \varepsilon^a\phi_a\}, \tag{21}$$

where $\varepsilon^a = \delta t(v'^a - v^a)$ are infinitesimal arbitrary parameters.

If we decided to transform every dynamical variable of our system according to the rule $\delta f \approx \{f, \varepsilon^a\phi_a\}$, we would still be describing the same state[4]. Then, we conclude

[4]This is so because there exists a *redundancy* in our description, which makes that the same state is described by a collection of sets of dynamical variables instead of by just one.

that the primary, first-class constraints generate infinitesimal contact transformations of the dynamical variables that do *not* alter the physical state.

Nonetheless, not only the *primary*, first-class constraints generate such transformations. In fact, *secondary*, first-class constraints do as well[5]. To realise this in a straightforward way, consider two infinitesimal transformations with parameters $\varepsilon^a$ and $\gamma^b$ ($b = 1, \dots, A$), respectively. Then, we apply them in different orders and see how the result changes. To illustrate this simple computation, let us do one of them explicitly. Consider the case where we apply the transformation with $\varepsilon^a$ first and the one with $\gamma^b$ afterwards.

$$
\begin{aligned}
&f \xmapsto{\varepsilon} f + \{f, \varepsilon^a \phi_a\} \xmapsto{\gamma} f + \{f, \varepsilon^a \phi_a\} + \{f + \{f, \varepsilon^a \phi_a\}, \gamma^b \phi_b\}, \\
&f \xmapsto{\gamma \circ \varepsilon} f + \{f, \varepsilon^a \phi_a\} + \{f, \gamma^b \phi_b\} + \{\{f, \varepsilon^a \phi_a\}, \gamma^b \phi_b\}.
\end{aligned} \tag{22}
$$

When the transformations are applied the other way around, the first two terms will appear and, in the third one, $\varepsilon^a \phi_a$ and $\gamma^b \phi_b$ will be interchanged. Hence, the difference between the two is

$$
\begin{aligned}
\Delta f &\approx \{\{f, \varepsilon^a \phi_a\}, \gamma^b \phi_b\} - \{\{f, \gamma^b \phi_b\}, \varepsilon^a \phi_a\} \\
&= \{\{f, \varepsilon^a \phi_a\}, \gamma^b \phi_b\} + \{\{\gamma^b \phi_b, f\}, \varepsilon^a \phi_a\} \\
&= -\{\{\varepsilon^a \phi_a, \gamma^b \phi_b\}, f\} \approx \{f, \varepsilon^a \gamma^b \{\phi_a, \phi_b\}\},
\end{aligned} \tag{23}
$$

where the third equality follows from the Jacobi identity that the Poisson bracket satisfies.

In this instance, the generators of these gauge transformations (in the sense that the physical degrees of freedom are unaffected by them) are $\{\phi_a, \phi_b\}$. Since the $\phi_a$ are first-class, $\{\phi_a, \phi_b\} \approx 0$, which means that the generators must be strongly equal to linear combinations of constraints (they are by definition the only independent quantities in our theory that are weakly zero):

$$
\{\phi_a, \phi_b\} = {c_{ab}}^j \phi_j, \tag{24}
$$

where ${c_{ab}}^j$ are unknown coefficients. It is easy to see that these must be first-class, although there is no restriction on whether they are primary or secondary. Indeed, let us prove that the Poisson bracket of two first-class variables $R$ and $S$ is first-class. By assumption, $R$ and $S$ weakly commute with all the constraints. Therefore,

$$
\{R, \phi_j\} \approx 0 \Rightarrow \{R, \phi_j\} = {r_j}^{j'} \phi_{j'}, \tag{25}
$$

$$
\{S, \phi_j\} \approx 0 \Rightarrow \{S, \phi_j\} = {s_j}^{j'} \phi_{j'}. \tag{26}
$$

By virtue of the Jacobi identity and the product law,

$$
\begin{aligned}
\{\{R, S\}, \phi_j\} &= \{\{R, \phi_j\}, S\} - \{\{S, \phi_j\}, R\} \\
&= \{{r_j}^{j'} \phi_{j'}, S\} - \{{s_j}^{j'} \phi_{j'}, R\} \\
&= {r_j}^{j'} \{\phi_{j'}, S\} - {s_j}^{j'} \{\phi_{j'}, R\} + \left(\{{r_j}^{j'}, S\} - \{{s_j}^{j'}, R\}\right) \phi_{j'},
\end{aligned} \tag{27}
$$

which is weakly zero because $R$ and $S$ are first-class and $\phi_{j'} \approx 0$ for all $j = 1, \dots, J$. Therefore, we have proven that

$$
\{R, \phi_j\} \approx 0, \quad \{S, \phi_j\} \approx 0 \quad \Rightarrow \quad \{\{R, S\}, \phi_j\} \approx 0. \tag{28}
$$

[5]As I commented before, the difference between primary and secondary constraints is not fundamental. The difference between first- and second-class, though, is crucial as we will see shortly.

In the light of this result, we infer that $\{\phi_a, \phi_b\} = c_{ab}{}^{j}\phi_j$ is a linear combination of first-class constraints, both primary and secondary. Then, we realise that *all* the first-class constraints can be thought of as the generators of infinitesimal *gauge transformations*, that is, transformations that modify the canonical variables without altering the physical state (on account of the redundancy in our mathematical description of the system).

This idea suggests that we should include in our notion of evolution the variations that lead to no change in the physical state. Then, we should generalise our equations of motion to encompass these transformations. This can be done by defining

$$\dot{f} := \{f, H_E\}, \tag{29}$$

where $H_E$ is an extended Hamiltonian given by

$$H_E = H_T + v'^{a'}\phi_{a'}. \tag{30}$$

The generators $\{\phi_{a'}\}$, which are not contained in $H_T$, are the secondary, first-class constraints.

In conclusion, the final picture from the classical viewpoint is that we end up with a total Hamiltonian which is written as the sum of a first-class Hamiltonian and a linear combination of the primary, first-class constraints. This Hamiltonian can be extended to include secondary, first-class constraints, which generate (as their primary counterparts) infinitesimal transformations of the dynamical variables that leave the physical state unchanged. Therefore, even though the extra terms produce further changes in the evolution of dynamical variables, these changes do not correspond to any alteration of the physical state itself.

## 2.2 Quantum theory

The objective of this subsection is to illustrate the quantisation procedure of a constrained system described classically using the formalism we have developed in Subsec. 2.1.

Let us begin by discussing the case when all the constraints of the system are first-class. Formally, the quantisation of a classical system (whose phase space is denoted by $\Gamma$) is performed following the steps sketched below [79]:

i) Make a selection of a subspace $\mathcal{S}$ of the (vector) space of smooth, complex functions on $\Gamma$ such that a) it is large enough[6] and contains the unit function '1', b) it is closed under Poisson brackets, and c) it is closed under complex conjugation. The elements of $\mathcal{S}$ can be thought of as elementary classical variables with well-defined quantum analogues that coordinatise the classical phase space.

ii) Define a linear map $\hat{}: \mathcal{S} \to \mathcal{O}$ that represents every classical variable $F$ by a linear operator $\hat{F}$ acting on the *kinematical* Hilbert space of the system, $\mathcal{H}^{\text{kin}}$. Such a map must represent the classical structure of Poisson brackets. That is, up to higher-order quantum corrections,

$$[\hat{F}\,, \hat{G}] = i\widehat{\{F, G\}}, \tag{31}$$

where $[\cdot\,, \cdot]$ denotes the operator commutator[7]. This is the so-called Dirac rule. This needs to be complemented with a representation rule or *factor ordering prescription*

[6]This means that any regular function on $\Gamma$ can be expressed as (possibly a limit of) a sum of products of elements in $\mathcal{S}$.

[7]Here, I am assuming that the classical variables are all independent. Otherwise, one would need to introduce the algebraic relations between them in the form of anticommutation relations. For details on this issue, see Ref. [79].

that specifies how to symmetrise nonlinear products of powers of classical variables. We will see the necessity of choosing a representation rule when dealing with the quantum representation of the first-class constraints.
This map is also required to transform the complex conjugation of elementary variables into the Hermitian conjugation of quantum operators. Hence, real classical variables would become self-adjoint operators upon quantisation.

iii) Impose the condition that the representation be irreducible (otherwise, it could be written as the direct sum of irreducible representations and extra information would be needed to select one of them).

Once we have represented our canonical variables by quantum operators satisfying the appropriate commutation relations, we write down a Schrödinger equation

$$i\frac{d\psi}{dt} = H'\psi, \tag{32}$$

where $\psi \in \mathcal{H}^{\mathrm{kin}}$ is a quantum state. Furthermore, we impose additional conditions on the quantum states: we require that physical states be annihilated by (possibly the adjoint action of) the operators that represent the constraints[8]

$$\hat{\phi}_j \psi^{\mathrm{phys}} = 0 \quad \forall\, j, \tag{33}$$

where $\psi^{\mathrm{phys}} \in \mathcal{H}^{\mathrm{phys}}$ is a *physical state* belonging to the *physical Hilbert space*.

We now have to verify that these requirements do not introduce inconsistencies. In order to do so, consider two constraints, $\hat{\phi}_j$ and $\hat{\phi}_{j'}$. Then, the difference between applying one first and then the other, or the other way around is

$$(\hat{\phi}_j\hat{\phi}_{j'} - \hat{\phi}_{j'}\hat{\phi}_j)\psi^{\mathrm{phys}} = [\hat{\phi}_j, \hat{\phi}_{j'}]\psi^{\mathrm{phys}} = 0. \tag{34}$$

We need this condition to hold for consistency. However, we want all the conditions on the physical states to be contained in Eq. (33). Thus, we must have

$$[\hat{\phi}_j, \hat{\phi}_{j'}]\psi^{\mathrm{phys}} = \hat{c}_{jj'}{}^{j''}\hat{\phi}_{j''}\psi^{\mathrm{phys}}. \tag{35}$$

Indeed, if Eq. (35) does hold, then the consistency condition (34) follows from the original requirement that the physical states be annihilated by the constraint operators. Recall that all the constraints are first-class by assumption. Therefore, $\{\phi_j, \phi_{j'}\} = -ic_{jj'}{}^{j''}\phi_{j''}$ is true at the classical level (the $-i$ is written to recover only $c_{jj'}{}^{j''}$ in the quantum expression). Nevertheless, this does not imply Eq. (35). What it does imply is

$$[\hat{\phi}_j, \hat{\phi}_{j'}]\psi^{\mathrm{phys}} = \widehat{c_{jj'}{}^{j''}\phi_{j''}}\psi^{\mathrm{phys}}. \tag{36}$$

Since the coefficients $c_{jj'}{}^{j''}$ can depend on the canonical variables, they may not commute with the constraint operators at the quantum level, leading to anomalies in the imposition of the constraints. This simple example also serves to illustrate one of the sources of ambiguity in the quantum theory: beyond the problem of anomalies, a certain classical expression may involve quantities that do not commute quantum mechanically and then we have to *choose* a factor ordering in the quantum theory. I will refer to the choice of a specific ordering as adopting a *quantisation prescription*.

[8]This physically means that the quantum states are invariant under the transformations the constraints generate: we are asking that the quantum theory inherits the symmetries of the classical theory.

In conclusion, if we manage to select a quantisation prescription such that all the coefficients appear to the left in Eq. (36), then we can successfully formulate a quantum theory of a classical Hamiltonian system bound only by first-class constraints.

Let us now analyse the effects of the second-class constraints in the system we want to quantise. It is instructive to consider a simple case in the first place.

Consider a two-dimensional system described by the canonical variables $x_1, p_1, x_2$, and $p_2$. Classically, the nontrivial Poisson brackets are $\{x_i, p_j\} = \delta_{ij}$. Imagine that the system was constrained to move on the direction 2, so that $x_1 = 0$ and $p_1 = 0$. It is trivial to realise that these two constraints are second-class, given that they do not commute under Poisson brackets ($\{x_1, p_1\} = 1$). These constraints cannot be imposed at the quantum level as we have done with the first-class ones. Indeed, if we try to do so, inconsistencies are introduced:

$$\left.\begin{array}{l}\hat{x}_1\psi = 0\\ \hat{p}_1\psi = 0\end{array}\right\} \longrightarrow (\hat{x}_1\hat{p}_1 - \hat{p}_1\hat{x}_1)\psi = 0 \quad \text{but} \quad [\hat{x}_1, \hat{p}_1]\psi = i\psi \neq 0. \tag{37}$$

In this simple case, it is immediate to see what the solution is: forget about the direction 1 and redefine the Poisson bracket to only take into account $x_2$ and $p_2$ (which are the only ones of physical interest). Once the second-class constraints have been imposed classically and the Poisson bracket has been appropriately redefined, we have a Hamiltonian system with only first-class constraints that we can proceed to quantise as discussed above.

In the same spirit, we can always use the second-class constraints to reduce the number of degrees of freedom of the system. A general method to do this was devised by Dirac [23]. I will not describe it fully for the sake of brevity.

In summary, the prescription that we will adopt is the following. When we have a constrained system, we will replace the constraints by independent linear combinations of them in such a way that we bring those combinations into the category of first-class constraints. The remaining second-class constraints (the constraints whose linear combinations can never be first-class) are imposed to reduce the number of degrees of freedom of the system while the first-class constraints are kept and imposed at the quantum level[9]. In practice, this is done by requiring that, once promoted to operators acting on the kinematical Hilbert space, they annihilate the physical states of the quantum theory.

## 2.3 The case of General Relativity

First of all, it is important to remark that, while the Lagrangian formulation of GR is manifestly covariant, its Hamiltonian formulation breaks the explicit covariance through the selection of a preferred notion of time. This is done via a process that receives the denomination of *ADM decomposition* [80, 81], named after the initials of its authors (Arnowitt, Deser, and Misner). I will briefly sketch this procedure in this subsection.

We consider globally hyperbolic spacetimes $(\mathcal{M}, g)$, where $\mathcal{M}$ is a four-dimensional differentiable manifold and $g$ is a Lorentzian metric. By definition, they admit a global time function $t$ and are characterised by the existence of a(n achronal[10]) Cauchy hypersurface $\Sigma$, that causally determines the whole spacetime [2]. Therefore, the spacetime is topologically $\mathcal{M} = \mathbb{R} \times \Sigma$. Additionally, there exists a future-oriented timelike vector $t^\mu$ such that

[9] In principle, we could also introduce a *gauge fixing condition* which is second-class with respect to one of the first-class constraints and proceed to the reduction of the number of degrees of freedom of the system. Nevertheless, this eliminates quantum fluctuations that would otherwise affect the quantum theory.

[10] Although this construct is valid for all nontimelike sections, I will focus on spacelike Cauchy hypersurfaces for definiteness.

$t^\mu \nabla_\mu t = 1$, where $\nabla$ is the covariant derivative associated with the Levi-Civita connection. The integral curves of $t^\mu$ only intersect once each of the Cauchy hypersurfaces, so that they can be parametrised by the time function $t$.

Once $\Sigma$ is given, virtually all the physically relevant information to determine the classical solutions is encoded in the spatial three-metric $h_{\mu\nu}$ induced on $\Sigma$, and in the corresponding extrinsic curvature

$$K_{\mu\nu} = \frac{1}{2}\mathcal{L}_n h_{\mu\nu}, \tag{38}$$

where $\mathcal{L}_n$ is the Lie derivative along the unit normal to $\Sigma$, $n^\mu$. Since $n^\mu$ has to be orthogonal to $\Sigma$ and future-oriented,

$$n^\mu = -N g^{\mu\nu} \nabla_\nu t, \tag{39}$$

where $N$ can be thought of (in this regard) as a normalisation factor called the lapse function. The timelike vector $t^\mu$ can then be decomposed as

$$t^\mu = N n^\mu + N^\mu, \tag{40}$$

where $N^\mu$, the projection of $t^\mu$ onto the Cauchy hypersurfaces, is the so-called shift vector.

The metric of a globally hyperbolic spacetime can always be written in the following form:

$$ds^2 = -(N^2 - N_a N^a)dt^2 + 2h_{ab}N^a dt dx^b + h_{ab}dx^a dx^b. \tag{41}$$

Hence, the four-dimensional metric can be described using the spatial three-metric $h_{ab}$ (where the information about the spatial geometry is stored), the lapse function $N$, and the shift vector $N^a$ (in which the information about the time evolution of the spatial sections is contained).

It is important to note that I have written the shift vector and the spatial three-metric with spatial indices (from the beginning of the Latin alphabet). This is because they are both tensor fields defined on the spatial sections (and, thus, they live in their corresponding range space $T^r_s\Sigma$). From now on, I will write these tensor fields with spatial indices (as well as others like $K_{ab}$), except when I wish to refer to their four-dimensional counterparts.

Let $S_{EH}$ be the Einstein-Hilbert action

$$S_{EH} = \int_{\mathcal{M}} d^4x\, \mathscr{L}_G = \frac{1}{16\pi G}\int_{\mathcal{M}} d^4x\, \sqrt{-\mathfrak{g}} R, \tag{42}$$

where $\mathscr{L}_G$ is the Einstein-Hilbert Lagrangian density, $G$ is Newton's gravitational constant, $\mathfrak{g}$ is the determinant of the spacetime metric, and $R$ is the Ricci scalar. Expressing $\mathfrak{g}$ and $R$ in terms of $h_{ab}$, $N$, and $N^a$, an ADM decomposition of the action can be carried out. Since we can read off the Lagrangian density from the action, the Hamiltonian density can be obtained from this decomposition through a Legendre transform.

The lapse function $N$ and the shift vector $N^a$ are relevant to this discussion inasmuch as they appear as Lagrange multipliers in the Hamiltonian of GR that results from this transformation. Indeed, it can be shown that they are not dynamical, i.e., there are no time derivatives of these functions in the Hamiltonian. Furthermore, apart from boundary terms, the Hamiltonian turns out to vanish on solutions, which means that it has the form of an integrated linear combination of the four constraints encoding the general covariance of the theory

$$H_{GR} = \int d^3x\, \left(N\mathcal{S} + N^a \mathcal{V}_a\right), \tag{43}$$

where $\mathcal{S}$ is the scalar constraint and $\mathcal{V}_a$ $(a = 1, 2, 3)$ are the three spatial diffeomorphism constraints. These four constraints are functions of the canonical variables: the spatial three-metric $h_{ab}$ and its conjugate momentum

$$\pi_{ab} = \frac{1}{16\pi G}\sqrt{\mathfrak{h}}(K_{ab} - K h_{ab}), \tag{44}$$

where $\mathfrak{h}$ is the determinant of the spatial three-metric and $K = h^{ab}K_{ab}$ is the trace of the extrinsic curvature. Whereas the spatial diffeomorphism constraints are linear (both in the spatial three-metric and the momentum), the Hamiltonian constraint is nonlinear, which will complicate enormously its implementation in general cases, as we will see.

Since no time derivatives of the lapse function or the shift vector appear in the Hilbert-Einstein action and the constraints only depend on $h_{ab}$ and $\pi_{ab}$, the equations of motion associated with $N$ and $N^a$ simply reduce to

$$\frac{\delta S_{EH}}{\delta N} = \mathcal{S} = 0, \qquad \frac{\delta S_{EH}}{\delta N^a} = \mathcal{V}_a = 0, \tag{45}$$

which state that $\mathcal{S}$ and $\mathcal{V}_a$ are indeed constraints on the canonical variables.

It is worth remarking once more that the explicit covariance of the theory has been broken in this process and we cannot be sure whether the genuine covariance has been compromised as well. Classically, when one reconstructs the theory from the algebra of constraints, the general covariance is restored. In the light of this result, we carry on with our quantisation programme and expect that the general covariance is recovered once the complete quantum theory is formulated and the constraints successfully implemented.

If we quantise the system employing $h_{ab}$ and $\pi_{ab}$ as canonical variables, and a *conventional* quantisation method, we arrive at a theory called *quantum geometrodynamics*, which suffers from certain problems[11] and whose analysis is not the objective of this thesis. Hence, we will adopt different variables instead, whose introduction is one of the objectives of the next section (Sec. 3).

[11]For instance, i) how to deal with the high nonlinearity of the theory is not well-understood, ii) it does not cure the singularities in generic peaked solutions, and iii) there is no well-controlled functional analysis on its associated configuration space (the space of three-geometries modulo spatial diffeomorphisms).

# 3 Rudiments of Loop Quantum Gravity

The objective of this section is to provide a very brief introduction to the concepts and techniques of canonical LQG, so that this thesis is as self-contained as possible. Furthermore, this will hopefully provide a clearer motivation for the treatment of cosmological spacetimes in subsequent sections. Although this information is covered in any introductory book on LQG (see, for instance, Ref. [77]), I will mainly follow the clear exposition of Ref. [32].

## 3.1 Triadic formulation

Instead of using the spatial geometry as a dynamical variable to describe the system, we can adopt an entirely equivalent formulation in terms of co-triads $e^i_a$ defined through

$$h_{ab} = e^i_a \delta_{ij} e^j_b. \tag{46}$$

As I already commented, Latin indices from the middle of the alphabet denote SU(2) indices[12] that take values from 1 to 3.

We can also define a triadic version of the extrinsic curvature as

$$K^i_a = K_{ab} e^b_j \delta^{ji}, \tag{47}$$

where $e^a_i$ is the inverse of the co-triad, the so-called *triad*, and is defined through

$$e^a_i e^j_a = \delta^j_i, \qquad e^a_i e^i_b = \delta^a_b. \tag{48}$$

Once we have reached this point, it is interesting to discuss the intuitive physical interpretation of the triad and the co-triad. It is transparent if we write the three-metric of the Cauchy hypersurfaces as

$$dl^2 = h_{ab} dx^a dx^b = e^i_a \delta_{ij} e^j_b dx^a dx^b = \delta_{ij} dy^i dy^j, \tag{49}$$

where $dy^i = e^i_a dx^a$ or, equivalently,

$$\frac{\partial y^i}{\partial x^a} = e^i_a. \tag{50}$$

Therefore, the components of the co-triad can be thought of as spatial 1-forms that, at each point of spacetime, solder the cotangent space $T^*\Sigma$ (defined as the dual of $T\Sigma$) with a local flat space. In this sense, they are also referred to as *soldering forms*.

With the two relations in Eq. (48), we can invert Eq. (46) by contracting it with $e^a_k e^b_l$. The result is the following:

$$h_{ab} e^a_k e^b_l = e^a_k e^i_a \delta_{ij} e^j_b e^b_l = \delta^i_k \delta_{ij} \delta^j_l = \delta_{kl}. \tag{51}$$

The equation above can be interpreted as an orthonormality relation for a set of three vector fields $\{e^a_i\}_{i=1,2,3}$. Then, the physical interpretation of the introduction of a triad is clear: we attach at each point in $\mathcal{M}$ a coordinate system (given by the three coordinate axes defined by the components of the triad) which is locally at free fall (i.e., the three-metric is locally

[12] This alternative triadic formalism allows for the coupling of fermions through the internal SU(2) indices, which we will have to do if we wish to formulate a theory of quantum geometry that interacts with quantum matter fields.

flat). In other words, a triad can be thought of as a set of coordinate axes corresponding to an inertial reference frame at each point of space.

Before moving on, it is important to note that, given a spatial three-metric, the choice of co-triad is not unique. Indeed, consider a certain co-triad $e^i_a$ satisfying Eq. (46). Then, any other co-triad obtained from $e^i_a$ as the result of a local (in space) internal rotation (meaning with respect to the index $i$) also satisfies Eq. (46). To directly realise this, consider a three-dimensional rotation matrix $R^i{}_j \in \mathrm{SO}(3)$. Rotating the co-triad $e^i_a$ solution of Eq. (46) trivially results in

$$\tilde{e}^j_a = R^j{}_i e^i_a. \tag{52}$$

Thus,

$$\tilde{e}^i_a \delta_{ij} \tilde{e}^j_a = R^i{}_k e^k_a \delta_{ij} R^j{}_l e^l_b = e^k_a R_{jk} R^j{}_l e^l_b = e^k_a R^T_{kj} R^j{}_l e^l_b = e^k_a (R^T R)_{kl} e^l_b, \tag{53}$$

where the superscript $T$ denotes the transpose. Since $R$ is an orthogonal matrix by definition, $(R^T R)_{ij} = \delta_{ij}$. As a result, we obtain

$$\tilde{e}^i_a \delta_{ij} \tilde{e}^j_a = e^k_a \delta_{kl} e^l_b = h_{ab}, \tag{54}$$

where the last equality follows from the assumption that the original co-triad satisfies Eq. (46). Given that we have made no assumptions on the nature of $R$ other than that it is a three-dimensional rotation, we conclude that all the co-triads related by a local internal rotation are equally valid and all of them describe the same spatial three-metric. Hence, we realise that there is a redundancy in our triadic description of the gravitational degrees of freedom: at each point in space we have the freedom of performing an internal SO(3) transformation and the physics remains unchanged. In conclusion, a triadic formulation of canonical GR introduces an extra symmetry (this time, local or *gauge*) under transformations of SO(3) or of its double universal cover SU(2), endowing the spacetime with the structure of an SU(2) principal bundle of three-dimensional reference frames[13]. This SU(2) symmetry that enlarges the symmetry group of the theory will give rise to an additional constraint on the dynamical variables, called the *Gauss* constraint.

Once we have analysed the advantages and consequences of appealing to a triadic formulation of GR, it is worth noting that the triad and the triadic extrinsic curvature do *not* provide a canonical pair (in the sense that their Poisson bracket is not proportional to the identity). However, an actual set of canonical variables for GR can be easily obtained by considering the densitised version of the triad instead

$$E^a_i := \sqrt{\mathfrak{h}}\, e^a_i. \tag{55}$$

Then, the densitised triad and the triadic extrinsic curvature have all the properties we were looking for: they are canonical variables for GR especially adapted for the coupling of fermionic fields. Indeed, their Poisson bracket is given by

$$\{K^i_a(x), E^b_j(y)\} = 8\pi G \delta^i_j \delta^b_a \delta(x-y), \tag{56}$$

where $\delta(\cdot)$ is the three-dimensional Dirac delta, and $x$ and $y$ are two generic points in $\Sigma$.

[13] It is for this reason that I refer to the $i, j, k$... indices as SU(2) indices.

## 3.2 Ashtekar-Barbero variables

To continue with the LQG programme, one introduces a connection valued 1-form to replace the triadic extrinsic curvature. In order to do this, it suffices to realise that the densitised triad determines an $\mathfrak{su}(2)$-connection (also called *spin connection*) $\Gamma^i_a$ compatible with it through the metricity condition

$$D_b E^a_i = \nabla^{(3)}_b E^a_i + \epsilon_{ij}{}^k \Gamma^j_b E^a_k = 0, \tag{57}$$

where $D_b$ is the minimally-coupled gauge covariant derivative, analogous to the standard covariant derivative in non-Abelian gauge field theories $D_a = \partial_a - T_i A^i_a$ but with a nonflat spatial background, which induces the replacement of the partial derivative by the covariant derivative $\nabla^{(3)}_a$ compatible with $h_{ab}$ .

In terms of the Christoffel symbols $\Gamma_{ab}{}^d = \frac{1}{2}h^{dc}(\partial_a h_{bc} + \partial_b h_{ac} - \partial_c h_{ab})$, the metricity condition reads

$$\begin{aligned} 0 &= \partial_b E^a_i + \Gamma_{cb}{}^a E^c_i - \Gamma_{cb}{}^c E^a_i + \epsilon_{ij}{}^k \Gamma^j_b E^a_k, \\ \epsilon_{ij}{}^k \Gamma^j_b E^a_k &= -(\partial_b E^a_i + \Gamma_{cb}{}^a E^c_i - \Gamma_{cb}{}^c E^a_i), \end{aligned} \tag{58}$$

where the third term of the gauge covariant derivative appears due to the fact that the densitised triad is a vector density of weight $-1$ (recall the square root of the determinant of $h_{ab}$ involved in its definition). If we contract Eq. (58) with $E'^l_a \epsilon^{im}{}_l$, the result is

$$\epsilon_{ij}{}^k \epsilon^{im}{}_l E^a_k E'^l_a \Gamma^j_b = -\epsilon^{im}{}_l E'^l_a (\partial_b E^a_i + \Gamma_{cb}{}^a E^c_i - \Gamma_{cb}{}^c E^a_i). \tag{59}$$

The definition of the densitised co-triad $E'^i_a$ is such that $E^a_k E'^l_a = \delta^l_k$. Using this definition and the property

$$\epsilon_{ijk}\epsilon^{ilm} = \delta^l_j \delta^m_k - \delta^m_j \delta^l_k, \tag{60}$$

we obtain

$$\begin{aligned} \epsilon_{ij}{}^l \epsilon^{im}{}_l \Gamma^j_b &= -\epsilon^{im}{}_l E'^l_a (\partial_b E^a_i + \Gamma_{cb}{}^a E^c_i - \Gamma_{cb}{}^c E^a_i), \\ (\delta^m_j \delta^l_l - \delta_{jl}\delta^{lm})\Gamma^j_b &= -\epsilon^{im}{}_l E'^l_a (\partial_b E^a_i + \Gamma_{cb}{}^a E^c_i - \Gamma_{cb}{}^c E^a_i), \\ 2\Gamma^m_b &= -\epsilon^{im}{}_j E'^j_a (\partial_b E^a_i + \Gamma_{cb}{}^a E^c_i - \Gamma_{cb}{}^c E^a_i). \end{aligned} \tag{61}$$

Thus, we have obtained a closed expression for the spin connection:

$$\Gamma^i_a = \frac{1}{2}\epsilon^{ik}{}_j E'^j_b (\partial_a E^b_k + \Gamma_{ca}{}^b E^c_k). \tag{62}$$

Notice that I have omitted the third term since it vanishes identically owing to the complete antisymmetry of the Levi-Civita symbol:

$$-\frac{1}{2}\epsilon^{ik}{}_j \Gamma_{ca}{}^c E'^j_b E^b_k = -\frac{1}{2}\epsilon^{ik}{}_j \Gamma_{ca}{}^c \delta^j_k = -\frac{1}{2}\epsilon^{ik}{}_k \Gamma_{ca}{}^c = 0 \; \square. \tag{63}$$

Then, we conclude that a spin connection is uniquely determined (up to gauge transformations) from the geometry of $\Sigma$. However, if we wish to replace the triadic extrinsic curvature by a connection in our canonical pair, such a connection must encode all the information about $K^i_a$ (i.e., about the time evolution of the spatial geometry). This can be achieved by realising that the sum of $\Gamma^i_a$ with any vector (both from the internal and external viewpoints) provides again an $\mathfrak{su}(2)$-connection valued 1-form. Therefore, we can simply consider

$$A^i_a = \Gamma^i_a + \gamma K^i_a, \tag{64}$$

which is the so-called *Ashtekar-Barbero* connection [20, 21]. The Immirzi parameter $\gamma$ is a free nonzero constant[14]. This connection, together with the densitised triad, provides a set of canonical variables, their Poisson bracket being given by

$$\{A^i_a(x), E^b_j(y)\} = 8\pi G\gamma \delta^b_a \delta^i_j \delta(x-y). \tag{65}$$

For the sake of a global vision of what we have done so far, let us summarise the steps we have followed up to this point:

- We have considered globally hyperbolic spacetimes in GR and performed an ADM decomposition thereof in order to construct a Hamiltonian formalism which can be readily quantised via a canonical approach.
- Instead of using the spatial metric and its conjugate momentum (related to the extrinsic curvature) as the dynamical variables, we have introduced a triad and a co-triad (which can be though of as the coordinate axes corresponding to an inertial frame of reference at each point of spacetime).
- Using the newly introduced triad and co-triad, we have defined a triadic version of the extrinsic curvature. Together with the densitised triad, the triadic extrinsic curvature provides a set of canonical variables for GR.
- Finally, we have replaced the triadic extrinsic curvature with an $\mathfrak{su}(2)$-connection valued 1-form composed by two pieces: a spin connection (defined from the densitised triad by a metricity condition) and the triadic extrinsic curvature. In this process, the Immirzi parameter (which is not fixed by the theory itself) is introduced.

In conclusion, we choose our canonical variables to be the densitised triad, which contains the information about the spatial geometry, and the Ashtekar-Barbero connection, that knows about how the spatial geometry changes with time.

It is important to remember that these variables are bound by a series of constraints[15] that generate the symmetries of (the triadic formulation of) GR: the spacetime diffeomorphisms and the gauge SU(2) transformations. First of all, let us begin by writing down the *Gauss constraint*, which generates SU(2) transformations:

$$\mathcal{G}_i := \frac{1}{8\pi G\gamma}(\partial_a E^a_i + \epsilon_{ij}{}^k A^j_a E^a_k) = 0. \tag{66}$$

The fact that GR is invariant under spatial diffeomorphisms is manifested in the *vector* or *spatial diffeomorphism constraint*:

$$\mathcal{V}_a := \frac{1}{8\pi G\gamma} F^i_{ab} E^b_i = 0, \tag{67}$$

where $F^i_{ab}$ is the curvature tensor of the Ashtekar-Barbero connection.

$$F^i_{ab} = 2\partial_{[a}A^i_{b]} + \epsilon^i{}_{jk} A^j_a A^k_b. \tag{68}$$

[14]The Immirzi parameter introduces an ambiguity in the quantisation, which is often resolved in LQG by appealing to the recovery of the Bekenstein-Hawking law for the entropy of black holes [82].

[15]The expressions of these constraints are considerably simplified by the introduction of the Ashtekar-Barbero gauge connection [83].

Finally, the invariance under time reparametrisation is reflected (up to spatial diffeomorphisms) in the *scalar* or *Hamiltonian constraint*. This constraint adopts the following form *in vacuo*:

$$\mathcal{S} := \frac{1}{16\pi G\sqrt{\mathfrak{h}}} E_i^a E_j^b (\epsilon^{ij}{}_k F_{ab}^k - 4K_{[a}^i K_{b]}^j). \tag{69}$$

The Hamiltonian constraint will play a central role in this thesis. The first piece of the expression above is often referred to as the *Euclidean part*, whereas the second one is the so-called *Lorentzian part*. We will discuss this distinction in detail later.

## 3.3 The holonomy-flux algebra

It should be noted that, given that the introduction of triads and co-triads results in the symmetry group of the theory being enlarged by the addition of a new SU(2) gauge symmetry, our mathematical description is *redundant*. This redundancy implies that there are gauge degrees of freedom with no physical relevance. Only the gauge invariant information has physical meaning. Thus, the question is how to successfully capture such information in our formalism.

We have discussed above how the triads and co-triads endow the spacetime with the structure of an SU(2) principal bundle. The spin connection $\Gamma_a^i$ extensively discussed above allows one to define a notion of parallel transport of elements of the fibres along a path. Such parallel transport is uniquely determined up to a gauge transformation at the initial and final points. Therefore, if we close the path, the gauge freedom is suppressed. This indicates that the gauge invariant information is encoded in closed paths or *loops* (this idea is closely related to the concept of Wilson loop appearing in Yang-Mills theories). In this manner, it seems natural to replace the connection with *holonomies* of the connection along edges, $e$

$$h_e = \mathcal{P}\mathrm{exp}\left(\int_e dx^a\, A_a^i \tau_i\right), \tag{70}$$

where $\mathcal{P}$ denotes the path-ordering operator. Here, $\tau_i = -i\sigma_i/2$ (with $\sigma_i$ being the Pauli matrices) are the generators of the defining representation of $SU(2)$ and, as such, verify $[\tau_i, \tau_j] = \epsilon_{ij}{}^k \tau_k$. It should be noted that two goals are achieved in this process:

i) The line integral in the exponent smears the connection along one dimension, partially alleviating the contact divergences ($x = y$) of the theory. See, for instance, Eq. (65).

ii) The gauge degrees of freedom are eliminated without the need of introducing a preferred background structure[16].

The most important divergences are expected to arise in the form of three-dimensional Dirac deltas in the Poisson brackets of the canonical variables. Since we have managed to smear the connection along one dimension, it seems reasonable to ask whether we can smear the densitised triad along two dimensions without paying the price of introducing a background structure. The answer is, in general, in the affirmative. For any surface $S$ and any smooth test function of SU(2) $f^i$, we define the *flux* of the densitised triad as

$$E(S, f) = \int_S dx^b dx^c\, \epsilon_{abc} f^i E_i^a. \tag{71}$$

Let us note that this is only possible because the densitised triad is a vector density (of weight $-1$) in $\Sigma$ and, therefore, its Hodge dual can be integrated over two-dimensional surfaces.

[16]By this we usually mean that no metric is needed to construct the object in question.

The holonomies of the Ashtekar-Barbero connection and the fluxes of the densitised triad form an algebra under Poisson brackets, which no longer has the distributional divergences of the canonical relations. This algebra is chosen in LQG to be represented over a kinematical Hilbert space. Thus, the quantisation of the theory as it is formulated consists in looking for a representation of the holonomy-flux algebra in the form of operators acting on a Hilbert space. On this representation, the diffeomorphism and scalar constraints must be imposed.

To close this subsection, let us briefly describe the kinematical Hilbert space of LQG. To begin with, we need to define a *cylindrical* function of the connection as a complex function that only depends on the connection through holonomies along a finite number of edges. The algebra of the cylindrical functions of the connection is identified in LQG as the configuration algebra. By virtue of the properties of this algebra when completed with a suitable norm, the configuration algebra is ensured to be isomorphic to the algebra of continuous functions on a compact space $\bar{\mathcal{A}}$ (called the spectrum) by Gel'fand theory [84]. The kinematical Hilbert space of any representation of the configuration algebra is that of square integrable functions on $\bar{\mathcal{A}}$, $L^2(\bar{\mathcal{A}}, d\mu)$, for some measure $d\mu$.

## 3.4 The LOST Theorem

The Lewandowski-Okolow-Sahlmann-Thiemann Theorem (or *LOST* Theorem, for short) is a crucial result in LQG. This theorem states the uniqueness (up to unitary equivalence) of a cyclic representation of the holonomy-flux algebra whose vacuum is invariant under diffeomorphisms [85]. In the language of the previous paragraph, this theorem ensures that there is a *unique* Hilbert space $L^2(\bar{\mathcal{A}}, d\mu_{AL})$ that supports a representation not only of the holonomies but also of the fluxes and such that the measure $d\mu_{AL}$ is invariant under diffeomorphisms[17].

Therefore, a *unique* family of unitarily equivalent quantisations is selected by the choice of canonical variables (motivated by the independence of background structures) and the identification of the invariance under diffeomorphisms as a fundamental symmetry.

To conclude this section concerning LQG, I want to briefly summarise (in a qualitative manner) the result one obtains when considering the representation of the holonomy-flux algebra that verifies the conditions above and whose existence is guaranteed by the LOST Theorem. For a technical and rigorous account, I refer to any standard reference on LQG (such as [18] or [19]).

The physical consequence of trying to quantise a theory of geometry is that space and time themselves are discrete. The LQG programme results in a picture where spacetime is granular and the geometric quantities (such as the area) are discrete.

The unique cyclic representation of the holonomy-flux algebra with a diffeomorphism invariant vacuum turns out not to be continuous [18]. This implies that we cannot obtain a representation of the connection (which appears in the exponent of the holonomy). This introduces a nonlocality in the theory, since physical observables will have to be expressed in terms of holonomies instead of connections. Another consequence of the discontinuity of the representation is that a generalisation of the Stone-von Neumann Theorem no longer holds and, thus, the representation of LQG is not equivalent to that of standard QM or QFT (usually referred to as *Schrödinger representation*).

In the quantum theory, the holonomies play the role of 'excitation lines' by means of which the excited states are generated from the vacuum. When one wants to compute the expected value of a given geometrical operator (the area of a surface, for instance), one

[17] This measure is usually referred to as the *Ashtekar-Lewandowski measure*.

obtains that the commutator of the holonomies with the densitised triad is nonzero and each 'punction' contributes with a quantum of area weighted with a certain representation of SU(2). The holonomy paths are embedded in the spacetime and regarded as equivalent under spatial diffeomorphisms. Then, one can view them as composed by straight edges that intersect. Recall that we wanted closed paths in order to retain only the physical degrees of freedom. Then, we obtain a network of straight edges that meet in vertices in such a way that no vertex is a 'dead end.' Each edge carries a representation of SU(2) (or *spin number*), $j$, and at each vertex there is an *intertwiner* (that is, a scheme of addition of representations that generalises the Clebsch-Gordan coefficients, intuitively speaking), so that the SU(2) invariance is respected. In total, we have a set of edges with different spin numbers that meet in vertices, where the 'angular momentum' is conserved. Such structures receive the name of *spin networks* and their time evolution are the so-called *spin foams*.

As of today, the Gauss and spatial diffeomorphism constraints have been implemented. The scalar constraint, however, remains to be solved, which prevents the obtention of the physical Hilbert space, thereby blocking the road towards the completion of the LQG quantisation programme.

# 4 Homogeneous LQC: Kinematics

In this section, we will review the standard loop quantum theory of two cosmological spacetimes which will play a central role in this thesis: Bianchi I and flat Friedmann-Lemaître-Robertson-Walker (FLRW) cosmologies. In particular, we will focus on their kinematical aspects.

Owing to their simplicity and their importance in cosmology, these models have been thoroughly studied both in GR and LQC. For details about these homogeneous cosmological models, a plethora of references can be consulted. See, e.g., Refs. [36, 37, 41, 46, 86].

## 4.1 Bianchi I cosmologies

The spacetimes of type Bianchi I are homogeneous but anisotropic and have flat spatial sections. In this regard, they can be thought of as the immediate anisotropic generalisation of flat FLRW spacetimes. For this reason, flat FLRW cosmologies are expected to be recovered in the isotropic limit of Bianchi I cosmologies (i.e., when the three spatial directions are identified). Even though this statement holds classically, its veracity at the quantum level depends critically on the quantisation prescription that we select to represent the Hamiltonian constraint. We will discuss this matter extensively in subsequent subsections.

In this subsection, we will summarise the classical and quantum kinematical aspects of the Bianchi I models that will be relevant for this thesis (leaving out the regularisation procedure of the Hamiltonian constraint, to which I will devote the following section).

Following the philosophy of LQG, we describe the system using Ashtekar-Barbero variables [44, 41, 46]. Usually, the definition of these variables require the introduction of a finite cell (which plays the role of an infrared regulator[18]) and a fiducial triad. Nevertheless, it was shown in Ref. [45] that, provided that one specialises to a diagonal gauge, an appropriate election of the Ashtekar-Barbero variables results in the physical quantities being independent of the choice of finite cell and fiducial metric. Therefore, for the sake of simplicity, we select a diagonal Euclidean triad and focus the discussion on spatial sections with a compact topology, namely, that of a three-torus $T^3$. Under these considerations, it seems natural to fix the finite cell as the whole of the $T^3$ section, with sides of coordinate length $2\pi$. In these circumstances, one arrives at the following Ashtekar-Barbero variables:

$$A_a^i = \frac{c^i}{2\pi}\delta_a^i, \qquad E_i^a = \frac{p_i}{4\pi^2}\delta_i^a, \tag{72}$$

where $c^i$ and $p_i$ are constants in $\Sigma$ (but not under time evolution) that encode all the geometric degrees of freedom.

When dealing with Bianchi I cosmologies, I will not use Einstein's summation convention *for the internal indices*, since I believe it is confusing owing to their repeated appearance in pairs. Therefore, I will be using the standard summation notation, $\sum$. However, Einstein's notation will still be applied in the case of spatial (and spacetime) indices.

The nontrivial canonical Poisson brackets on the phase space of the model adopt the following form in terms of $c^i$ and $p_i$:

$$\{c^i, p_j\} = 8\pi G\gamma\delta_j^i. \tag{73}$$

[18]Indeed, owing to the spatial homogeneity of the models we will be considering, certain quantities (such as the Hamiltonian itself) diverge upon being integrated over noncompact spatial sections.

It is important to notice that, due to the fact that we have chosen a diagonal system, the internal $SU(2)$ and spatial indices can be identified, and we will for convenience.

Using circular coordinates $\{x^i\} = \{\theta, \sigma, \delta\}$, $x^i \in S^1$, we can write the spacetime metric as

$$ds^2 = -N^2 dt^2 + \frac{V^2}{4\pi^2} \sum_{i=\theta,\sigma,\delta} \frac{(dx^i)^2}{p_i^2}, \tag{74}$$

where $N$ is the lapse function and

$$V = \sqrt{|p_\theta p_\sigma p_\delta|} \tag{75}$$

is the physical volume of the Universe.

In homogeneous LQC, we characterise the configuration space using holonomies of the Ashtekar-Barbero connection $A_a^i$ along straight edges. In the case of Bianchi I, these edges are oriented along the fiducial directions (labeled by $i = \theta, \sigma, \delta$) and have lengths $2\pi\mu_i \in \mathbb{R}$, respectively. In this manner, we get the basic holonomies

$$h_i^{\mu_i}(c^i) = \exp\{\mu_i c^i \tau_i\}, \tag{76}$$

whose explicit expression will be computed in the next section (Sec. 5).

The description of the phase space is then completed with the fluxes of the densitised triad through the fiducial rectangles composed by edges of the holonomies. The area of the rectangle formed by two edges oriented along two different fiducial directions $j$ and $k$ (both orthogonal to the direction $i$) turns out to be proportional to $p_i$. Indeed, the triad flux associated with a rectangular surface of this kind is given by

$$E(S_i) = \frac{p_i}{4\pi^2} S_i, \tag{77}$$

where $S_i$ is the fiducial area of the rectangular surface.

The configuration algebra is given by sums of products of the matrix elements of the irreducible representations of the holonomies. It is well known [32] that this algebra is the algebra of almost-periodic functions of the connection variables $c^i$. Such an algebra is generated, as I said before, by the holonomy matrix elements

$$\prod \mathcal{N}_{\mu_i}(c^i) = \prod e^{i\mu_i c^i/2}. \tag{78}$$

In the previous expression, the product is to be taken over the three fiducial directions $(i = \theta, \sigma, \delta)$ and $\mu_i \in \mathbb{R}$ is any real number.

Upon quantisation, these exponentials will be represented by a ket state[19] $|\mu_i\rangle$. We can define the analogue of the space of cylindrical functions in LQG as [50]

$$\mathrm{Cyl}_{\mathrm{S}}^{\mathrm{BI}} = \mathrm{span}\left\{|\mu_\theta, \mu_\sigma, \mu_\delta\rangle\right\}, \tag{79}$$

where

$$|\mu_\theta, \mu_\sigma, \mu_\delta\rangle = |\mu_\theta\rangle \otimes |\mu_\sigma\rangle \otimes |\mu_\delta\rangle \tag{80}$$

denotes the tensor product of the states corresponding to the three different spatial directions. The kinematical Hilbert space of a Bianchi I cosmology, ${}^{(\mathrm{BI})}\mathcal{H}_{\mathrm{grav}}^{\mathrm{kin}} = \otimes_i \mathcal{H}_{\mathrm{grav},i}^{\mathrm{kin}}$, will be given by the completion of $\mathrm{Cyl}_{\mathrm{S}}^{\mathrm{BI}}$ with respect to the discrete inner product

$$\langle\mu_i|\mu_i'\rangle = \delta_{\mu_i,\mu_i'} \tag{81}$$

[19]From now on, I will use Dirac's bra-ket notation.

in each direction. Clearly, a basis of the kinematical Hilbert space is provided by the states $|\mu_\theta, \mu_\sigma, \mu_\delta\rangle$ introduced above. The action of the fundamental operators on these states is simple: they are eigenstates of $\hat{p}_i$ (associated, as we saw, with triad fluxes across rectangular surfaces orthogonal to the $i$th fiducial direction), and the operators $\hat{\mathcal{N}}_{\mu_i}$ shift their labels.

$$\hat{p}_i \,|\mu_i\rangle = 4\pi\gamma l_p^2 \mu_i \,|\mu_i\rangle \,, \tag{82}$$

$$\hat{\mathcal{N}}_{\mu_i'} \,|\mu_i\rangle = |\mu_i + \mu_i'\rangle \,, \tag{83}$$

where $l_p = \sqrt{G}$ is the Planck length. Of course, these operators act trivially on states belonging to the Hilbert spaces associated with the fiducial directions orthogonal to the $i$th direction. In this sense, when I write $\hat{\mathcal{N}}_i$, I am referring to $\hat{\mathcal{N}}_i \otimes \mathbb{I}_j \otimes \mathbb{I}_k$. Nevertheless, in most cases we will omit the trivial actions for brevity.

In LQG, the area spectrum is discrete and the limit of zero area cannot be attained [18]: there exists an area gap $\Delta$, which is commonly identified with the quantity

$$\Delta = 4\sqrt{3}\pi\gamma l_p^2. \tag{84}$$

It has been argued that this fact should be taken into account in LQC as well. In particular, this nonzero area gap is imported in the form of a minimum coordinate length of the edges of the holonomies. Although different prescriptions exist concerning the implementation of this minimum length, the most widespread one is the so-called *$\bar{\mu}$-scheme* or *improved dynamics prescription* [36]. It states that the minimum coordinate length for each direction should be fixed by requiring that the edges of the holonomies form rectangles of minimum nonzero area $\Delta$ [41]

$$\bar{\mu}_j \bar{\mu}_k |p_i| = \Delta, \tag{85}$$

with $i \neq j \neq k$. We can write similar expressions for rectangles orthogonal to the directions $j$ and $k$: $\bar{\mu}_i \bar{\mu}_k |p_j| = \Delta$ and $\bar{\mu}_i \bar{\mu}_j |p_k| = \Delta$. Multiplying the last two conditions and dividing the result by the first one yields

$$\bar{\mu}_i = \sqrt{\frac{|p_i|}{|p_j p_k|}\Delta}. \tag{86}$$

The fact that this minimum coordinate length depends on the variables $p_i$ for the three spatial directions implies that the shift produced by $\hat{\mathcal{N}}_{\bar{\mu}_i}$ depends on the state it acts upon. However, it is possible to rewrite these holonomy operators in such a way that their action is considerably simplified. This is normally done by introducing an affine parameter $\lambda_i$ for each spatial direction, such that

$$\lambda_i = \mathrm{sgn}(p_i)\frac{\sqrt{|p_i|}}{(4\pi\gamma l_p^2\sqrt{\Delta})^{1/3}} \Rightarrow (4\pi\gamma l_p^2\sqrt{\Delta})^{1/3} d\lambda_i = \mathrm{sgn}(p_i) d|p_i|^{1/2}. \tag{87}$$

In the previous equation, $\mathrm{sgn}(\cdot)$ denotes the sign function.

We can represent $i\bar{\mu}_i c^i$ in the exponent of the holonomies by the differential operator $8\pi\gamma G \bar{\mu}_i \partial_{p_i}$ (as usual in the $p$-representation, $c^i$ is represented by the differential operator $\hat{c^i} = -iC\partial_{p_i}$, where $C$ is the constant appearing in the canonical commutation relations through $[\hat{c}^i, \hat{p}_j] = iC\delta^i_j$). It can be shown that such an operator can be recast as [41, 46]

$$8\pi\gamma G \bar{\mu}_i \partial_{p_i} = \frac{1}{|\lambda_j \lambda_k|}\partial_{\lambda_i}, \tag{88}$$

where the three directions appearing in the expression above are different from one another. Indeed,

$$
\begin{aligned}
\bar{\mu}_i \partial_{p_i} &= \frac{\sqrt{\Delta}}{\sqrt{|p_j p_k|}} \mathrm{sgn}(p_i) \sqrt{|p_i|} \frac{\partial}{\partial |p_i|} = \frac{\sqrt{\Delta}}{2\sqrt{|p_j p_k|}} \mathrm{sgn}(p_i) \frac{\partial}{\partial |p_i|^{1/2}} \\
&= \frac{\sqrt{\Delta}}{2(4\pi\gamma l_p^2 \sqrt{\Delta})^{1/3}} \frac{1}{\sqrt{|p_j|}} \frac{1}{\sqrt{|p_k|}} \partial_{\lambda_i} \\
&= \frac{\sqrt{\Delta}}{2(4\pi\gamma l_p^2 \sqrt{\Delta})^{1/3}} \frac{1}{(4\pi\gamma l_p^2 \sqrt{\Delta})^{1/3} |\lambda_j|} \frac{1}{(4\pi\gamma l_p^2 \sqrt{\Delta})^{1/3} |\lambda_k|} \partial_{\lambda_i} \\
&= \frac{1}{8\pi\gamma l_p^2} \frac{1}{|\lambda_j \lambda_k|} \partial_{\lambda_i}, \\
\frac{1}{2} i \bar{\mu}_i c^i \to \frac{1}{2} 8\pi G \gamma \bar{\mu}_i \partial_{p_i} &= \frac{1}{2|\lambda_j \lambda_k|} \partial_{\lambda_i} \; \square.
\end{aligned} \tag{89}
$$

Then, it seems natural to relabel the states of the $|\mu_\theta, \mu_\sigma, \mu_\delta\rangle$-basis using the $\lambda$-parameters instead, $|\lambda_\theta, \lambda_\sigma, \lambda_\delta\rangle$. The action of the fundamental holonomy operators is now written as follows [50]

$$
\hat{\mathcal{N}}_{\pm\bar{\mu}_\theta} |\lambda_\theta, \lambda_\sigma, \lambda_\delta\rangle = \left| \lambda_\theta \pm \frac{1}{2|\lambda_\sigma \lambda_\delta|}, \lambda_\sigma, \lambda_\delta \right\rangle, \tag{90}
$$

$$
\hat{\mathcal{N}}_{\pm\bar{\mu}_\sigma} |\lambda_\theta, \lambda_\sigma, \lambda_\delta\rangle = \left| \lambda_\theta, \lambda_\sigma \pm \frac{1}{2|\lambda_\theta \lambda_\delta|}, \lambda_\delta \right\rangle, \tag{91}
$$

$$
\hat{\mathcal{N}}_{\pm\bar{\mu}_\delta} |\lambda_\theta, \lambda_\sigma, \lambda_\delta\rangle = \left| \lambda_\theta, \lambda_\sigma, \lambda_\delta \pm \frac{1}{2|\lambda_\theta \lambda_\sigma|} \right\rangle. \tag{92}
$$

Once we have reached this point of the discussion (where we have completed the description of the kinematical Hilbert space of the system), I will summarise the steps we have followed in order to see the parallelism with the strategy adopted in LQG.

1. We have begun by describing the gravitational degrees of freedom using a gauge connection and a densitised triad. In this process, we have selected a fiducial cell adapted to the choice of (compact) $T^3$ topology for the spatial sections and we have selected a gauge with diagonal variables (recall that this is motivated by the fact that it has been proven that the physical results are independent of these choices).
2. We have defined the holonomies of the connection along edges of a certain coordinate length and the fluxes of the densitised triad across rectangular surfaces.
3. We have identified the configuration algebra (which is given by the sums of products of the holonomy matrix elements) with the algebra of almost-periodic functions of the connection variables $c^i$.
4. We have represented each of the exponentials by a ket state. Then, we have defined the space of cylindrical functions as the linear span of these ket states and the kinematical Hilbert space as its completion with respect to a discrete inner product in each fiducial direction.
5. We have represented the classical variables (that is, the holonomy matrix elements and the triad variables $p_i$) by operators acting on the kinematical Hilbert space and we have written their action on the basis provided by the ket states introduced above.
6. Finally, we have argued that a minimum coordinate length should exist in LQC, appealing to the fact that there is a nonzero area gap in LQG. We have discussed how

this minimum coordinate length is implemented according to the improved dynamics prescription. This process results in the action of the fundamental holonomy operators becoming state-dependent. For this reason, we have devised an alternative relabelling of the ket states such that the action of the fundamental operators is simplified.

The next step in the quantisation programme is the representation of the Hamiltonian constraint, which is the only nontrivial constraint in a flat homogeneous cosmology for the introduced diagonal scenario. In particular, we must regularise it classically to express it in terms of the holonomies of the Ashtekar-Barbero connection and then quantise it by choosing a factor ordering prescription. I will devote the next three sections to analysing these two procedures.

## 4.2 FLRW cosmologies

Before that, let us briefly discuss the isotropic limit of Bianchi I cosmologies, that is, the limit in which the three fiducial directions behave in the same manner and, thus, become equivalent. As mentioned in Sec. 4, in this process one reaches a flat FLRW cosmology. For further details on the quantisation of models in LQC, one can consult, e.g., [35, 36, 37].

In the isotropic case (i.e., $p_i = p$ and $c^i = c$ for all $i$), the Ashtekar-Barbero variables reduce to

$$A^i_a = \frac{c}{2\pi}\delta^i_a, \qquad E^a_i = \frac{p}{4\pi^2}\delta^a_i. \tag{93}$$

The only nontrivial Poisson bracket is given by

$$\{c, p\} = \frac{8\pi G\gamma}{3}. \tag{94}$$

Notice the extra factor 1/3 in the Poisson bracket of $c$ and $p$ with respect to its analogue in Bianchi I cosmologies. The identification of the *three* pairs $(c^i, p_i)$ corresponding to each spatial direction is the origin of this difference.

The expressions above are valid if one chooses a Euclidean fiducial metric and a diagonal fiducial triad. This fixes the spatial diffeomorphism and the gauge freedoms, so that the Hamiltonian constraint is again the only constraint whose content is nontrivial. It is known that the LQC model that results from these choices is in fact independent of the fiducial structures [35, 36].

In the next paragraphs, we will follow a procedure that is identical to that already presented in the previous subsection for the case of Bianchi I cosmologies. However, owing to the isotropy of the model we are currently working with, this case is considerably simpler.

Let us introduce holonomies along edges of coordinate length $2\pi\mu$ and triad fluxes through squares formed by these edges. The configuration algebra is then the algebra of almost-periodic functions of the connection variable $c$, which is generated by the holonomy matrix elements

$$\mathcal{N}_\mu(c) = e^{i\mu c/2}. \tag{95}$$

As before, the states $|\mu\rangle$ are the quantum representation of these exponentials. The span of these states defines the analogue of the space of cylindrical functions of the connection variable $\mathrm{Cyl_S} = \mathrm{span}\{|\mu\rangle\}$. The completion of $\mathrm{Cyl_S}$ with respect to the discrete inner product $\langle\mu|\mu'\rangle = \delta_{\mu,\mu'}$ results in the kinematical Hilbert space of a FLRW spacetime, $\mathcal{H}^{\mathrm{kin}}_{\mathrm{grav}}$.

The fundamental operators have a straightforward action on the $|\mu\rangle$-basis. Indeed, these states are eigenstates of the operator $\hat{p}$, and their labels are shifted by $\hat{\mathcal{N}}_\mu$:

$$\hat{p}\,|\mu\rangle = \frac{4\pi\gamma l_p^2}{3}\mu\,|\mu\rangle\,, \tag{96}$$

$$\hat{\mathcal{N}}_{\mu'}\,|\mu\rangle = |\mu+\mu'\rangle\,. \tag{97}$$

We adopt the improved dynamics prescription to determine the coordinate length of the edges of the holonomies. Then, we require that they form squares whose area is equal to the area gap in LQG, $\bar{\mu}^2|p| = \Delta$. From this condition, we recover the minimum coordinate length of the edges of the holonomies

$$\bar{\mu} = \sqrt{\frac{\Delta}{|p|}}. \tag{98}$$

It is easy to realise that this expression reproduces the result we obtained in Bianchi I cosmologies when all the fiducial directions are equivalent. As in the anisotropic case, the fact that $\bar{\mu}$ depends on $p$ results in the fundamental holonomy operators producing state-depend shifts. Once more, we can introduce an affine parameter $v$ to solve this inconvenience. For this, we require that the differential operator corresponding to $i\bar{\mu}c/2$ is $\partial_v$ [36]. This amounts to imposing that

$$i\bar{\mu}c \to \frac{8\pi G\gamma}{3}\bar{\mu}\partial_p = 2\partial_v. \tag{99}$$

Manipulating this equation yields

$$dv = \frac{3}{4\pi l_p^2\gamma}\frac{dp}{\bar{\mu}(p)} = \frac{3}{4\pi l_p^2\gamma\sqrt{\Delta}}\sqrt{|p|}dp = (2\pi G\gamma\sqrt{\Delta})^{-1}\mathrm{sgn}(p)d|p|^{3/2}, \tag{100}$$

which can be easily integrated:

$$v = (2\pi l_p^2\gamma\sqrt{\Delta})^{-1}\mathrm{sgn}(p)|p|^{3/2}, \tag{101}$$

$$p = (2\pi l_p^2\gamma\sqrt{\Delta})^{2/3}\mathrm{sgn}(v)|v|^{2/3}. \tag{102}$$

Notice that, in the light of Eq. (101), $v$ has a very clear physical interpretation: it is an adimensional parameter that is proportional to the physical volume of the Universe. Indeed, taking the isotropic limit of the line element (74), one realises that the volume operator can be defined in this setting as

$$\hat{V} = \widehat{|p|}^{3/2} \tag{103}$$

and, hence,

$$\hat{V}\,|v\rangle = 2\pi\gamma l_p^2\sqrt{\Delta}\,|v|\,|v\rangle = \sqrt{16\sqrt{3}\pi^3\gamma^3}\,l_p^3|v|\,|v\rangle\,. \tag{104}$$

Therefore, $v$ essentially gives the physical volume in units of the Planck volume $l_p^3$ (except for a factor $[16\sqrt{3}\pi^3\gamma^3]^{-1/2} \approx 0.29$, with the value usually taken for the Immirzi parameter).

Finally, if we relabel the states $|\mu\rangle$ using the quantity $v$ instead, we obtain the following simple actions:

$$\hat{p}\,|v\rangle = (2\pi\gamma l_p^2\sqrt{\Delta})^{2/3}\mathrm{sgn}(v)|v|^{2/3}\,|v\rangle\,, \tag{105}$$

$$\hat{\mathcal{N}}_{\bar{\mu}}\,|v\rangle = |v+1\rangle\,. \tag{106}$$

With this we complete the description of the kinematical Hilbert space of FLRW cosmologies. In the next section (Sec. 5), I will present the standard regularisation procedure of the Hamiltonian constraint in flat, homogeneous scenarios.

# 5 The standard regularisation procedure

In this section, we will discuss the first step in the implementation of the quantum Hamiltonian constraint: the regularisation procedure. More precisely, we will discuss how the Hamiltonian constraint is usually regularised in the context of flat, homogeneous LQC. Throughout this thesis, I will refer to this procedure as the *standard* one, in the sense that it is the one which has been extensively used in the community since the foundation of LQC. However, we will see that this regularisation scheme differs from the one followed in LQG in that it is based on a peculiarity of the kind of systems under consideration.

I want to begin by noting that the Hamiltonian constraint is the only nontrivial constraint in homogeneous spacetimes. Indeed, the spatial diffeomorphism constraint is trivially satisfied owing to the spatial homogeneity of the cosmologies we are considering and the gauge freedom has been eliminated once we have chosen a set of diagonal variables.

In LQG, the (gravitational part of the) Hamiltonian constraint $H_{gr}$ is composed of two distinct pieces: the Euclidean part $H_E$ and the Lorentzian part $H_L$. The reason behind this nomenclature is straightforward: its origin lies in the fact that the first piece (that is, the Euclidean one) is the only one that appears in Euclidean gravity. Therefore, the second piece is intimately related to the Lorentzian nature of gravitation.

Explicitly, $H_{gr}(N) = N(H_E + H_L)$, with

$$H_E = \frac{1}{16\pi G}\int d^3x\, e^{-1}\sum_{i,j,k}\epsilon^{ij}{}_k E^a_i E^b_j F^k{}_{ab}\,, \tag{107}$$

$$H_L = -\frac{1+\gamma^2}{8\pi G}\int d^3x\, e^{-1}\sum_{i,j} E^a_i E^b_j K^i_{[a}K^j_{b]}. \tag{108}$$

Here, $e = \sqrt{|\det(E)|} = \sqrt{\mathfrak{h}}$. Recall that the Ashtekar-Barbero connection is defined as the sum of the spin connection and the triadic extrinsic curvature (multiplied by the Immirzi parameter $\gamma$). Therefore, we have classically that $\gamma K^i_a = A^i_a - \Gamma^i_a$.

When the spatial sections are flat, the spin connection $\Gamma^i_a$ vanishes identically and, then, the Ashtekar-Barbero connection reduces to the triadic extrinsic curvature multiplied by the Immirzi parameter. Moreover, for homogeneous cosmologies, the extrinsic curvature is equal at all points of each spatial section (although it may vary under time evolution). This implies that

$$\partial_a A^i_b = \gamma\partial_a K^i_b = 0. \tag{109}$$

Thus, in the case of the symmetry reduced models we are considering (both of which are flat and homogeneous), the curvature tensor of the Ashtekar-Barbero connection can be written as

$$F^k{}_{ab} = \gamma^2\sum_{l,m}\epsilon^k{}_{lm}K^l_{[a}K^m_{b]}. \tag{110}$$

As a result, when contracted with $\epsilon^{ij}{}_k$, $H_L$ turns out to be proportional to $H_E$. By virtue of

Eq. (60),

$$\begin{aligned}
16\pi G\, H_E &= \gamma^2 \int d^3x\, e^{-1} \sum_{i,j,l,m} E^a_i E^b_j \left( \sum_k \epsilon^{ij}{}_k \epsilon^k{}_{lm} \right) K^l_{[a} K^m_{b]} \\
&= \gamma^2 \int d^3x\, e^{-1} \sum_{i,j,l,m} E^a_i E^b_j (\delta^i_l \delta^j_m - \delta^i_m \delta^j_l) K^l_{[a} K^m_{b]} \\
&= \gamma^2 \int d^3x\, e^{-1} \sum_{i,j,l,m} E^a_i E^b_j (2\delta^i_l \delta^j_m) K^l_{[a} K^m_{b]} \\
&= 2\gamma^2 \int d^3x\, e^{-1} \sum_{i,j} E^a_i E^b_j K^i_{[a} K^j_{b]} = -8\pi G \frac{2\gamma^2}{1+\gamma^2} H_L, \\
\Rightarrow H_L &= -\frac{1+\gamma^2}{\gamma^2} H_E \;\square.
\end{aligned} \tag{111}$$

Then, when dealing with flat, homogeneous cosmologies; the gravitational Hamiltonian constraint can be written as being proportional to the Euclidean part alone.

$$H_{gr}(N) = N(H_E + H_L) = N\left(1 - \frac{1+\gamma^2}{\gamma^2}\right) H_E = -\frac{N}{\gamma^2} H_E. \tag{112}$$

Owing to this fact, the most common regularisation method in LQC has consisted in regularising the Euclidean part and employing the identity above. I remark that it is only valid in flat and homogeneous scenarios. Throughout this thesis, I will refer to this process as the ‘standard regularisation procedure.’ In this section, I will sketch how this regularisation scheme is implemented, reproducing the results obtained in the literature.

## 5.1 Standard Hamiltonian in Bianchi I cosmologies

We want to express the Euclidean part of the Hamiltonian constraint in terms of the holonomies of the connection and the densitised triad. In order to achieve this objective, we need to deal with the curvature tensor first. For this, we employ the so-called *Thiemann identities*, which Thiemann devised in the context of LQG. These classical identities usually involve the Poisson brackets of the holonomies with other quantities, as we will see. These identities are inherited by LQC (together with the rest of techniques inspired by LQG) and can be used in particular to regularise the curvature tensor. We will use the following identity, valid in our diagonal model,

$$^{(\mathrm{BI})}F^i{}_{ab} = -2 \sum_{j,k} \mathrm{tr}\left( \frac{h^{\bar\mu}_{\square_{jk}} - \delta_{jk}}{4\pi^2 \bar\mu_j \bar\mu_k} \tau^i \right) \delta^j_a \delta^k_b, \tag{113}$$

where $i \neq j \neq k$. Besides,

$$h^{\bar\mu}_{\square_{jk}} := h^{\bar\mu_j}_j h^{\bar\mu_k}_k (h^{\bar\mu_j}_j)^{-1} (h^{\bar\mu_k}_k)^{-1} \tag{114}$$

is the holonomy along a rectangular circuit whose sides (of coordinate lengths $2\pi\bar\mu_i$ and $2\pi\bar\mu_j$) are oriented along the fiducial directions $i$ and $j$, respectively.

For the sake of a complete illustration of the regularisation procedure, let us do this computation in detail.

The holonomies along an edge of fiducial length $2\pi\bar{\mu}_i \in \mathbb{R}$ oriented along the $i$th fiducial direction is

$$h_i^{\bar{\mu}_i} = \exp(\bar{\mu}_i c^i \tau_i) = \sum_{n=0}^{\infty} (-i)^n \left(\frac{\bar{\mu}_i c^i}{2}\right)^2 \sigma_i^n$$
$$= \sum_{n=0}^{\infty} (-1)^n \bar{x}_i^{2n} \sigma_i^{2n} - i \sum_{m=0}^{\infty} (-1)^m \bar{x}_i^{2m+1} \sigma_i^{2m+1}, \tag{115}$$

where $\bar{x}_i = \bar{\mu}_i c^i/2$. Since $\sigma_i^2 = \mathbb{I}$ (where $\mathbb{I}$ is the $2\times 2$ identity matrix), it follows trivially that, by using the Taylor expansions of the sine and cosine functions,

$$h_i^{\bar{\mu}_i} = \cos\bar{x}_i \mathbb{I} - i\sin\bar{x}_i \sigma_i. \tag{116}$$

Writing this expression in components results in

$$h_i^{\bar{\mu}_i} = \begin{pmatrix} \cos\bar{x}_i - i\sin\bar{x}_i\delta_{i\delta} & -\sin\bar{x}_i(\delta_{i\sigma} + i\delta_{i\theta}) \\ \sin\bar{x}_i(\delta_{i\sigma} - i\delta_{i\theta}) & \cos\bar{x}_i + i\sin\bar{x}_i\delta_{i\delta} \end{pmatrix}. \tag{117}$$

From this, it follows that the determinant of $h_i^{\bar{\mu}_i}$ is given by

$$\det(h_i^{\bar{\mu}_i}) = \cos^2\bar{x}_i + \sin^2\bar{x}_i \sum_{j=\theta,\sigma,\delta} \delta_{ij} = \cos^2\bar{x}_i + \sin^2\bar{x}_i = 1 \quad \forall\, i. \tag{118}$$

In conclusion, the inverse of $h_i^{\bar{\mu}_i}$ is simply its adjoint

$$(h_i^{\bar{\mu}_i})^{-1} = \mathrm{adj}(h_i^{\bar{\mu}_i}) = \begin{pmatrix} \cos\bar{x}_i + i\sin\bar{x}_i\delta_{i\delta} & \sin\bar{x}_i(\delta_{i\sigma} + i\delta_{i\theta}) \\ -\sin\bar{x}_i(\delta_{i\sigma} - i\delta_{i\theta}) & \cos\bar{x}_i - i\sin\bar{x}_i\delta_{i\delta} \end{pmatrix}$$
$$= \cos\bar{x}_i \mathbb{I} + i\sin\bar{x}_i\sigma_i. \tag{119}$$

With these explicit expressions at hand, we are ready to compute the holonomy along a rectangular circuit:

$$h_{\square_{jk}}^{\bar{\mu}} = h_j^{\bar{\mu}_j}[h_k^{\bar{\mu}_k}, (h_j^{\bar{\mu}_j})^{-1}](h_k^{\bar{\mu}_k})^{-1} + h_j^{\bar{\mu}_j}(h_j^{\bar{\mu}_j})^{-1} h_k^{\bar{\mu}_k}(h_k^{\bar{\mu}_k})^{-1},$$
$$h_{\square_{jk}}^{\bar{\mu}} - \mathbb{I} = h_j^{\bar{\mu}_j}[h_k^{\bar{\mu}_k}, (h_j^{\bar{\mu}_j})^{-1}](h_k^{\bar{\mu}_k})^{-1}. \tag{120}$$

Given that the $\cos\bar{x}_i$ in the holonomies appear together with the identity matrix, they will not appear in the commutator. Hence,

$$h_{\square_{jk}}^{\bar{\mu}} - \mathbb{I} = \sin\bar{x}_j \sin\bar{x}_k\, h_j^{\bar{\mu}_j}[\sigma_k, \sigma_j](h_k^{\bar{\mu}_k})^{-1}$$
$$= -2i\sin\bar{x}_j\sin\bar{x}_k \sum_l \epsilon_{jk}{}^l h_j^{\bar{\mu}_j}\sigma_l(h_k^{\bar{\mu}_k})^{-1}. \tag{121}$$

Multiplying this by $\tau^i = -i\sigma^i/2$ and taking the trace yields

$$-\mathrm{tr}\left[(h_{\square_{jk}}^{\bar{\mu}} - \mathbb{I})\tau^i\right] = \sin\bar{x}_j\sin\bar{x}_k \sum_l \epsilon_{jk}{}^l \mathrm{tr}\left[h_j^{\bar{\mu}_j}\sigma_l(h_k^{\bar{\mu}_k})^{-1}\sigma^i\right]. \tag{122}$$

There are three types of terms in this expression: the ones concerning the trace of two, three or four Pauli matrices. Therefore, we will need the following identities:

$$\mathrm{tr}(\sigma_i\sigma_j) = 2\delta_{ij}, \tag{123}$$
$$\mathrm{tr}(\sigma_i\sigma_j\sigma_k) = 2i\epsilon_{ijk}, \tag{124}$$
$$\mathrm{tr}(\sigma_i\sigma_j\sigma_k\sigma_l) = 2(\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{125}$$

Using these, one arrives at

$$ {}^{(\mathrm{BI})}F^i_{ab} = \frac{1}{\pi^2}\frac{\sin\bar{x}_a}{\bar{\mu}_a}\frac{\sin\bar{x}_b}{\bar{\mu}_b}\sum_l \epsilon_{ab}{}^l \left\{\cos\bar{x}_a\cos\bar{x}_b\delta^i_l + \epsilon_{al}{}^i\sin\bar{x}_a\cos\bar{x}_b \right. $$
$$ \left. - \epsilon_{lb}{}^i\cos\bar{x}_a\sin\bar{x}_b + \sin\bar{x}_a\sin\bar{x}_b(\delta_{al}\delta^i_b - \delta_{ab}\delta^i_l + \delta^i_a\delta_{lb})\right\}. \tag{126} $$

Note that the only terms that do not vanish are those where $a$, $b$, and $l$ are different from one another. That means that the last term (the one that comes from the trace of four Pauli matrices) identically vanishes. As a result, we have that the curvature tensor for a Bianchi I cosmology can be written as

$$ \begin{aligned} {}^{(\mathrm{BI})}F^i_{ab} &= \frac{1}{\pi^2}\frac{\sin\bar{x}_a}{\bar{\mu}_a}\frac{\sin\bar{x}_b}{\bar{\mu}_b}\sum_l \epsilon_{ab}{}^l(\cos\bar{x}_a\cos\bar{x}_b\delta^i_l - \epsilon_{la}{}^i\sin\bar{x}_a\cos\bar{x}_b - \epsilon_{lb}{}^i\cos\bar{x}_a\sin\bar{x}_b) \\ &= \frac{1}{4\pi^2}\frac{\sin 2\bar{x}_a}{\bar{\mu}_a}\frac{\sin 2\bar{x}_b}{\bar{\mu}_b}\epsilon_{ab}{}^i + \frac{1}{2\pi^2}\left(\frac{\sin 2\bar{x}_a}{\bar{\mu}_a}\frac{\sin^2\bar{x}_b}{\bar{\mu}_b}\delta^i_a - \frac{\sin^2\bar{x}_a}{\bar{\mu}_a}\frac{\sin 2\bar{x}_b}{\bar{\mu}_b}\delta^i_b\right). \end{aligned} \tag{127} $$

The last two terms will not contribute to the computation of the Euclidean part of the Hamiltonian constraint. It is easy to realise why. In Eq. (107), we see that $H_E$ is proportional to the integral of $\sum_{a,b}\epsilon^{ij}{}_k E^a_i E^b_j\,{}^{(\mathrm{BI})}F^k_{ab}$. Owing to our choice of diagonal variables, this quantity is proportional to $\epsilon^{ij}{}_k\,{}^{(\mathrm{BI})}F^k_{ij}$. Recall that the second and third terms of the Bianchi I curvature tensor (which are proportional to $\delta^k_i$ and $\delta^k_j$, respectively) are symmetric. Therefore, those contributions will vanish owing to the presence of the totally antisymmetric symbol.

We are finally ready to compute the Euclidean part of the Hamiltonian constraint, $H_E^{\mathrm{BI}}$. Owing to the spatial homogeneity of Bianchi I cosmologies, the integration will simply result in the product of the integrand by the volume of the finite fiducial cell, $(2\pi)^3$. Hence,

$$ \begin{aligned} 16\pi G\, H_E^{\mathrm{BI}} &= (2\pi)^3 e^{-1}\sum_{i,j,k}\epsilon^{ij}{}_k\frac{p_i}{4\pi^2}\frac{p_j}{4\pi^2}\,{}^{(\mathrm{BI})}F^k_{ij} \\ &= \frac{e^{-1}}{2\pi}\sum_{i,j}p_ip_j\frac{1}{4\pi^2}\frac{\sin 2\bar{x}_i}{\bar{\mu}_i}\frac{\sin 2\bar{x}_j}{\bar{\mu}_j}\sum_k \epsilon^{ij}{}_k\epsilon_{ij}{}^k \\ &= \frac{e^{-1}}{(2\pi)^3}\sum_{i,j}(\delta^i_i\delta^j_j - \delta^i_j\delta^j_i)\,p_i\frac{\sin 2\bar{x}_i}{\bar{\mu}_i}p_j\frac{\sin 2\bar{x}_j}{\bar{\mu}_j} \\ &= \frac{e^{-1}}{(2\pi)^3}\sum_i p_i\frac{\sin 2\bar{x}_i}{\bar{\mu}_i}\sum_j(1-\delta^i_j)\,p_j\frac{\sin 2\bar{x}_j}{\bar{\mu}_j} \\ &= \frac{e^{-1}}{(2\pi)^3}\sum_i p_i\frac{\sin 2\bar{x}_i}{\bar{\mu}_i}\sum_{j\neq i}p_j\frac{\sin 2\bar{x}_j}{\bar{\mu}_j}. \end{aligned} \tag{128} $$

It only remains to compute the determinant of the densitised triad:

$$ \begin{aligned} \det(E) &= \det\begin{pmatrix} \frac{p_\theta}{(2\pi)^2} & 0 & 0 \\ 0 & \frac{p_\sigma}{(2\pi)^2} & 0 \\ 0 & 0 & \frac{p_\delta}{(2\pi)^2} \end{pmatrix} = \frac{p_\theta p_\sigma p_\delta}{(2\pi)^6}, \\ e &= \sqrt{|\det(E)|} = \frac{\sqrt{|p_\theta p_\sigma p_\delta|}}{(2\pi)^3} = \frac{V}{(2\pi)^3} \Rightarrow \frac{e^{-1}}{(2\pi)^3} = \frac{1}{V}. \end{aligned} \tag{129} $$

Using this result, the Euclidean part of the gravitational Hamiltonian in a Bianchi I cosmology is

$$H_E^{\mathrm{BI}} = \frac{1}{16\pi G}\frac{1}{V}\sum_i p_i \frac{\sin \bar{\mu}_i c^i}{\bar{\mu}_i}\sum_{j\neq i} p_j \frac{\sin \bar{\mu}_j c^j}{\bar{\mu}_j}, \tag{130}$$

where we recall that $\bar{\mu}_i = \sqrt{\Delta|p_i|}/\sqrt{|p_j p_k|}$.

In the standard approach to LQC, the gravitational Hamiltonian is written only in terms of the Euclidean part, as we saw before. This results in the gravitational Hamiltonian being

$$H_{gr}^{\mathrm{BI}}(N) = -\frac{N}{16\pi G\gamma^2}\frac{1}{V}\sum_i p_i \frac{\sin \bar{\mu}_i c^i}{\bar{\mu}_i}\sum_{j\neq i} p_j \frac{\sin \bar{\mu}_j c^j}{\bar{\mu}_j}. \tag{131}$$

## 5.2 Standard Hamiltonian constraint in FLRW cosmologies

In principle, we would have to carry out the same process presented above in an isotropic scenario.

1. Use an appropriate Thiemann identity to express the curvature tensor in terms of the holonomies. This typically involves the computation of a holonomy along a closed circuit (this time, a square one). Indeed,

$$F_{ab}^i = -2\sum_{j,k} \mathrm{tr}\left(\frac{h_{\square_{jk}}^{\bar{\mu}} - \delta_{jk}}{4\pi^2\bar{\mu}^2}\tau^i\right)\delta_a^j\delta_b^k, \tag{132}$$

   which is entirely analogous to the identity we employed in the anisotropic scenario.
2. Obtain the Euclidean part of the Hamiltonian constraint by introducing the result of the previous computation in Eq. (107). For this, we make use of the form of the densitised triad in FLRW cosmologies and of the spatial homogeneity.
3. Lastly, insert the Euclidean piece in Eq. (112) to obtain the standard regularised gravitational Hamiltonian of a flat FLRW cosmology.

Nevertheless, it is immediate to realise that there is no need to go over the whole computation again. Indeed, as I commented above, it is classically true that flat FLRW spacetimes are the isotropic limit of Bianchi I cosmologies. Therefore, it suffices to set $p_i = p$, $c^i = c$ and $\bar{\mu}_i = \bar{\mu}$ for all $i \in \{\theta, \sigma, \delta\}$ in Eq. (130). If we do this, $\sum_i \sum_{j\neq i} \to 6$, given that the six terms in $H_E^{\mathrm{BI}}$ are equal in the isotropic limit. In conclusion[20],

$$H_E = \frac{3}{8\pi G V}\left(\mathrm{sgn}(p)|p|\frac{\sin(\bar{\mu}c)}{\bar{\mu}}\right)\left(\mathrm{sgn}(p)|p|\frac{\sin(\bar{\mu}c)}{\bar{\mu}}\right). \tag{133}$$

I choose to keep this structure explicitly (although there appears a sign function squared) to facilitate the quantum representation of the Hamiltonian constraint according to the MMO prescription in Sec. 7.

Finally, we can obtain the standard gravitational Hamiltonian constraint as before, using that it is proportional to $H_E$ in spatially flat and homogeneous cosmologies:

$$H_{gr} = -\frac{3N}{8\pi G\gamma^2}\frac{1}{V}\left(\mathrm{sgn}(p)|p|\frac{\sin(\bar{\mu}c)}{\bar{\mu}}\right)\left(\mathrm{sgn}(p)|p|\frac{\sin(\bar{\mu}c)}{\bar{\mu}}\right). \tag{134}$$

[20] Notice that I have omitted any reference to the fact that we are considering FLRW cosmologies to simplify the notation.

# 6 The full Hamiltonian constraint

Once we have reviewed the regularisation procedure of the Euclidean part of the Hamiltonian constraint, I will discuss in this section the regularisation of the Lorentzian part (108). Together with the regularised Euclidean part constructed in Sec. 5, this will allow us to write the full Hamiltonian constraint without relying on a peculiarity of the models under consideration (namely, spatial flatness and homogeneity). After carrying out this computation in a Bianchi I cosmology, we will take the isotropic limit to obtain the full gravitational Hamiltonian constraint in an FLRW cosmology, which we will proceed to quantise in Sec. 7.

## 6.1 Lorentzian part in Bianchi I cosmologies

We have seen in Sec. 5 that the Lorentzian part of the Hamiltonian constraint becomes proportional to the Euclidean one in homogeneous scenarios and in absence of spatial curvature. For this reason, the whole Hamiltonian constraint has usually been regularised (and then quantised) as being proportional to $H_E$. Nevertheless, as we will see in this section, the imposition of symmetries and the regularisation scheme do not commute. In other words, the result of regularising the most general Hamiltonian and imposing the symmetries afterwards is not the same as the result presented above (in Eq. (131) for Bianchi I cosmologies or in Eq. (134) for FLRW spacetimes). In this sense, it is interesting to study a regularisation procedure which is closer to the one used in full LQG (where $H_E$ and $H_L$ are regularised in a different manner). This would be enlightening inasmuch as it would give an insight into a cosmological dynamics that actually lies closer to the one in LQG. In Sec. 8, we will compare the effective cosmological dynamics arising from both models.

In the same way as the Euclidean part contains the curvature tensor, the Lorentzian part is proportional to two powers of the triadic extrinsic curvature. Therefore, the regularisation procedure starts from a classical identity that allows us to reexpress $K_a^i$ in terms of holonomies. Indeed, it is based on the following identity:

$$K_a^i = \frac{1}{8\pi G\gamma^3}\{A_a^i, \{H_E, V\}\}. \tag{135}$$

The Poisson bracket of the volume and the regularised Euclidean part for the Bianchi I model can be written as

$$\begin{aligned}\{H_E^{\mathrm{BI}}, V\} &= 8\pi G\gamma \sum_i \frac{\partial H_E^{\mathrm{BI}}}{\partial c^i}\frac{\partial V}{\partial p_i} = 4\pi G\gamma \sum_i \mathrm{sgn}(p_i)\sqrt{\left|\frac{p_j p_k}{p_i}\right|}\frac{\partial H_E^{\mathrm{BI}}}{\partial c^i} \\ &= \frac{\gamma}{2}\sum_i p_i \frac{\sin 2\bar{x}_i}{\bar{\mu}_i}\sum_{j\neq i}\cos 2\bar{x}_j,\end{aligned} \tag{136}$$

where $i \neq j \neq k$. Hence,

$$\begin{aligned}\{A_a^i, \{H_E^{\mathrm{BI}}, V\}\} &= 8\pi G\gamma \sum_k \frac{\partial A_a^i}{\partial c^k}\frac{\partial}{\partial p_k}\{H_E^{\mathrm{BI}}, V\} = 4G\gamma \frac{\partial}{\partial p_i}\{H_E^{\mathrm{BI}}, V\}\,\delta_a^i \\ &= 2G\gamma^2\,\frac{\sin 2\bar{x}_i}{\bar{\mu}_i}\left(\sum_{j\neq i}\cos 2\bar{x}_j\right)\delta_a^i.\end{aligned} \tag{137}$$

From this result, we conclude that the triadic extrinsic curvature can be expressed as

$${}^{(\mathrm{BI})}K_a^i = \frac{1}{8\pi G\gamma^3}\{A_a^i, \{H_E^{\mathrm{BI}}, V\}\} = \frac{1}{4\pi\gamma}\frac{\sin 2\bar{x}_i}{\bar{\mu}_i}\left(\sum_{j\neq i}\cos 2\bar{x}_j\right)\delta_a^i. \tag{138}$$

The Lorentzian part of the gravitational Hamiltonian of a Bianchi I cosmology can be written as

$$H_L^{\mathrm{BI}} = -\frac{1+\gamma^2}{2G}\frac{\pi}{V}\sum_{i,j} p_i p_j \, {}^{(\mathrm{BI})}K^i_{[i} \, {}^{(\mathrm{BI})}K^j_{j]}, \tag{139}$$

where the integral over the finite cell has already been performed. Inserting in this expression the regularised triadic extrinsic curvature of Eq. (138) yields

$$H_L^{\mathrm{BI}} = -\frac{1+\gamma^2}{\gamma^2}\frac{1}{64\pi G}\frac{1}{V}\sum_{i,j} p_i p_j (R^i_i R^j_j - R^i_j R^j_i), \tag{140}$$

where $R^i_j = 4\pi\gamma \, {}^{(\mathrm{BI})}K^i_j$. By virtue of Eq. (138),

$$\begin{aligned}\sum_{i,j} p_i p_j (R^i_i R^j_j - R^i_j R^j_i) = & \left[\sum_i p_i \frac{\sin 2\bar{x}_i}{\bar{\mu}_i}\left(\sum_{k\neq i}\cos 2\bar{x}_k\right)\right]^2 \\ & - \sum_i p_i^2 \frac{\sin^2 2\bar{x}_i}{\bar{\mu}_i^2}\left(\sum_{k\neq i}\cos 2\bar{x}_k\right)^2 \\ = & \sum_i p_i \frac{\sin 2\bar{x}_i}{\bar{\mu}_i}\left(\sum_{k\neq i}\cos \bar{2}x_k\right)\sum_{j\neq i} p_j \frac{\sin 2\bar{x}_j}{\bar{\mu}_j}\left(\sum_{l\neq j}\cos \bar{2}x_l\right).\end{aligned} \tag{141}$$

In conclusion, the regularised Lorentzian part is given by

$$H_L^{\mathrm{BI}} = -\frac{1}{64\pi G}\frac{1+\gamma^2}{\gamma^2}\frac{1}{V}\sum_i p_i \frac{\sin 2\bar{x}_i}{\bar{\mu}_i}\sum_{j\neq i} p_j \frac{\sin 2\bar{x}_j}{\bar{\mu}_j}\sum_{k\neq i}\cos 2\bar{x}_k \sum_{l\neq j}\cos 2\bar{x}_l. \tag{142}$$

Finally, if we combine the Lorentzian part obtained above with the Euclidean part obtained in the previous section, we arrive at the following expression for the gravitational Hamiltonian regularised according to the modified procedure:

$$H_{gr}^{\mathrm{BI}} = \frac{N}{16\pi G V}\sum_i p_i \frac{\sin \bar{\mu}_i c^i}{\bar{\mu}_i}\sum_{j\neq i} p_j \frac{\sin \bar{\mu}_j c^j}{\bar{\mu}_j}\left\{1 - \frac{1+\gamma^2}{4\gamma^2}\sum_{k\neq i}\cos \bar{\mu}_k c^k \sum_{l\neq j}\cos \bar{\mu}_l c^l\right\}. \tag{143}$$

As we will discuss thoroughly in the next section, the motivation for studying Bianchi I cosmologies in this context was the identification of a natural symmetrisation structure which is apparent in anisotropic scenarios. For this reason, it is crucial to emphasise that the gravitational Hamiltonian presented above these lines is of the form

$$\sum_{N=1,2}\left[\sum_i \mathrm{sgn}(p_i) F_i^{(N)}(|p|, c)\sum_{j\neq i}\mathrm{sgn}(p_j) F_j^{(N)}(|p|, c)\right]. \tag{144}$$

For each value of $i$ and $N$, the functions $F_i^{(N)}(|p|, c)$ only depend on the *norm* of the triad variables $|p_l|$ and the three connection variables $c^l$ (with $l = \theta, \sigma, \delta$). Indeed, all the dependence on the signs of the triad variables is factored out and contained in $\mathrm{sgn}(p_i)\,\mathrm{sgn}(p_j)$. Notice that this conclusion is valid both in the standard and in the modified regularisation schemes (i.e., the Lorentzian part has the same sign structure as the Euclidean part).

Owing to the fact that the three spatial directions are in general not equivalent, $\mathrm{sgn}(p_i)$ needs not be equal to $\mathrm{sgn}(p_j)$ if $i \neq j$. Therefore, $\mathrm{sgn}(p_i)\mathrm{sgn}(p_j) \neq 1$. Furthermore, the

Poisson bracket of the sign of the triad variables with the connection variables is nonzero, in general.

Based on these remarks, it seems natural to symmetrise the products of these variables upon quantisation. Additionally, it also seems natural that the isotropic model inherits this symmetrisation prescription, if we wish to regard FLRW cosmologies as the limit of Bianchi I cosmologies where all the spatial directions behave in the same way. This choice of symmetrisation and its preservation for isotropic situations is the cornerstone of the *MMO quantisation prescription*, that I will use to represent the full Hamiltonian constraint in Sec. 7. Other quantisation prescriptions (see, for instance, Ref. [36]) seek to rearrange the commented products to obtain factors quadratic in signs, which would equal the unit in an isotropic scenario.

## 6.2 Lorentzian part in FLRW spacetimes: the isotropic case

If we set $c_i = c$, $p_i = p$, and $\bar{\mu}_i = \bar{\mu}$ for all spatial directions $i$, as we did in Secs. 4.2 and 5.2, the isotropic limit of the Lorentzian part of the Hamiltonian constraint yields

$$H_L = -\frac{3}{8\pi GV}\frac{1+\gamma^2}{4\gamma^2}\left(\mathrm{sgn}(p)|p|\frac{\sin(2\bar{\mu}c)}{\bar{\mu}}\right)\left(\mathrm{sgn}(p)|p|\frac{\sin(2\bar{\mu}c)}{\bar{\mu}}\right). \tag{145}$$

Hence, the gravitational part of the Hamiltonian constraint for a flat FLRW cosmology is, in fact, a difference of squares:

$$\begin{aligned} H_{gr} = \frac{3N}{8\pi GV}\Bigg\{&\left(\mathrm{sgn}(p)|p|\frac{\sin\bar{\mu}c}{\bar{\mu}}\right)\left(\mathrm{sgn}(p)|p|\frac{\sin\bar{\mu}c}{\bar{\mu}}\right) \\ &-\frac{1+\gamma^2}{\gamma^2}\left(\mathrm{sgn}(p)|p|\frac{\sin 2\bar{\mu}c}{2\bar{\mu}}\right)\left(\mathrm{sgn}(p)|p|\frac{\sin 2\bar{\mu}c}{2\bar{\mu}}\right)\Bigg\}. \end{aligned} \tag{146}$$

Once again, I have chosen to keep the sign structure explicitly in spite of the classical nature of the expression.

Notice that, for small $\bar{\mu}$ (or small $\Delta$), this Hamiltonian equals at leading order the standard LQC Hamiltonian constraint. Indeed,

$$H_{gr} \approx -\frac{3N}{8\pi G\gamma^2 V}\left(\mathrm{sgn}(p)|p|\frac{\sin\bar{\mu}c}{\bar{\mu}}\right)\left(\mathrm{sgn}(p)|p|\frac{\sin\bar{\mu}c}{\bar{\mu}}\right) \tag{147}$$

when $\bar{\mu}c \ll 1$. Likewise, as expected, we retrieve the gravitational Hamiltonian constraint of GR for isotropic and homogeneous cosmologies in the (classical) limit $\bar{\mu} \to 0$,

$$\lim_{\bar{\mu}\to 0} H_{gr} = H_{gr}^{\mathrm{GR}} = -\frac{3N}{8\pi G\gamma^2}c^2\sqrt{|p|}. \tag{148}$$

In the light of these observations, we expect to recover the defining aspects and results of standard (classical) cosmology and effective LQC in the limit of small minimum coordinate length.

This remark appears to suggest that the inclusion of the Lorentzian term into the regularisation scheme results in small modifications in the form of higher-order corrections to the standard formalism in LQC. Therefore, at first glance, one may be led to expect no qualitative changes in the dynamics. However, this conclusion is far from being correct. In fact, we will show in Sec. 7 that the number of formal eigensolutions of this modified Hamiltonian seems to be doubled compared to those of the standard gravitational Hamiltonian of LQC.

# 7 The quantum Hamiltonian

The next step in the quantisation programme of LQC is the quantum representation of the gravitational Hamiltonian constraint (146) by an operator that acts on the kinematical Hilbert space of the system. As we noted in Sec. 2, there exist several sources of ambiguity in this process. In other words, there are nonequivalent ways of quantising the system which are *a priori* equally valid. One of these sources is the choice of a quantisation prescription or factor ordering prescription, which becomes relevant when one wishes to represent a classical expression composed by pieces that do not commute quantum mechanically.

In this section, we will quantise the gravitational Hamiltonian constraint derived in the previous sections (in particular, in Secs. 5 and 6) according to the MMO prescription. For this reason, we will begin by summarising the core features of this prescription. Then, we will perform the actual quantisation and compute the action of the gravitational Hamiltonian operator on the basis provided by the eigenstates of the volume operator, $\{|v\rangle\}$. Furthermore, we will analyse the superselection sectors defined by the action of this operator. We will close this section with a discussion of its generalised eigenstates.

## 7.1 The MMO quantisation prescription

In the MMO prescription, one selects a specific symmetric prescription, thereby removing the factor ordering ambiguity in the quantum representation of the gravitational Hamiltonian constraint. The origin of this prescription lies in an exhaustive analysis of the loop quantisation of Bianchi I cosmologies [46, 47], which motivates the fact that Bianchi I cosmologies have been the starting point of this thesis (having been treated in Secs. 4.1, 5.1 and 6.1). In these anisotropic scenarios, the signs of the triad variables (which are the reflection of the orientation of the triad) play a central role. Indeed, due to the fact that the three spatial directions behave differently, the product of two signs of the triad variables is not necessarily equal to one. Consequently, the sign structure becomes apparent in anisotropic scenarios. In this respect, FLRW cosmologies are different: since all three spatial directions are identified, the product of two signs is classically equal to the unit. For this reason, if we wish to regard Bianchi I cosmologies as the immediate anisotropic generalisation of flat FLRW spacetimes, this issue must be accounted for in the quantum representation of the Hamiltonian constraint. The MMO prescription is inspired by this observation.

To summarise, this quantisation prescription is based on two main rules concerning the factor ordering ambiguity:

i) The products of powers of $\widehat{|p|}$ and $\widehat{1/\sqrt{|p|}}$ with holonomies and signs of the triad variables are ordered via an algebraic symmetrisation in the $|p|$-operators. In other words, the powers of $\widehat{|p|}$ and $\widehat{1/\sqrt{|p|}}$ (which are nonnegative operators) are reordered in a symmetric fashion to the left and to the right.

ii) The products of the sign of $p$ with the holonomies $\sin n\bar{\mu}c$ are symmetrised as

$$\sin n\bar{\mu}c\ \mathrm{sgn}(p) \longrightarrow \frac{1}{2}\left\{\widehat{\sin n\bar{\mu}c}\ \widehat{\mathrm{sgn}(p)} + \widehat{\mathrm{sgn}(p)}\ \widehat{\sin n\bar{\mu}c}\right\}, \tag{149}$$

for any integer $n$.

By adopting these rules, it is easy to see that

$$
\begin{aligned}
|p|\mathrm{sgn}(p)\frac{\sin n\bar{\mu}c}{\bar{\mu}} &= \frac{1}{\sqrt{\Delta}}\left[\frac{1}{\sqrt{|p|}}\right]^{-1} |p|\,\mathrm{sgn}(p)\sin n\bar{\mu}c \\
\xrightarrow{\text{i)}} &\frac{1}{\sqrt{\Delta}}\left[\widehat{\frac{1}{\sqrt{|p|}}}\right]^{-1/2}\widehat{\sqrt{|p|}}(\widehat{\mathrm{sgn}(p)}\,\widehat{\sin n\bar{\mu}c})\widehat{\sqrt{|p|}}\left[\widehat{\frac{1}{\sqrt{|p|}}}\right]^{-1/2} \\
\xrightarrow{\text{ii)}} &\frac{1}{2\sqrt{\Delta}}\left[\widehat{\frac{1}{\sqrt{|p|}}}\right]^{-1/2}\widehat{\sqrt{|p|}}\left(\widehat{\sin n\bar{\mu}c}\,\widehat{\mathrm{sgn}(p)}+\widehat{\mathrm{sgn}(p)}\,\widehat{\sin n\bar{\mu}c}\right)\widehat{\sqrt{|p|}}\left[\widehat{\frac{1}{\sqrt{|p|}}}\right]^{-1/2}, \qquad (150)
\end{aligned}
$$

where

$$\widehat{\sin n\bar{\mu}c} = \frac{1}{2i}(\widehat{e^{in\bar{\mu}c}} - \widehat{e^{-in\bar{\mu}c}}) = \frac{1}{2i}\left(\hat{\mathcal{N}}_{2n\bar{\mu}} - \hat{\mathcal{N}}_{-2n\bar{\mu}}\right). \qquad (151)$$

We introduce the convenient notation

$$\hat{\Omega}_{n\bar{\mu}} = \frac{1}{4i\sqrt{\Delta}}\left[\widehat{\frac{1}{\sqrt{|p|}}}\right]^{-1/2}\widehat{\sqrt{|p|}}\left[(\hat{\mathcal{N}}_{n\bar{\mu}} - \hat{\mathcal{N}}_{-n\bar{\mu}})\,,\,\widehat{\mathrm{sgn}(p)}\right]_+\widehat{\sqrt{|p|}}\left[\widehat{\frac{1}{\sqrt{|p|}}}\right]^{-1/2}, \qquad (152)$$

for any label $n \in \mathbb{Z}$. In the previous expression, $[\,\cdot\,,\cdot\,]_+$ denotes the anticommutator, defined by $[A\,,B]_+ = AB + BA$. Then, following the factor ordering rules that characterise the MMO prescription, we arrive at

$$|p|\,\mathrm{sgn}(p)\,\frac{\sin\bar{\mu}c}{\bar{\mu}} \longrightarrow \hat{\Omega}_{2\bar{\mu}}. \qquad (153)$$

As an immediate result, we represent the Euclidean part of the gravitational scalar constraint by the operator

$$\hat{H}_E = \frac{3}{8\pi G}\left[\widehat{\frac{1}{V}}\right]^{1/2}\hat{\Omega}^2_{2\bar{\mu}}\left[\widehat{\frac{1}{V}}\right]^{1/2}. \qquad (154)$$

Notice that the inverse volume operator is ordered via an algebraic symmetrisation because it only contains powers of $\widehat{1/\sqrt{|p|}}$. Indeed,

$$\widehat{\frac{1}{V}} = \left[\widehat{\frac{1}{\sqrt{|p|}}}\right]^3 \qquad (155)$$

and

$$\widehat{\frac{1}{\sqrt{|p|}}} = \frac{3}{4\pi G\gamma\sqrt{\Delta}}\widehat{\mathrm{sgn}(p)}\widehat{\sqrt{|p|}}\left(\hat{\mathcal{N}}_{-\bar{\mu}}\widehat{\sqrt{|p|}}\hat{\mathcal{N}}_{\bar{\mu}} - \hat{\mathcal{N}}_{\bar{\mu}}\widehat{\sqrt{|p|}}\hat{\mathcal{N}}_{-\bar{\mu}}\right), \qquad (156)$$

which is known to be self-adjoint (and nonnegative, as we have already commented) and where $\widehat{\sqrt{|p|}}$ is defined from Eq. (105) in the sense of the spectral theorem [5, 87], i.e.,

$$\widehat{\sqrt{|p|}}\,|v\rangle := (2\pi\gamma l_p^2\sqrt{\Delta})^{1/3}|v|^{1/3}\,|v\rangle\,. \qquad (157)$$

Before proceeding to describe the quantisation of the Lorentzian part, I want to briefly discuss the origin of the definition in Eq. (156). As with the curvature tensor, $\widehat{1/\sqrt{|p|}}$ is defined using a classical Thiemann identity as the starting point. It is straightforward to verify that the following relation holds classically for any $\bar{\mu} \in \mathbb{R}$:

$$\frac{1}{\sqrt{|p|}} = \frac{1}{2\pi G\gamma}\frac{\mathrm{sgn(p)}}{\bar{\mu}}\sum_i \mathrm{tr}\left(\tau^i h_i^{\bar{\mu}}\left\{(h_i^{\bar{\mu}})^{-1}, \sqrt{|p|}\right\}\right). \tag{158}$$

From this identity, Eq. (156) can be derived easily. To do this: i) replace the Poisson bracket by $-i$ times the commutator, ii) recall that $1/\bar{\mu} = \sqrt{|p|}/\sqrt{\Delta}$, and iii) use the fact that the Pauli matrices are traceless. I will skip the detailed calculation for the sake of brevity.

After making this matter clear, we can go back to quantising the Hamiltonian constraint. It is obvious from Eq. (146) that the Lorentzian and Euclidean parts have identical structures and, in fact, they coincide (up to constant multiplicative factors) if $\bar{\mu}$ is replaced by $2\bar{\mu}$. As a result of this similarity, both pieces will be represented by symmetric operators with the same structure.

Then, owing to the observation in the previous paragraph, it is immediate to see that we can represent $H_L$ by the operator [76]

$$\hat{H}_L = -\frac{3}{8\pi G}\frac{1+\gamma^2}{4\gamma^2}\left[\widehat{\frac{1}{V}}\right]^{1/2}\hat{\Omega}^2_{4\bar{\mu}}\left[\widehat{\frac{1}{V}}\right]^{1/2}. \tag{159}$$

In conclusion, in the MMO prescription, the full gravitational Hamiltonian constraint operator is [76]

$$\hat{H}_{gr}(N) = \frac{3N}{8\pi G}\left[\widehat{\frac{1}{V}}\right]^{1/2}\left\{\hat{\Omega}^2_{2\bar{\mu}} - \frac{1+\gamma^2}{4\gamma^2}\hat{\Omega}^2_{4\bar{\mu}}\right\}\left[\widehat{\frac{1}{V}}\right]^{1/2}. \tag{160}$$

## 7.2 Action on the volume eigenbasis

Notice that, in our factor ordering prescription, the Hamiltonian constraint operator has powers of $\widehat{1/\sqrt{|p|}}$ both to the left and to the right[21]. Therefore, when the Hamiltonian constraint acts on any given state, the operator $\widehat{1/\sqrt{|p|}}$ (or, rather, a power thereof) is the first and the last to act on the state. Using the definitions in Eqs. (97), (156) and (157); let us compute its action on a generic volume eigenstate $|v\rangle$:

$$\begin{aligned}\widehat{\frac{1}{\sqrt{|p|}}}\,|v\rangle &= \frac{3}{4\pi G\gamma\sqrt{\Delta}}\widehat{\mathrm{sgn}(p)}\widehat{\sqrt{|p|}}\left(\hat{\mathcal{N}}_{-\bar{\mu}}\widehat{\sqrt{|p|}}\,|v+1\rangle - \hat{\mathcal{N}}_{\bar{\mu}}\widehat{\sqrt{|p|}}\,|v-1\rangle\right)\\ &= \frac{3}{2(2\pi G\gamma\sqrt{\Delta})^{2/3}}\left(|v+1|^{1/3} - |v-1|^{1/3}\right)\widehat{\mathrm{sgn}(p)}\widehat{\sqrt{|p|}}\,|v\rangle\\ &= \frac{3}{2(2\pi G\gamma\sqrt{\Delta})^{1/3}}|v|^{1/3}\left||v+1|^{1/3} - |v-1|^{1/3}\right|\,|v\rangle\,, \end{aligned} \tag{161}$$

which follows from the fact that $\mathrm{sgn}(v) = \mathrm{sgn}\left(|v+1|^{1/3} - |v-1|^{1/3}\right)$, as can be verified easily.

From the action computed above, we realise that the operator (161) is diagonal in the $|v\rangle$-basis and, therefore, it indeed commutes with $\hat{v}$. Moreover, we see that the eigenstate

[21] Recall that the inverse volume operator is defined as the cube of $\widehat{1/\sqrt{|p|}}$. See Eq. (155).

of vanishing volume $|v=0\rangle$ (that is, the quantum analogue of the classical singularity) is *annihilated*, and that it provides the entire kernel of the introduced operator. Furthermore, given that its action is diagonal, the orthogonal complement of $|v=0\rangle$ (hereafter referred to as $\tilde{\mathcal{H}}^{\text{kin}}_{\text{grav}}$) is left invariant. Together with the fact that the inverse volume operator is at the left and right ends of $\hat{H}_{gr}$, this means that we can restrict the quantum constraint to $\tilde{\mathcal{H}}^{\text{kin}}_{\text{grav}}$ in a well-defined manner. Notice that we can (and will) do so because we are interested in finding nontrivial solutions of the Hamiltonian constraint. Therefore, as a result of the factor ordering that characterises the MMO prescription, the quantum analogue of the singular state *decouples* and we can search for nontrivial physical solutions in its orthogonal complement[22]. It is in this sense that one often says that the classical singularity is cured already at the kinematical level in the MMO prescription[23]. However, the singularity resolution is something even stronger: the quantum dynamics of any semiclassical universe is found to be nonsingular (in the sense that no physical observable diverges in the region where the classical singularity is found). Although I will not perform the whole numerical simulation owing to the lack of space (the numerical results in standard LQC can be found in Refs. [35] and [36]), we will see how the singularity no longer occurs in the effective dynamics approach in Sec. 8.

After the removal of the kernel of the inverse volume operator, we can define a densitised version of the constraint, $\hat{\mathscr{H}}_{gr}$. The experience accumulated in the study of other cosmological settings tells us that the physical states are, in general, not renormalisable in the kinematical Hilbert space (this is due to the fact that the vanishing eigenvalue of the constraint operator belongs to the continuous spectrum). Therefore, we consider a larger space instead. There exists a choice that is natural in what concerns the gravitational part of the system: the completion of the algebraic dual of $\widetilde{\text{Cyl}}_{\text{S}}$ [37]. The next step is finding a one-to-one correspondence between any $\langle\phi|$ annihilated by the adjoint of $\hat{H}_{gr}$ and the corresponding $\langle\phi'| = \langle\phi|\,[\widehat{1/V}]^{1/2}$, which is annihilated by the adjoint of the densitised constraint

$$\hat{\mathscr{H}}_{gr}(N) = \frac{3N}{8\pi G}\left\{\hat{\Omega}^2_{2\bar{\mu}} - \frac{1+\gamma^2}{4\gamma^2}\hat{\Omega}^2_{4\bar{\mu}}\right\}. \tag{162}$$

Henceforth, when I say ‘Hamiltonian constraint’ or simply ‘Hamiltonian’, I will be referring to this densitised operator in all cases. For this reason, I omit any additional specifications in the following.

In the light of the expression of the Hamiltonian, the computation of its action on any given state $|v\rangle$ is determined once we compute the action of the operators $\hat{\Omega}^2_{n\bar{\mu}}$ for $n=2,4$ (which encode the functional form of the Euclidean and Lorentzian parts, respectively). Some definitions facilitate enormously such computation:

$$g(v) = \begin{cases} 0 & \text{if } v=0, \\ \left|\left|1+\dfrac{1}{v}\right|^{1/3} - \left|1-\dfrac{1}{v}\right|^{1/3}\right|^{-1/2} & \text{if } v\neq 0, \end{cases} \tag{163}$$

$$s^{(n)}_{\pm}(v) = \text{sgn}(v) + \text{sgn}(v\pm n), \tag{164}$$

$$f^{(n)}_{\pm}(v) = \frac{\pi G\gamma}{3} g(v) s^{(n)}_{\pm}(v) g(v\pm n). \tag{165}$$

[22]Note that $\tilde{\mathcal{H}}^{\text{kin}}_{\text{grav}}$ is merely the completion of $\widetilde{\text{Cyl}}_{\text{S}} = \text{span}\{|v\rangle\,,\, v\neq 0\}$ with respect to the discrete inner product $\langle v|v'\rangle = \delta_{v,v'}$.

[23] We are assuming that the inclusion of a matter contribution to the constraint does not alter this conclusion.

We notice that $f_{\pm}^{(n)}(v \mp n) = f_{\mp}^{(n)}(v)$.

Let us begin by obtaining the action of $\hat{\Omega}_{n\bar{\mu}}$ on an arbitrary volume eigenstate. Using Eq. (152) and the functions defined above yields

$$\hat{\Omega}_{n\bar{\mu}} \left| v \right\rangle = -i \left[ f_{+}^{(n)}(v) \left| v+n \right\rangle - f_{-}^{(n)}(v) \left| v-n \right\rangle \right]. \tag{166}$$

The action of $\hat{\Omega}^2_{n\bar{\mu}}$ follows trivially:

$$\begin{aligned} \hat{\Omega}^2_{n\bar{\mu}} \left| v \right\rangle = &- f_{+}^{(n)}(v) f_{+}^{(n)}(v+n) \left| v+2n \right\rangle \\ &+ \left\{ \left[ f_{+}^{(n)}(v) \right]^2 + \left[ f_{-}^{(n)}(v) \right]^2 \right\} \left| v \right\rangle - f_{-}^{(n)}(v) f_{-}^{(n)}(v-n) \left| v-2n \right\rangle. \end{aligned} \tag{167}$$

Considering that the volume eigenstates provide an orthonormal basis of the kinematical Hilbert space $\tilde{\mathcal{H}}^{\text{kin}}_{\text{grav}}$, the action of the Hamiltonian constraint is completely characterised by the equation above.

Particularising for $n = 2$, we obtain the action of the Euclidean part of the Hamiltonian (up to constant multiplicative factors). We realise that it either preserves the label of the state it acts upon or produces shifts of four units (towards either smaller or larger volumes). A similar behaviour is displayed by the Lorentzian part ($n = 4$). However, instead of shifts of four units, it gives rise to shifts of *eight* units. In conclusion, owing to the fact that the volume representation is discrete, the action of the full Hamiltonian constraint on a certain volume eigenstate $\left| v \right\rangle$ can be cast as an equation in finite differences that relates five eigenstates: $\left| v \right\rangle$, $\left| v \pm 4 \right\rangle$ and $\left| v \pm 8 \right\rangle$.

Notice that this conclusion is in contrast with that found using the standard regularisation procedure. Indeed, since only the Euclidean part intervenes in such a case, the action of the Hamiltonian constraint results in an equation in finite differences that relates a total of *three* volume eigenstates instead. This difference will have important consequences, as we will see later on.

## 7.3 Superselection sectors

In standard LQC, we obtain that certain Hilbert subspaces are invariant under the action of the Hamiltonian constraint (including the matter term) and of the relevant physical observables (see Refs. [34, 35, 36, 88, 89, 90]), which results in the existence of superselection sectors. The details about these superselection sectors partially depend on the prescription used to represent the Hamiltonian constraint. For instance, the superselection sectors found with the prescription of Ref. [36] are the Hilbert spaces with support on (discrete) lattices of step four. In the case of the MMO prescription, the superselection sectors turn out to be simpler. The choice of factor ordering that characterises the prescription results in the decoupling of the positive and negative semilattices [37]. In other words, no eigenstate belonging to the positive semilattice (that is, $v > 0$) will be sent to the negative one by the action of the Hamiltonian constraint and *vice versa*. Therefore, the Hamiltonian superselects dicrete *semi*lattices of step four, as opposed to entire lattices. This feature is usually regarded as one of the strengths of the prescription we are discussing in this thesis. This subsection will be devoted to verifying whether this nice feature is still present when the Hamiltonian is regularised according to the modified procedure.

At least, the superselection sectors are ensured not to be more complicated than the ones appearing in standard isotropic LQC: discrete lattices of step four *are* left invariant under the action of $\hat{\mathscr{H}}_{gr}$. This is due to the fact that the Lorentzian term has the same structure as the Euclidean one but it produces shifts twice as large, leading to eigenstates which still belong to the same lattice (two points away instead of one, though).

In fact, we can see that simpler Hilbert spaces are superselected. This is a result of some very special properties of the coefficients $f_{\pm}^{(n)}(v)f_{\pm}^{(n)}(v \pm n)$. In the light of the definition in Eq. (165), it can be shown that

$$\begin{aligned} f_{+}^{(n)}(v)f_{+}^{(n)}(v+n) &= 0 \quad \forall\, v \in [-2n, 0), \\ f_{-}^{(n)}(v)f_{-}^{(n)}(v-n) &= 0 \quad \forall\, v \in (0, 2n]. \end{aligned} \tag{168}$$

These identities hold because the combination $f_{\pm}^{(n)}(v)f_{\pm}^{(n)}(v \pm n)$ is trivially proportional to $s_{\pm}^{(n)}(v)s_{\pm}^{(n)}(v \pm n)$, which vanishes when $v$ belongs to the intervals detailed above.

This result shows that the discrete lattices of step four actually *split* into two separate semilattices under the action of $\hat{\mathscr{H}}_{gr}$. This implies that the decoupling of the positive and negative semilattices takes place in this setting as well. Hence, the superselection sectors are Hilbert spaces with support on the positive or negative discrete semilattices. In a more precise fashion, the superselection sectors (to which we will refer as $\mathcal{H}_{\varepsilon}^{\pm}$) are given by the (Cauchy) completion with respect to the discrete inner product $\langle v|v'\rangle = \delta_{v,v'}$ of $\mathrm{Cyl}_{\varepsilon}^{\pm} = \mathrm{span}\{|v\rangle\,,\, v \in \mathcal{L}_{\varepsilon}^{\pm}\}$, $\mathcal{L}_{\varepsilon}^{\pm}$ being semilattices of step four:

$$\mathcal{L}_{\varepsilon}^{\pm} = \{v = \pm(\varepsilon + 4n),\, \varepsilon \in (0, 4],\, n \in \mathbb{N}\}. \tag{169}$$

Note that we can write the nonseparable kinematical Hilbert space $\tilde{\mathcal{H}}_{\mathrm{grav}}^{\mathrm{kin}}$ as the direct sum of separable subspaces $\tilde{\mathcal{H}}_{\mathrm{grav}}^{\mathrm{kin}} = \oplus_{\varepsilon}(\mathcal{H}_{\varepsilon}^{+} \oplus \mathcal{H}_{\varepsilon}^{-})$.

The fact that the superselection sectors are Hilbert spaces supported on semilattices is a direct consequence of the properties in Eq. (168). In turn, these identities hold (as I have commented above) owing to the precise combination of signs of the triad variable, which results from the special symmetrisation of the Hamiltonian constraint that is dictated by the MMO prescription. Therefore, we conclude that the simplicity of the superselection sectors $\mathcal{H}_{\varepsilon}^{\pm}$ is originated from the specific way in which we have treated the orientation of the triad: it is a key feature of the prescription, which is *de facto* robust under the modification of the regularisation procedure that we have considered in this work.

## 7.4 Generalised eigenfunctions

In standard loop quantum FLRW cosmologies, the Hamiltonian constraint operator has been shown to be essentially self-adjoint [89, 37] or, at least, to admit self-adjoint extensions. Furthermore, its continuous spectrum is generally nonempty. In the case of modified LQC, it has been shown very recently that the gravitational part of the modified Hamiltonian constraint admits a family of self-adjoint extensions [69]. However, this has been shown by restricting the analysis to the semilattice starting at $\varepsilon = 4$ and decoupling by hand the eigenstate of vanishing eigenvolume[24]. The other semilattices lead to some technical difficulties in the proof but the same result is expected to hold for them.

Bearing this caveat in mind, let us concentrate on the continuous part of the spectrum of the Hamiltonian constraint and study the form of its generalised eigenstates. Let

$$|e_{\lambda}^{\varepsilon}\rangle = \sum_{v' \in \mathcal{L}_{\varepsilon}^{\pm}} e_{\lambda}^{\varepsilon}(v')\,|v'\rangle\,, \qquad \left[\hat{\Omega}_{2\bar{\mu}}^{2} - \frac{1+\gamma^2}{4\gamma^2}\hat{\Omega}_{4\bar{\mu}}^{2}\right]|e_{\lambda}^{\varepsilon}\rangle = \lambda\,|e_{\lambda}^{\varepsilon}\rangle\,, \tag{170}$$

[24] This is needed because the authors use the prescription of Ref. [36], where the singular state does not decouple naturally at the kinematical level.

be a generalised eigenstate corresponding to the eigenvalue $3N\lambda/8\pi G$. It should be noted that $\varepsilon$ is fixed in the previous expression. Given that we can restrict our analysis to any superselection sector without loss of generality, I choose the one with support on the positive semilattice $\mathcal{L}_\varepsilon^+$ (with $\varepsilon$ fixed).

Taking the inner product of $\hat{\mathscr{H}}_{gr}\,|e_\lambda^\varepsilon\rangle$ with $\langle v|$, we can find an equation relating the values of the generalised eigenfunction $e_\lambda^\epsilon$ at five points in the semilattice. Notably, when the Hamiltonian constraint acts upon the volume eigenstate which is the closest to the origin (that is, the one with eigenvolume $v = \varepsilon$), the relation that we are discussing does not involve five values but only *three* —namely; $e_\lambda^\varepsilon(\varepsilon)$, $e_\lambda^\varepsilon(\varepsilon{+}4)$ and $e_\lambda^\varepsilon(\varepsilon{+}8)$. This is a direct consequence of the properties (168) examined above: the two other values that would in principle appear in the relation —$e_\lambda^\varepsilon(\varepsilon - 4)$ and $e_\lambda^\varepsilon(\varepsilon - 8)$— lie in the negative semilattice[25] and, therefore, they do not contribute (their respective coefficients vanish). As a conclusion, the value of the eigenfunction at the third point of the semilattice is uniquely determined once we give $e_\lambda^\varepsilon(\varepsilon)$ and $e_\lambda^\varepsilon(\varepsilon+4)$, as long as $|e_\lambda^\varepsilon\rangle$ is required to be a generalised eigenstate of the quantum Hamiltonian.

The picture changes when we displace the action of the Hamiltonian to the next point in our semilattice, that is, $v = \varepsilon + 4$. This time, the relation will involve four values (indeed, $v - 4 = \varepsilon > 0$ lies in the positive semilattice now). As a result, we will obtain a (linear) relation between $e_\lambda^\varepsilon(\varepsilon)$, $e_\lambda^\varepsilon(\varepsilon + 4)$, $e_\lambda^\varepsilon(\varepsilon + 8)$, and $e_\lambda^\varepsilon(\varepsilon + 12)$. Recall that three of these are already fixed (the first two specified by us and the third determined by the fact that $|e_\lambda^\varepsilon\rangle$ is an eigenstate of $\hat{\mathscr{H}}_{gr}$). Therefore, the fourth is fixed as well by this relation. Notice that we can extend this reasoning *ad infinitum.* This argument makes us conclude that the values of the generalised eigenfunction $e_\lambda^\varepsilon$ at *all* points in the semilattice are fixed once we give the two first values. Therefore, only *two* pieces of data are undetermined, in principle.

It is important to emphasise that this result contrasts with the one found in standard LQC with the MMO quantisation prescription. When the standard renormalisation procedure is considered, the densitised Hamiltonian constraint only contains the operator $\hat{\Omega}_{2\bar{\mu}}^2$, which relates three values of the generalised eigenfunction. Then, when we particularise for $v = \varepsilon$, $\tilde{e}_\lambda^\varepsilon(\varepsilon - 4)$ does not appear in the relation and only the values at *two* points are involved[26]. As a result, fixing one of them freely suffices to determine completely the generalised eigenfunction (this can be seen following a reasoning entirely equivalent to the one discussed in the previous paragraph). Therefore, instead of two, there is *one* piece of data available in the construction, which can be absorbed up to a phase by appropriately normalising the generalised eigenfunction [37].

In the light of this comparison between our results and the standard results in the polymeric quantisation of flat FLRW spacetimes, we are in the position of concluding what is the dynamical effect of considering a modification of the Hamiltonian constraint: the number of formal solutions is increased. Owing to this key difference, we argue in Ref. [76] that the inclusion of the Lorentzian term results in more than a simple modification of the details of the solutions found using the standard approach: new formal eigensolutions emerge from our modified regularisation procedure. This is the reflection of the appearance of de Sitter branches of Planckian curvature in the Dapor-Liegener model, analysed in Refs. [67, 73, 70, 71, 91], which alter the self-adjointness properties of the Hamiltonian operator [69].

To close this analysis of the quantum Hamiltonian, I will derive a closed expression that allows us to compute the eigenfunction at any point in the semilattice once its values at the

[25] Recall that $\varepsilon \leq 4$ and $|v = 0\rangle \notin \tilde{\mathcal{H}}^{\text{kin}}$.

[26] By $\tilde{e}_\lambda^\varepsilon(v) := \langle v|\tilde{e}_\lambda^\varepsilon\rangle$ I refer to the eigenfunction associated with a generalised eigenstate of $\hat{\Omega}_{2\bar{\mu}}^2$, $|\tilde{e}_\lambda^\varepsilon\rangle$.

two first points are given. By reason of the size of such an expression, it is convenient to define the following functions,

$$F^0_\lambda(v) = \frac{4\gamma^2}{1+\gamma^2}\frac{\lambda - \left\{\left[f^{(2)}_+(v)\right]^2 + \left[f^{(2)}_-(v)\right]^2\right\}}{f^{(4)}_-(v+8)f^{(4)}_-(v+4)} + \frac{\left[f^{(4)}_+(v)\right]^2 + \left[f^{(4)}_-(v)\right]^2}{f^{(4)}_-(v+8)f^{(4)}_-(v+4)}, \tag{171}$$

$$F^{\pm 4}(v) = \frac{4\gamma^2}{1+\gamma^2}\frac{f^{(2)}_\mp(v\pm 4)f^{(2)}_\mp(v\pm 2)}{f^{(4)}_-(v+8)f^{(4)}_-(v+4)}, \tag{172}$$

$$F^{-8}(v) = -\frac{f^{(4)}_+(v-8)f^{(4)}_+(v-4)}{f^{(4)}_-(v+8)f^{(4)}_-(v+4)}. \tag{173}$$

These definitions are not arbitrary. If we write down explicitly the generalised eigenvalue equation of the densitised Hamiltonian constraint (leaving out the constant prefactors), project it on $|v\rangle$, and divide the whole equation by the coefficient of $e^\varepsilon_\lambda(v+8)$; the result is

$$e^\varepsilon_\lambda(v+8) = F^{+4}(v)e^\varepsilon_\lambda(v+4) + F^0_\lambda(v)e^\varepsilon_\lambda(v) + F^{-4}(v)e^\varepsilon_\lambda(v-4) + F^{-8}(v)e^\varepsilon_\lambda(v-8). \tag{174}$$

In terms of the functions (171)-(173) that we just defined, we can write the value of a generalised eigenfunction at any point of the semilattice $\mathcal{L}^+_\varepsilon$ as[27]

$$\begin{aligned} e^\varepsilon_\lambda(\varepsilon+4n) = \sum_{m=0,1}\sum_{O(m\to n)}\Bigg\{&\prod_{\{r_m\}}F^{+4}[\varepsilon+4(r_m-1)]\prod_{\{s\}}F^0_\lambda[\varepsilon+4s] \\ &\times\prod_{\{t\}}F^{-4}[\varepsilon+4(t+1)]\prod_{\{u\}}F^{-8}[\varepsilon+4(u+2)]\Bigg\}\, e^\varepsilon_\lambda(\varepsilon+4m). \end{aligned} \tag{175}$$

In the above expression, $O(p\to q)$ is the set of paths connecting two points $p$ and $q$ on a semilattice of step one that contain jumps of one, two, three, or four units. Such paths are understood as sets of intermediate points between $p$ and $q$. Let $\{r\}$, $\{s\}$, $\{t\}$, and $\{u\}$ be the subsets of these intermediate points such that, in a given path, they are followed by jumps of one unit, two units, three units, and four units, respectively.

For clarity, let us write down explicitly a simple example. Consider the case where $p=0$ and $q=3$. There is a total of four possible paths if we allow jumps of one, two, three, and four units: i) a jump of three units directly from 0 to 3; ii) a jump of two units from 0 to 2 and, then, a jump of one unit from 2 to 3; iii) a jump of one unit from 0 to 1 followed by a jump of two units from 1 to 3; and iv) three consecutive jumps of one unit. Once we have identified all the possible paths connecting $p$ and $q$, we can write down the sets $\{r\}$, $\{s\}$, $\{t\}$, and $\{u\}$ for each of them. Given that no jump of four units can be performed in the example under consideration, $\{u\}$ is the empty set for the four paths. The remaining sets are detailed below.

i) $\{r\}=\emptyset$, $\{s\}=\emptyset$, and $\{t\}=\{0\}$ (this path contains a single jump of three units starting from the point 0).
ii) $\{r\}=\{2\}$, $\{s\}=\{0\}$, and $\{t\}=\emptyset$ (there is a jump of two units starting from 0 and, then, a jump of one unit starting from the target of the previous jump, i.e., from the point 2).

[27]A similar expression can be found for case of the superselection sectors with support on the negative semilattices.

iii) $\{r\} = \{0\}$, $\{s\} = \{1\}$, and $\{t\} = \emptyset$.
iv) $\{r\} = \{0, 1, 2\}$, $\{s\} = \emptyset$ and, $\{t\} = \emptyset$.

We note that there is an important difference in Eq. (175) as far as $\{r\}$ is concerned. Indeed, we must distinguish the case of the paths starting at 0 (i.e., $\{r_0\}$) from the case of the paths that start at 1 (i.e., $\{r_1\}$). In fact, the point 0 cannot belong to $\{r_0\}$, whereas 1 may reside in $\{r_1\}$. The reason why is straightforward: if 0 did belong to $\{r_0\}$, it would imply that there exists a path connecting the integers 0 and 1. Then, substituting $n = 1$ in Eq. (175), we would obtain that the value of the eigenfunction at $\varepsilon + 4$ would directly depend on the value at $\varepsilon$:

$$e_\lambda^\varepsilon(\varepsilon + 4) = F^{+4}(\varepsilon - 4) e_\lambda^\varepsilon(\varepsilon). \tag{176}$$

This would mean that the number of pieces of data that are available to us is reduced back to one. However, this conclusion is in contradiction with the argument above, which proves that $0 \notin \{r_0\}$.

Being mindful of this peculiarity, the closed expression (175) allows us to analytically obtain the values of the generalised eigenfunction corresponding to any given eigenvalue at an arbitrary (finite) point of the semilattice under consideration (depending on the superselection sector to which we restrict our study). In practice, this can be achieved by identifying all the possible paths that link the integers 0 and 1 with other integers. The fact that we can compute the gravitational generalised eigenfunctions exactly is an especially attractive feature of the MMO prescription: it can be done in standard LQC and we have shown that it is still possible when the Hamiltonian is modified in the manner we have been discussing. In this respect, our results are in sharp contrast with the options existing when other prescriptions are chosen. In Ref. [36], where the other predominant prescription is employed, the gravitational eigenfunctions were obtained in an iterative way and computed numerically[28].

[28] Moreover, the authors of this work considered the standard regularisation procedure, which implies that our results are more potent even when considering a more complicated gravitational Hamiltonian.

# 8 Effective cosmological dynamics

In this final section, we will compare the different effective cosmological dynamics arising from classical GR, standard LQC, and modified LQC (mLQC). Although the effective dynamics of these models has been discussed to some extent in several references, I will essentially reproduce some of the results from Ref. [70]. To achieve this purpose, I will compute the time evolution of certain physical quantities (the volume, the energy density, and the Hubble parameter) using the *effective* Hamiltonian as the generator of the evolution. In this context, by effective Hamiltonian I refer to the result of substituting each operator by its classical counterpart (in terms of holonomies and densitised triads) in the quantum Hamiltonian. Once the effective equations of motion are explicitly obtained for each case, I will integrate them numerically with the help of Mathematica. This will hopefully provide a clearer visualisation of how the physical cosmological picture is modified with respect to the one in classical GR, in particular as far as the resolution of the Big Bang singularity is concerned[29].

I would like to begin by writing down explicitly the effective Euclidean and Lorentzian parts of the Hamiltonian. For this purpose, it suffices to take the expressions of Eqs. (133) and (145):

$$H_E^{\text{eff}} = \frac{3V}{8\pi G\lambda^2}\sin^2(\lambda b), \tag{177}$$

$$H_L^{\text{eff}} = -\frac{3V}{8\pi G\lambda^2}\frac{1+\gamma^2}{4\gamma^2}\sin^2(2\lambda b), \tag{178}$$

where $b = c/|p|^{1/2}$ (recall as well that the physical volume of the Universe is given by $V = |p|^{3/2}$). We introduce here the notation $\lambda := \sqrt{\Delta}$ for convenience. From the definition of the variable $b$, we obtain

$$\{b, V\} = \frac{8\pi G\gamma}{3}\frac{\partial b}{\partial c}\frac{dV}{dp} = \frac{8\pi G\gamma}{3}|p|^{-1/2}\frac{d|p|^{3/2}}{dp} = 4\pi G\gamma. \tag{179}$$

Since they provide a pair of canonical variables, we will use $b$ and $V$ to describe the classical phase space. With these ingredients we are ready to construct the effective gravitational Hamiltonian, both in the standard and in the modified cases.

Nevertheless, this is not yet enough. Since an empty FLRW cosmology has trivial dynamics, we will consider an extra term in the Hamiltonian coming from the matter content. For this purpose, we select the simplest matter content that yields a nontrivial evolution: a massless scalar field, $\phi$. The corresponding Hamiltonian is given by [70]

$$H_{\text{matter}} = \frac{\pi_\phi^2}{2V}, \tag{180}$$

where $\pi_\phi$ is the canonical momentum associated with $\phi$, and $\{\phi, \pi_\phi\} = 1$. At this point, we can write down the effective Hamiltonian $H_{gr}^{\text{eff}} + H_{\text{matter}}$ for each case (GR, LQC, and mLQC) and proceed to the computation of the effective equations of motion. It should be noted that the only difference between each of the cases lies in the gravitational sector. For this reason,

[29]Notice that the relevance of this discussion rests on two assumptions. The first of them is the existence of physical states with a suitable semiclassical behaviour at large volumes. The second one has to do with the effective dynamics being a good approximation to the underlying fully quantum dynamics. The latter is supported by extensive numerical simulations in the past decades (see, for instance, Refs. [35, 36]).

the equations of motion of the matter sector are common to all of them. Computing the time evolution following the method discussed in Sec. 2 results in

$$\dot{\pi}_\phi = \{\pi_\phi, H^{\text{eff}}\} = -\frac{\partial H^{\text{eff}}}{\partial \phi} = -\frac{\partial H_{\text{matter}}}{\partial \phi} = 0 \Rightarrow \pi_\phi = \pi_\phi^0, \tag{181}$$

$$\dot{\phi} = \{\phi, H^{\text{eff}}\} = \frac{\partial H^{\text{eff}}}{\partial \pi_\phi} = \frac{\partial H_{\text{matter}}}{\partial \pi_\phi} = \frac{\pi_\phi^0}{V}, \tag{182}$$

where $\pi_\phi^0$ is a constant that labels different solutions and $\dot{x}$ represents the derivative of a dynamical variable $x$ with respect to the cosmic time $t$.

## 8.1 Effective equations of motion in modified LQC

The effective Hamiltonian constraint (whose gravitational contribution has been regularised according to the modified scheme) can be written as

$$H_{\text{mLQC}}^{\text{eff}} = \frac{3V}{8\pi G\lambda^2}\left[\sin^2(\lambda b) - \frac{1+\gamma^2}{4\gamma^2}\sin^2(2\lambda b)\right] + \frac{(\pi_\phi^0)^2}{2V}. \tag{183}$$

The effective equations of motion can be obtained in a straightforward manner. Let us begin by computing the time evolution of the physical volume:

$$\begin{aligned}
\dot{V} = \{V, H_{\text{mLQC}}^{\text{eff}}\} &= -4\pi G\gamma \frac{\partial H_{\text{mLQC}}^{\text{eff}}}{\partial b} \\
&= -4\pi G\gamma \frac{3V}{8\pi G\lambda^2}\left[\lambda\sin(2\lambda b) - \frac{1+\gamma^2}{\gamma^2}\lambda\sin(2\lambda b)\cos(2\lambda b)\right] \\
&= \frac{3V}{2\gamma\lambda}\sin(2\lambda b)\left[(1+\gamma^2)\cos(2\lambda b) - \gamma^2\right].
\end{aligned} \tag{184}$$

The effective equation of motion associated with $b$ is given by

$$\begin{aligned}
\dot{b} = \{b, H_{\text{mLQC}}^{\text{eff}}\} &= 4\pi G\gamma \frac{\partial H_{\text{mLQC}}^{\text{eff}}}{\partial V} \\
&= 4\pi G\gamma \frac{3}{8\pi G\lambda^2}\left[\sin^2(\lambda b) - \frac{1+\gamma^2}{4\gamma^2}\sin^2(2\lambda b)\right] - 4\pi G\gamma \frac{(\pi_\phi^0)^2}{2V^2} \\
&= \frac{3}{2\gamma\lambda^2}\sin^2(\lambda b)\left[\gamma^2 - (1+\gamma^2)\cos^2(\lambda b)\right] - 2\pi G\gamma\left(\frac{\pi_\phi^0}{V}\right)^2 \\
&= \frac{3}{2\gamma\lambda^2}\sin^2(\lambda b)\left[\gamma^2\sin^2(\lambda b) - \cos^2(\lambda b)\right] - 2\pi G\gamma\left(\frac{\pi_\phi^0}{V}\right)^2.
\end{aligned} \tag{185}$$

Note that the last term comes from $\partial H_{\text{matter}}/\partial V$ and, thus, it is the same for all the regularisations of the gravitational Hamiltonian.

## 8.2 Effective equations of motion in standard LQC

The effective Hamiltonian in this case is the one whose gravitational contribution is purely Euclidean. Therefore,

$$H_{\text{LQC}}^{\text{eff}} = -\frac{3V}{8\pi G\gamma^2\lambda^2}\sin^2(\lambda b) + \frac{(\pi_\phi^0)^2}{2V}. \tag{186}$$

In this model, the time evolution of the physical volume is given by

$$
\begin{aligned}
\dot{V} = \{V, H^{\mathrm{eff}}_{\mathrm{LQC}}\} &= -4\pi G\gamma \frac{\partial H^{\mathrm{eff}}_{\mathrm{LQC}}}{\partial b} \\
&= 4\pi G\gamma \frac{3V}{8\pi G\gamma^2\lambda^2} \lambda \sin(2\lambda b) \\
&= \frac{3V}{2\gamma\lambda} \sin(2\lambda b).
\end{aligned}
\tag{187}
$$

Similarly, the time evolution of the variable $b$ is

$$
\begin{aligned}
\dot{b} = \{b, H^{\mathrm{eff}}_{\mathrm{mLQC}}\} &= 4\pi G\gamma \frac{\partial H^{\mathrm{eff}}_{\mathrm{mLQC}}}{\partial V} \\
&= -4\pi G\gamma \frac{3}{8\pi G\gamma^2\lambda^2} \sin^2(\lambda b) - 2\pi G\gamma \left(\frac{\pi^0_\phi}{V}\right)^2 \\
&= -\frac{3}{2\gamma\lambda^2} \sin^2(\lambda b) - 2\pi G\gamma \left(\frac{\pi^0_\phi}{V}\right)^2 .
\end{aligned}
\tag{188}
$$

## 8.3 Effective equations of motion in GR

As we have already done in Sec. 6.2, we can take the (classical) limit $\lambda \to 0$ in order to recover the results for symmetry reduced GR (that is, homogeneous and isotropic GR). Using this strategy, we obtain the effective Hamiltonian

$$
H^{\mathrm{eff}}_{\mathrm{GR}} = -\frac{3Vb^2}{8\pi G\gamma^2} + \frac{(\pi^0_\phi)^2}{2V}. \tag{189}
$$

Instead of going through the computation of the Poisson brackets once more, we can directly take the classical limit of the effective equations of motion obtained in the two previous subsections (the classical limit of both sets of equations coincide, naturally). The result of this limit is presented below these lines:

$$
\dot{V} = \frac{3}{\gamma} V b, \tag{190}
$$

$$
\dot{b} = -\frac{3b^2}{2\gamma} - 2\pi G\gamma \left(\frac{\pi^0_\phi}{V}\right)^2 . \tag{191}
$$

It is also interesting to discuss the physical meaning of $b$ in this scenario, where it becomes transparent. Let $a$ be the *scale factor* of the Universe (in my conventions, the scale factor today, $a_0$, is taken to be one). In terms of $a$, the volume of the Universe can be written as $V = V_0 a^3$, where $V_0$ is the physical volume of the Universe today. From the scale factor, one usually defines the *Hubble parameter* $H = \dot{a}/a$, which measures the expansion rate of the Universe. It is trivial to write $H$ in terms of the physical volume instead. One finds

$$
H = \frac{\dot{V}}{3V} = \frac{b}{\gamma}, \tag{192}
$$

where the last equality follows from Eq. (190). Therefore, we can think of $b$ as a variable that measures the expansion rate of the Universe, and that coincides with the Hubble parameter up to a factor of $\gamma$.

## 8.4 Numerical integration and plots

In the previous subsections, we have explicitly computed the effective equations of motion governing the cosmological dynamics in GR, LQC and mLQC[30]. These provide three systems of coupled ordinary differential equations. To solve them, we need to give an appropriate number of initial conditions. Owing to the fact that they are first-order differential equations, we only need to provide a value of $V(t_i)$ and $b(t_i)$ for a suitably chosen $t_i$ that will serve as the initial time in our simulations.

Nonetheless notice that, once the constant $\pi_\phi^0$ is given, $V_i \equiv V(t_i)$ and $b_i \equiv b(t_i)$ cannot be chosen independently: once one is fixed, the other is as well if the Hamiltonian constraint is to be satisfied! In the following, we will choose $V_i$ and fix $b_i$ in such a way that the Hamiltonian constraint vanishes.

Let us consider the equations of modified LQC. The condition that the constraint is satisfied at $t_i$ is given by

$$\begin{aligned} 0 &= \frac{3V_i}{8\pi G\lambda^2}\left[\sin^2(\lambda b_i) - \frac{1+\gamma^2}{4\gamma^2}\sin^2(2\lambda b_i)\right] + \frac{(\pi_\phi^0)^2}{2V_i}, \\ 0 &= \sin^2(\lambda b_i)\left[1 - \frac{1+\gamma^2}{\gamma^2}\cos^2(\lambda b_i)\right] + \frac{8\pi G\lambda^2}{3}\frac{(\pi_\phi^0)^2}{2V_i^2}, \\ 0 &= \sin^2(\lambda b_i)\left[(1+\gamma^2)\sin^2(\lambda b_i) - 1\right] + \frac{8\pi G\gamma^2\lambda^2}{3}\rho_i, \\ 0 &= (1+\gamma^2)\sin^4(\lambda b_i) - \sin^2(\lambda b_i) + \frac{8\pi G\gamma^2\lambda^2}{3}\rho_i, \\ \sin^2(\lambda b_i^\pm) &= \frac{1 \pm \sqrt{1-\rho_i/\tilde{\rho}_c}}{2(1+\gamma^2)}. \end{aligned} \tag{193}$$

Therefore, there are two branches of solutions, one corresponding to $b_i^+$ and the other corresponding to $b_i^-$. In Eq. (193), $\rho_i$ and $\tilde{\rho}_c$ are defined as

$$\rho_i = \frac{(\pi_\phi^0)^2}{2V_i^2}, \tag{194}$$

$$\tilde{\rho}_c = \frac{3}{32\pi G\Delta\gamma^2(1+\gamma^2)}, \tag{195}$$

and have units of energy density. Indeed, it is immediate to see that the energy density can be defined from the matter Hamiltonian as

$$\rho = \frac{H_{\text{matter}}}{V} = \frac{(\pi_\phi^0)^2}{2V^2}. \tag{196}$$

As a result, we realise that $\rho_i$ is nothing but $\rho(t_i)$.

On the other hand, $\tilde{\rho}_c$ has the meaning of a critical density. Inserting $\gamma = 0.2375$ and using the usual value of $\Delta$, we obtain $\tilde{\rho}_c \approx 0.10\rho_p$ (where $\rho_p = G^{-2}$ is the Planck density). We can interpret $\tilde{\rho}_c$ physically by computing the time derivative of $\rho$ when $\rho = \tilde{\rho}_c = (\pi_\phi^0)^2/(2\tilde{V}_c^2)$:

$$\dot{\rho}\Big|_{\rho=\tilde{\rho}_c} = -\left(\frac{\pi_\phi^0}{V_c}\right)^2\frac{\dot{V}}{V} = -\left(\frac{\pi_\phi^0}{V}\right)^2\frac{3}{2\gamma\lambda}\sin\!\left(2\lambda\tilde{b}_c\right)[(1+\gamma^2)\cos\!\left(2\lambda\tilde{b}_c\right) - \gamma^2], \tag{197}$$

[30] In practice, we are going to dispense with the equation of motion corresponding to $\phi$. Hence, only the ones associated with $V$ and $b$ will be integrated numerically.

where $\tilde{b}_c$ is fixed by the requirement that $H_{eff}\big|_{\rho=\tilde{\rho}_c} = 0$. From a relation similar to Eq. (193) (derived from the fact that the Hamiltonian must vanish at all times), it follows that

$$\sin^2(\lambda\tilde{b}_c) = \frac{1}{2(1+\gamma^2)}, \tag{198}$$

$$\cos\Big(2\lambda\tilde{b}_c\Big) = \cos^2(\lambda\tilde{b}_c) - \sin^2(\lambda\tilde{b}_c) = 1 - 2\sin^2(\lambda\tilde{b}_c) = 1 - \frac{1}{1+\gamma^2} = \frac{\gamma^2}{1+\gamma^2}. \tag{199}$$

Hence, $(1+\gamma^2)\cos\Big(2\lambda\tilde{b}_c\Big) - \gamma^2 = 0$ and $\dot{\rho}\big|_{\rho=\tilde{\rho}_c} = 0$. In conclusion, $\tilde{\rho}_c$ is either a maximum or a minimum of the energy density. It can be shown that, in the physical branch, $\tilde{\rho}_c$ is a global maximum (this implies, in turn, that the volume is bounded below, as can be seen in Eq. (197)). The 'physical branch' is defined as the branch (either the $b_i^+$-one or the $b_i^-$-one) which describes an expanding universe for $t = t_i$. Thus, we can determine which branch is the physical one by requiring $\dot{V}(t_i) > 0$. Using Eq. (184) at $t = t_i$, we obtain

$$\begin{aligned}
\dot{V}(t_i) > 0 \Rightarrow 0 &< (1+\gamma^2)\cos\big(2\lambda b_i^\pm\big) - \gamma^2, \\
\frac{\gamma^2}{1+\gamma^2} &< \cos\big(2\lambda b_i^\pm\big) = \cos^2(\lambda b_i^\pm) - \sin^2(\lambda b_i^\pm) = 1 - 2\sin^2(\lambda b_i^\pm), \\
\frac{\gamma^2}{1+\gamma^2} &< 1 - \frac{1 \pm \sqrt{1-\rho_i/\tilde{\rho}_c}}{1+\gamma^2} = 1 - \frac{1}{1+\gamma^2} \mp \frac{\sqrt{1-\rho_i/\tilde{\rho}_c}}{1+\gamma^2}, \\
0 &< \mp\frac{\sqrt{1-\rho_i/\tilde{\rho}_c}}{1+\gamma^2}.
\end{aligned} \tag{200}$$

This result makes us conclude that only the lower sign yields an expanding universe at $t = t_i$. Therefore, the physical branch is the one corresponding to $b_i^-$.

At this point of the discussion, we are in a position to give a complete set of initial conditions. Following the authors in Ref. [70], we will select $\pi_\phi^0 = 1$, $t_i = 11.5\, l_p$, and $\rho_i = 10^{-4}\rho_p$. The corresponding $b_i^-$ is

$$b_i^- = \frac{1}{\lambda}\sin^{-1}\sqrt{\frac{1-\sqrt{1-\rho_i/\tilde{\rho}_c}}{2(1+\gamma^2)}} \approx 6.9\cdot 10^{-3}. \tag{201}$$

Notice that we can set $\pi_\phi^0 = 1$ without loss of generality because all the dependence on $\pi_\phi^0$ of the equations of motion happens through $\pi_\phi^0/V$. Thus, $\pi_\phi^0$ can be put to one by an appropriate rescaling of the volume $V \to \pi_\phi^0 V$.

In summary, we take $(\pi_\phi^0, \rho_i, b_i) = (1, 10^{-4}, 6.9\cdot 10^{-3})$. We will use these initial conditions for the three cases. This is possible because $H_{\rm LQC}^{\rm eff}$ and $H_{\rm GR}^{\rm eff}$ vanish to a very good approximation ($|H_{\rm LQC,GR}^{\rm eff}| \sim 10^{-6}$) when these initial conditions are employed. Indeed, I have plotted the magnitude of the Hamiltonian constraint throughout the whole integration region to make sure that the effective constraints are consistent under evolution.

Once we have verified that we can use these initial conditions, we proceed to the numerical integration of the effective equations of motion. The result of this procedure is presented in Figs. 2-4. Everything is expressed in Planck units for simplicity. I will conclude by briefly commenting the differences in the physical pictures that result from each description.

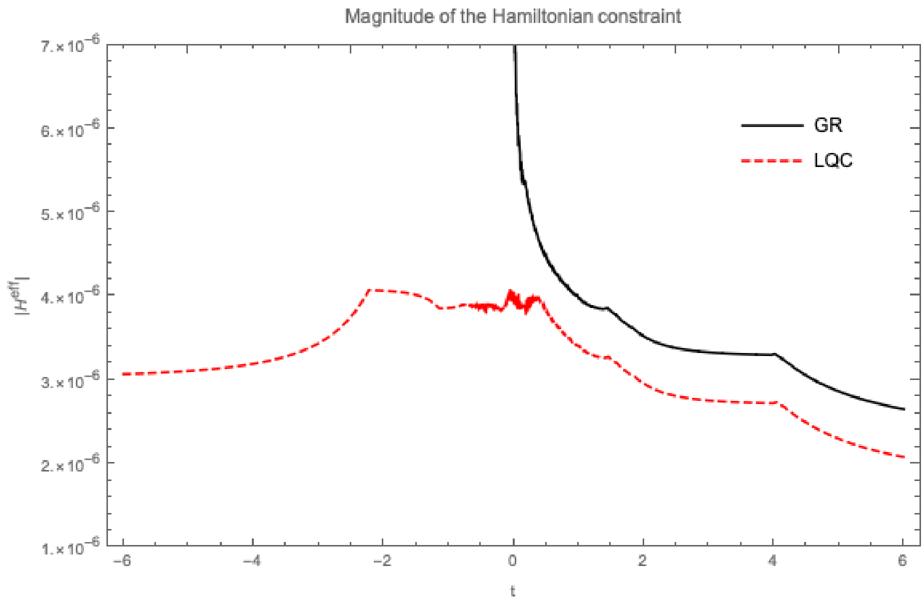


Figure 1: The absolute value of the effective Hamiltonian constraint is plotted as a function of the cosmic time in standard LQC and GR. The fact that it remains small in the whole time interval in which we have integrated numerically the equations of motion implies that we can use consistently the initial conditions written above.

In the case of GR (which is represented by a black solid line), we see in Figs. 2-4 that at around $t \approx 0$ the Big Bang singularity takes place: the volume of the Universe shrinks to zero, the energy density becomes infinite and the expansion rate diverges as well.

In the other two homogeneous and isotropic models, however, this does not occur. Whereas the three descriptions coincide remarkably well for large volumes and small energy densities (in the region of validity of GR), they differ greatly as $t$ approaches zero. Instead of collapsing, the two universes described by a loop effective dynamics attain a minimum in physical volume and start expanding again (I am describing the plots in backwards evolution). Hence, the classical Big Bang singularity is replaced by a quantum bounce (the so-called *Big Bounce*) that joins a contracting prebounce branch and an expanding postbounce branch. The appearance of this bounce is produced by an emergent 'repulsive behaviour' of gravity due to the quantum nature of geometry at the Planck scale (as can be seen in Fig. 3, the repulsive effects do not become dominant until the energy density reaches a value of $\sim 0.01\rho_p$). We observe that GR becomes an extremely good approximation just a few Planck times after the bounce.

Even though the two loop quantum models exhibit a quantum bounce, the respective bounces differ enormously. To begin with, the critical densities are obviously different. While they are of the same order of magnitude, the one obtained in standard LQC is larger than the one in modified LQC. Indeed, we found that $\tilde{\rho}_c \approx 0.10\rho_p$. We can also compute the critical density in standard LQC. Although it can be calculated in several ways, the simplest one is to compute the value of $b$ for which $\dot{V} = 0$. Then, substituting this value in $\rho$, we obtain

$$\rho_c = \frac{3}{8\pi G\gamma^2\Delta} \approx 0.41\rho_p, \tag{202}$$

which coincides with the value observed in Fig. 3. We see that $\tilde{\rho}_c$ is suppressed by a factor of $1/[4(1+\gamma^2)] \approx 0.24$ with respect to $\rho_c$.

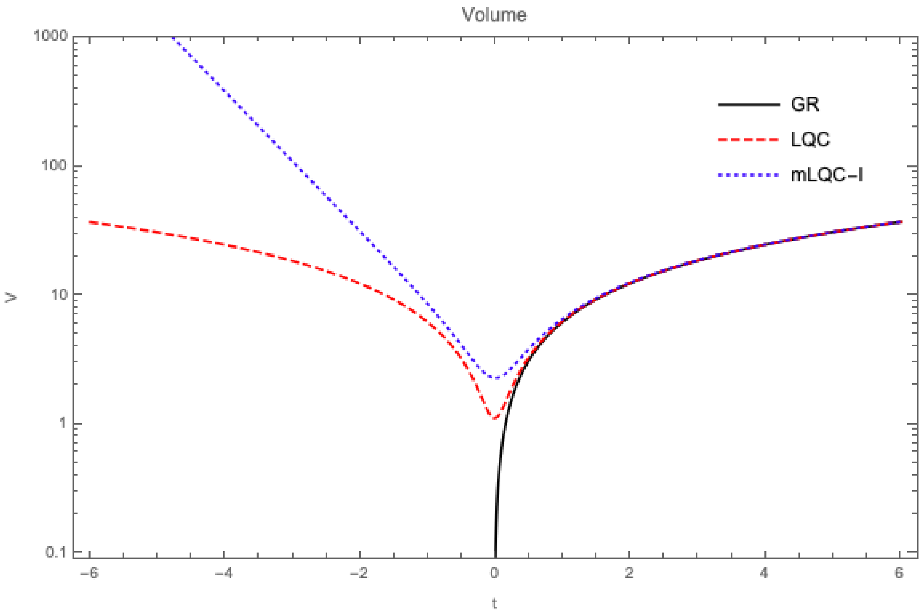


Figure 2: The physical volume of the Universe is plotted as a function of the cosmic time in GR, standard LQC, and modified LQC.

Finally, I want to mention another fundamental difference. The bounce found in standard LQC is symmetric: it joins two similar classical universes, in the sense that they become large and have a small spacetime curvature at late times. However, the bounce found in modified LQC is asymmetric: whereas the postbounce branch remains classical, the prebounce branch expands exponentially (i.e., in a straight line in a logarithmic scale; see Fig. 2) and its Hubble parameter is of Planckian order [70]. Therefore, the standard bouncing mechanism is modified not only quantitatively (the numerical value of the critical density is changed) but also *qualitatively*: it is asymmetric and joins a prebounce de Sitter branch (a Planckian cosmological constant emerges in the prebounce era) with a postbounce classical branch[31].

There exist other differences between the two loop description that can be seen directly from the Friedmann-Raychaudhuri equations. However, I will not cover them in this work. For further details, I refer to the original article [70].

[31]It would also be possible that the two branches were ordered the other way around. However, such a possibility could not describe our Universe: it is already ruled out by observation [70].

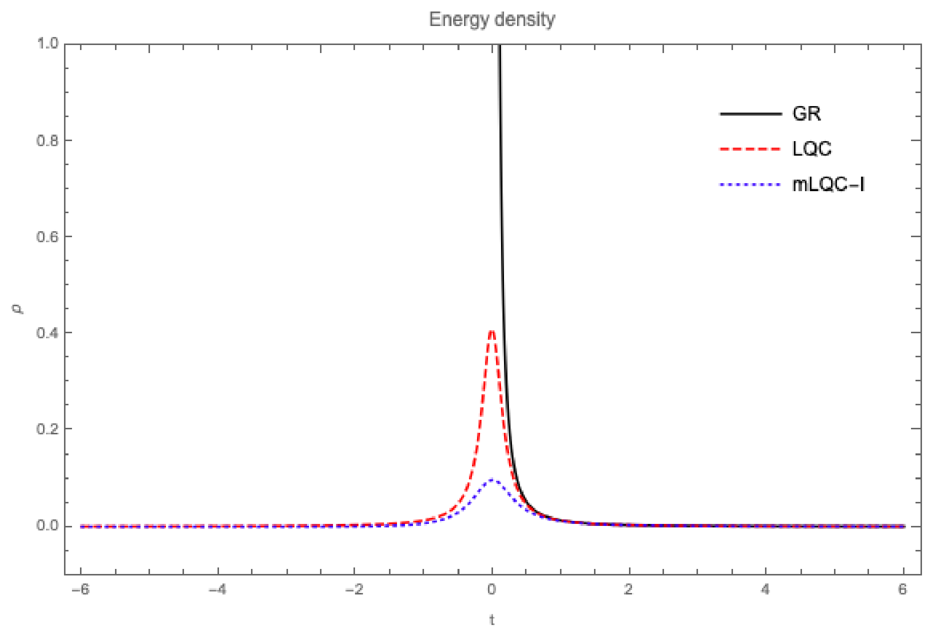


Figure 3: The energy density of the Universe as a function of cosmic time in GR, standard LQC, and modified LQC.

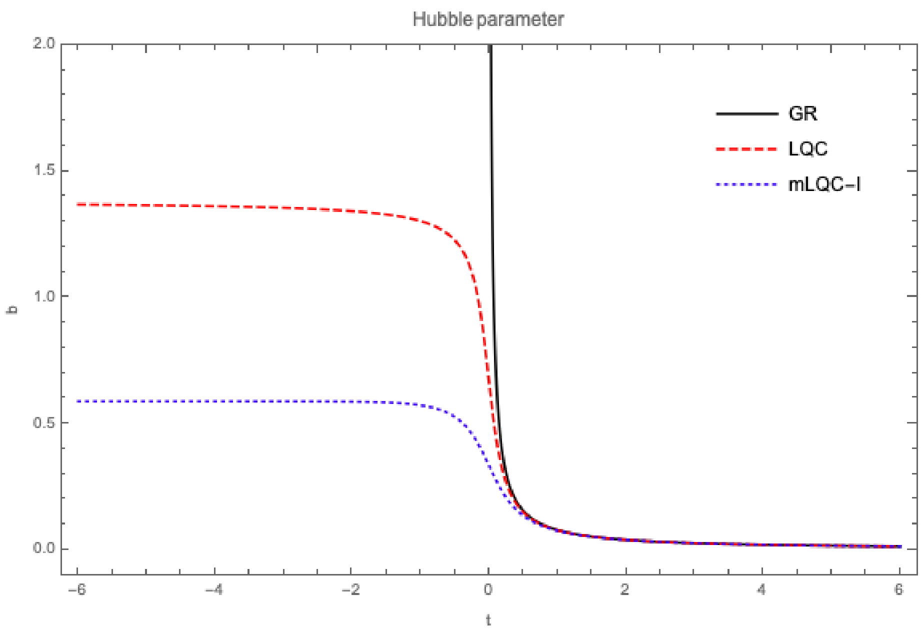


Figure 4: The Hubble parameter (up to a factor of $\gamma$) is plotted as a function of cosmic time in GR, standard LQC, and modified LQC.

# 9 Conclusions

After almost twenty years marked by a major development of LQC, a new line of research has sparked the interest of the community recently: the examination of the foundations of the LQC formalism and the discussion of the ambiguities that may affect its construction. A prominent example of these ambiguities is the procedure to regularise the Hamiltonian constraint. The analysis of these mathematical ambiguities not only is interesting by itself, but also may lead to alternative formalisms that entail nontrivial modifications with respect to the standard approach to LQC. More concretely, it is compelling to determine how these modification alter the (potentially testable) physical predictions of the theory. Among the physical predictions of LQC, one stands out: the resolution of the classical Big Bang singularity, which is replaced by a quantum bounce. Owing to the relevance of this result, it seems natural to wonder whether it is robust under these ambiguities (i.e., whether it remains present in alternative formalisms). This question is especially interesting when the alternatives under consideration make use of techniques that are closer to LQG, in the sense that they are inspired by those employed in the full theory and are adapted to the cosmological scenario without suffering any substantial modifications. I highlight the relevance of these cases because the relation between LQG and LQC is not fully settled yet: it is not known to which extent the physical cosmological dynamics (presumably computable within the framework of LQG) is captured by LQC. This is the main motivation for exploring alternative quantisations of cosmological spacetimes that follow more faithfully the precepts of LQG.

Dapor and Liegener have recently put forward a modified formalism of this kind [65]. To do so, they obtained the gravitational Hamiltonian constraint within full LQG and computed its expected value on certain coherent states representing homogeneous and isotropic spacetimes. The effective Hamiltonian resulting from this procedure turned out to coincide (at dominant order) with one already considered by Yang, Ding, and Ma [64]. In collaboration with other authors, they showed [67] that such a Hamiltonian could also be obtained within LQC as a result of regularising the Euclidean and Lorentzian parts of the Hamiltonian constraint independently. A considerable number of papers have been dedicated to the study of this modified Hamiltonian and the extraction of its phenomenological consequences. Concerning the effective cosmological dynamics resulting from this Hamiltonian, it has been determined that, while the classical singularity is still replaced by a quantum bounce joining deterministically two branches of the Universe (a prebounce one that contracts and a postbounce one that expands), the bounce picture is qualitatively different: whereas one of the branches is a large classical universe (as in the standard case), the other branch is necessarily replaced by a de Sitter universe with an emergent cosmological contant of Planckian order.

Nevertheless, the selection of a regularisation scheme is *not* the only origin of mathematical ambiguities in the construction of a loop quantum theory of cosmological spacetimes. This process also involves a *choice* of quantisation prescription for the factor ordering of the terms determined by the employed regularisation. Two predominant prescriptions exist in the literature of standard LQC (see Refs. [36, 37]). The main original contribution that I have wanted to cover in this Master's Thesis is related to the implementation of the MMO prescription in the alternative formalism of Dapor and Liegener [76]. In particular, my objective has been to determine whether the appealing features of this prescription in standard LQC hold under this modification of the Hamiltonian constraint. To achieve this purpose, I have aimed to answer the following questions: i) Does (the quantum analogue of) the classical singularity decouple already at the kinematical level? ii) Do the superselection sectors defined by the action of the quantum Hamiltonian remain simpler than those obtained using other prescriptions? iii) Is it still possible to find a closed expression that allows us to explicitly construct the generalised eigenfunctions of the gravitational Hamiltonian constraint? iv) If the answer to the previous question is in the affirmative, how many available pieces of data appear in the construction of such eigenfunctions? It should be noted that the number of these pieces of data for a fixed eigenvalue can be regarded as an indication of the degeneracy of (the gravitational contribution of) the Hamiltonian constraint operator.

With these questions in mind, I have begun by introducing the Dirac formalism for the quantisation of constrained systems (GR being an example thereof) and some preliminary concepts on LQG. This was done in order to motivate the treatment of cosmological spacetimes, which are the protagonists of this thesis. After this introduction, I have reviewed the kinematical aspects of both flat FLRW and Bianchi I cosmologies, which are well-known in the LQC community. Although the main concern of this work is the quantisation of flat FLRW spacetimes, we consider Bianchi I cosmologies in parallel so that we may identify the sign structure appearing in anisotropic scenarios. Indeed, this sign structure in Bianchi I cosmologies inspired the proposal of the MMO prescription in the first place.

Once the kinematical Hilbert space has been constructed in both cases and the action of the fundamental operators on an orthonormal basis has been computed, I have dealt with the regularisation of the Hamiltonian constraint. In the first place, I have reviewed the standard regularisation procedure in order to see how it departs from the more general one adopted in LQG. To illustrate this process, I have explicitly regularised the Hamiltonian constraint in Bianchi I cosmologies according to the standard method, i.e., only considering its Euclidean part. After completing the computation and noting how the signs of the components of the triad appear in the resulting expression, I have taken the isotropic limit (carefully conserving the sign structure) to recover the standard Hamiltonian constraint in flat FLRW spacetimes. Then, I have proceeded to regularise the Lorentzian part in a similar manner, first in Bianchi I cosmologies and taking the isotropic limit afterwards. I have noticed that the sign structure is in fact identical to the one arising in the Euclidean part, so that it can be factored out and results in a global sign structure that suggests a natural symmetrisation upon quantisation.

Once the full (modified) Hamiltonian in FLRW cosmologies has been constructed, I have represented it by a quantum operator according to the MMO prescription. When computing its action on the volume eigenbasis, I have noticed that the quantum Hamiltonian annihilates the state of vanishing eigenvolume and leaves invariant its orthogonal complement. This fact allows us to restrict the Hamiltonian constraint to the orthogonal complement in a well-defined manner: the 'classically singular' state is decoupled at the kinematical level. Besides, after the removal of the singularity, we have densitised the constraint in (the algebraic dual of) the Hilbert space with support on the orthogonal complement discussed above. Then, I have obtained that the action of the densitised Hamiltonian results in a fourth-order difference equation that relates five volume eigenstates. This is in contrast with the standard result in LQC, where a *second-order* difference equation relating *three* eigenstates follows from the same computation. The reason behind the relation between five eigenstates is that the modified Hamiltonian produces shifts of four or eight units (if any) in the label of the volume eigenstates, linking $v$ with $v \pm 4$ and $v \pm 8$. From this observation, I have concluded that the modified Hamiltonian constraint is ensured to leave invariant the Hilbert spaces with support on lattices of step four: the superselection sectors will not be more involved than those obtained in standard LQC with other prescriptions. However, by virtue of the attributes of the MMO prescription, smaller spaces are left invariant by the action of the constraint. As occurs in standard LQC, the lattices split into two owing to the special treatment of the signs of the triad variables: the positive and negative semilattices are left invariant separately. Hence, I confirm that the superselection sectors are simpler than the ones obtained using the prescription of Ref. [36], even when the Hamiltonian under consideration has a more complicated functional form.

The crucial point about this splitting is that there exists in each superselection sector a point with minimum (and nonvanishing) eigenvolume. This has direct consequences in the study of the generalised eigenfunctions of the gravitational Hamiltonian. Indeed, this implies that it is possible to write a relation between the values of the generalised eigenfunction at the first three points of the semilattice. The other two points that would *a priori* be involved in the relation do not contribute because they lie in the negative semilattice. Therefore, once two of these values are given, the third is uniquely determined by the requirement that the generalised eigenvalue equation be satisfied. Then, as we displace the action of the Hamiltonian to points in the semilattice corresponding to eigenstates of increasing (in absolute value) volume, we realise that every value of the eigenfunction is fixed by the first two. This made us conclude that there are two pieces of data available in principle in the construction of the generalised eigenfunction associated with a given eigenvalue. This is again in contrast with the single piece of data available in standard LQC, and indicates the existence of subtleties in the self-adjoint extensions of the quantum Hamiltonian if its degeneracy is not doubled by the introduction of the Lorentzian part in the regularisation procedure.

To close the analysis of the quantum Hamiltonian, I have derived a closed expression that allows us to obtain the exact form of the generalised eigenfunctions of the gravitational Hamiltonian constraint. This appears to be a defining feature of the prescription, since it can also be done when the standard regularisation scheme is adopted instead. However, using other prescriptions, one needs to retort to numerical tools in order to analyse the generalised eigenfunctions of the Hamiltonian. The reason why is straightforward: the closed expression relies on the fact that the first two values (at most) determine the rest, which is only true when the splitting of the superselection sectors takes place. Recall that this is a direct consequence of the special treatment of the sign functions (which defines the MMO prescription in the first place) and no extra conditions are needed.

I have also reviewed the most basic aspects of the effective dynamics [70] arising from the modified Hamiltonian constraint and compared the results with the ones obtained using standard LQC and GR.

The results presented in this thesis lead to an univocal conclusion: the MMO prescription presents attractive features that make it stand out from the other existing proposals, even after including a modification in the Hamiltonian motivated by the construction of an LQC formalism that lies closer to full LQG.

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