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Evolutionary Minisuperspace Quantum Dynamics in the WKB approach

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Abstract

This Thesis deals with the application of the Vilenkin idea of a probabilistic interpretation of the Universe wavefunction, firstly proposed in the 1969, to the Bianchi models exploiting in particular two different quantization procedures: the Standard one and the Polymer Quantum Mechanics. The whole work can be divided in three research areas.

The first one is the study of the Taub Cosmology, a particular case of the Bianchi IX model in which there are two equal cosmic scale factors. We developed a suitable technical algorithm to implement a separation of the Minisuperspace configurational variables into quasi-classical and purely quantum degrees of freedom, in the framework of both a Standard quantization procedure and a Polymer quantum Mechanics reformulation of the canonical dynamics. We then implemented this technique to a Taub Universe with a massless scalar field. We used a set of Misner-Chitrè-like variables. We have identified the volume of the Universe and a function of the scalar field as quasi-classical variables; while we have identified the Universe anisotropy as purely quantum degree of freedom.

The resulting evolution (Schrödinger) equation for this anisotropy variable has, in the spirit of this analysis, two main physical implications. Firstly, the Taub model is reduced to a cyclical Universe, evolving between a minimum and a maximum value of the Universe volume. This offers an intriguing paradigm for the physical implementation of a cosmological history: clearly the maximum volume turning point is expected to live in a classical domain of the Universe dynamics, while the Bounce turning point has a pure quantum character, in the sense of a Polymer regularization. Then the Universe anisotropy is always finite in value as a result of the singularity regularization and its specific value in the Bounce turning point depends on the initial conditions of the system, but in principle, it can be restricted to small enough values to make the Bounce dynamics unaffected by their behavior. This ensures the applicability of the Born-Oppenheimer approximation. This study permitted us to submit an article, whose title is "WKB approximation for the Polymer quantization of the Taub Model", that is undergoing the refereeing procedure.

In the second part, we analyzed the Bianchi IX Universe dynamics within the corner region associated to the potential term which the spatial curvature induces in the Minisuperspace. The study was done in two different cases: in the vacuum and in the presence of a massless scalar field plus a cosmological constant term. We investigated the dynamics in terms of WKB scenario for which the isotropic Misner variables (the volume) and one of the two anisotropic ones (and the scalar field when present) are treated on a semi-classical level, while the remaining anisotropy degree of freedom, the one trapped in the corner, is described on a pure quantum level. The quantum dynamics always reduced to the one of a time dependent Schrödinger equation for a harmonic potential with a time dependent frequency. The vacuum case is treated in the limits of both a collapsing and an expanding Universe, while the dynamics in presence of massless scalar field and cosmological constant is studied only in the case of crescent time. In both analysis, the quantum dynamics of the anisotropy variable is associated to a decaying standard deviation of its probability density, corresponding to a suppression of the quantum anisotropy

associated. In the vacuum case, the corner configuration becomes an attractor for the dynamics and the evolution resembles that one of a Taub cosmology in the limit of a non-singular initial Universe. This suggests that if the Bianchi dynamics enters enough the potential corner then the initial singularity is removed and a Taub picture emerges. The case when the scalar field and the cosmological constant are present well mimics the De-Sitter phase of an inflationary Universe. We showed that both the classical and quantum anisotropies are exponentially suppressed, so that the resulting dynamics corresponded to an isotropic closed Robertson-Walker geometry. This study permitted us to submit an article, whose title is “Quantum dynamics of the corner of the Bianchi IX model in the WKB approximation”, that has been published in Physical Review D 102.

Contents

Chapter 1

Introduction

Quantum Cosmology began as the idea of applying Quantum Mechanics to every aspect of Nature, Universe included; although a similar quantization procedure is, even now, in its early stages since the General Relativity Theory states that not only matter but also space and time become physical objects and not mere background. This means that Quantum Cosmology is inexorably linked to Quantum Gravity, i.e. the quantum theory of gravitation as a whole; such a theory, unfortunately, is still incomplete and it contributes to give an unclear theoretical foundation to cosmology. Despite being studied a lot in the last century, this is not the only issue of this fascinating theory.

General Relativity demonstrated that the space-time is physical and dynamic, and interacts with matter; since the last one is described by Quantum Mechanics, a suitable matching would require the exact quantization of the space-time, but the structure of its microscopic degrees of freedom remains obscure. In this theory, the space-time is characterized by its symmetries, they are not accidental but rather they guarantee the intrinsic meaning of the theory, in the sense that the predictions have to be independent of the choice of the observer and the mathematical description of the coordinates. What we need to require to a healthy quantization of the gravitational field is that it should preserve the classical symmetries in order to maintain the self-consistency of the theory; although it can be an obvious request, this results in one of the greatest challenges.

The canonical approach to Quantum Cosmology consists in considering the quantization of a certain space-time in presence of some symmetries that help its description. Such a procedure takes to a configuration space with a finite number of degrees of freedom, called minisuperspace. Another problem deals with a rather sensitive case; Quantum Mechanics requires a system quantized in space and the existence of a time in which the system evolves as an external parameter, while General Relativity states that time has to be the same of all the others coordinates, and so a first attempt to match those two different perspectives would necessarily bring to the loss of the intrinsic covariance of the theory. This issue naturally requires a new interpretation of the concept of time.

Given a self consistent quantum model of *bricks* of space, a suitable quantum space would be the union of all the portions of the space described above, which on long distances could accurately reproduce the curved Relativistic space-time. This union could also be also viewed as an approximation of an inhomogeneous space-time with a series of homogeneous surfaces; a more acute analysis could interpret it as a physical decomposition of the space, if the quantum theory of gravitation will require discrete structures.

As a consequence there are two different tasks we have to deal with:

- find the exact quantum theory of the single patch of space, similarly to the dynamics of a single particle;

- determine the rules for the matching of different patches in a more complex system that includes two or more patches, this is the comparable to the case of interacting multi-body systems;

only once we solve both of them, we could say that we have a Quantum Cosmology theory and it will be merely necessary to find a way to make direct observations in order to test its consistency.

The simplest interpretation of the single patch is the classical description of a homogeneous and isotropic space-time. Such a system is described by the Friedman equations, and the canonical approach is the one that involves their direct quantization. It is important to highlight that the point of view of the single patch theories is not the same of traditional minisuperspace quantization, although both of them quantize the Friedman equations and in some cases are formally equivalent. In the minisuperspace models one tends to interpret the single patch as the entire Universe; the traditional approach, however, brought to a series of issues, especially in the case of discrete theories that give birth to some corrections which depend on the size of the patch, while in the minisuperspace models a measure of these corrections is not properly given, since the size of the patch is set as the size of the Observable Universe.

A strong and valid argument in favor of these *multipatch-theories* is the so called BKL conjecture originally formulated in [11]. In their work the physicists stated that going towards the singularity, the terms that contain time derivatives in the Einstein equations dominate over the one with spatial derivatives; this means that the system of partial differential equations (PDE) can be well approximated by a system of ordinary differential equations (ODE) and the dynamics becomes local and oscillatory. So the time evolution of fields, analyzed in every spatial point, is well approximated by the homogeneous cosmologies in the Bianchi classification, in particular the Bianchi IX model. At the beginning such a conjecture was strongly criticized but firstly the pioneering work of Ashtekar and then modern numerical studies on black holes gave more strength to the BKL analysis, prompting researchers to accurately address the issues of the quantum cosmology theory.

In my PhD thesis,I have put particular interest in the generalization of a probabilistic approach to Quantum Cosmology, that was initially developed by A. Vilenkin [54], to a more general class of cosmological models than the Friedman ones, i.e. the homogeneous but anisotropic Universes. Such models play a crucial intermediate role in the developing of the so called General Cosmological Solution, namely a solution of the Einstein equations without particular symmetries. I found a solid formulation that allows to demonstrate the general validity of such an approach. Therefore, in this context, I will analyze some applications to the Bianchi I model and to few particular cases of the Bianchi IX model, i.e. Taub model and the right corner of the Bianchi IX potential. This discussion will be divided in two separated parts: in the first, I will utilize the standard representation for the Quantum Mechanics, while in the second one, I will adopt a more complex representation, the Polymer one, that is non-equivalent to the Schrödinger one.

Polymer Quantum Mechanics allows to greatly simplify the formulation by giving a Physical interpretation of the treated system. As we will see in the following the results obtained in both of the representations will be consistent with each other, obviously bearing in mind the differences given by their intrinsic characteristics. The conclusions on the quantum nature of the studied models have been validated by the study of Gaussian Packets, built on the basis of the wavefunction that is solution of the Schrödinger equation, and compared with the expectation values given by the Ehrenfest Theorem, obtaining, in the relevant cases, a good correspondence between them.

The Thesis is composed in the following way.

In chapter (2) will be introduced the homogeneous cosmological models and the Bianchi classification, taking particular care in the description of three important Universes:

- Bianchi I that is the simplest cosmological model;
- Taub Model that is a very peculiar case of the more complex Bianchi IX Universe;
- Bianchi IX model

I will present the dynamics of those Universes from a critical point of view.

In the last part of this chapter, I will also introduce the canonical quantization of the Gravitational Field starting from its historical iter, in order to describe the modern discussion on such a theory with largely used instruments such as the Wheeler-DeWitt equation, the ADM formalism and its counterpart: the original Vilenkin approach. At the end, I will present even the Polymer representation of the Quantum Mechanics and some open issues in Modern Quantum Cosmology, these last parts will be especially relevant for the following.

In chapter (3) and (4), I will describe the works made during my PhD and they represents all the efforts of the last years.

In the first one, I will demonstrate firstly how to generalize the Vilenkin Approach to more complex cosmological models with particular maths; then I will diversify the treatment between the two different quantum representation and they will be presented in parallel and only after I will compare the results once thoroughly studied. Finally, I will adopt this generalized approach to two different cosmological models, Bianchi I and the Taub model. While for the former it will not be useful, for the latter I will analyze the dynamics of a Gaussian Packet and use it in order to reveal the behavior of the Particle-Universe in his early stages. This study also aims to demonstrate that the Polymer Quantum Dynamics can be used instead of the standard one in the case where the last one isn't predictive, without altering the system description.

The work explores the possibility to deal with a cosmological model in which the singularity is regularized via a Polymer Quantum Mechanics approach and a time dependence of the Universe wave function is defined via a Born-Oppenheimer decomposition of the quantum dynamics. The non trivial technical question we address here is to reconcile the momentum representation of the quantum dynamics, mandatory for a Polymer quantization, as developed in [19] for the continuum limit and the WKB scheme, thought in the coordinate representation. The crucial point is that the potential term emerging in the Minisuperspace model is, in general, non quadratic in the configurational variables, like instead in general is the Kinetic part of the Hamiltonian in the momenta. To overcome this difficulty, we introduce a suitable and general algorithm and then we implement it in the particular and important case of a Taub Cosmological model [40, 47].

Furthermore, the Taub cosmology has a non-trivial meaning for the physics of the early Universe. It corresponds to a Bianchi IX model with two scale factor equal to each other, and it is well-known that the Bianchi dynamics in the "corner" of the spatial curvature induced potential [15, 48] closely resembles small oscillations around a Taub configuration. Thus the generality of the Bianchi IX cosmology, versus a generic inhomogeneous cosmological model [47], justifies the interest for the present analysis. Finally, implementing the polymer paradigm within a WKB decomposition of the Minisuperspace dynamics, we aim to clarify the behavior of the anisotropy degree of freedom when a Big-Bounce emerges.

The case of a vacuum Taub cosmology, when the polymer quantum mechanics is implemented on the anisotropy dynamics only, was analyzed in [5], showing how the cosmological singularity is not removed, but only probabilistic weakened. The merit of such an investigation consists in clarifying that the emergence of a bouncing cosmology requires that the polymer reformulation also involves the Universe volume. In this respect, the present analysis is the conceptual continuation of the study in [5]. We include in the quantum dynamics a massless scalar field in order to deal with a relational time variable giving a material nature [32].

In the second one, we analyze the Bianchi IX Universe dynamics within the corner region associated to the potential term which the spatial curvature induces in the Minisuperspace. We analyze the diagonal Bianchi IX Universe both in vacuum and in the presence of a massless scalar field and a cosmological constant term. The dynamics is always analyzed in terms of a WKB scenario.

The Bianchi IX model [11, 2, 47] has a relevant role in the study of the cosmological dynamics since, despite its spatial homogeneity, it possesses typical features of the generic cosmological solution [9, 29, 45], like a chaotic time evolution of the cosmic scale factors near the cosmological singularity [25, 47]. Approaching the cosmological singularity, the potential term of the Bianchi IX dynamics resembles an infinite well having the morphology of an equilateral triangle. In the presented analysis, we study the situation in which the Bianchi IX dynamics is trapped in a corner of the potential, but the oscillating small degree of anisotropy is in a quantum regime.

In the vacuum case, the corner configuration becomes an attractor for the dynamics to the singularity and the evolution resembles that one of a Taub cosmology in the limit of a non-singular initial Universe. The case when the scalar field is present well mimics the De-Sitter phase of an inflationary Universe and we show that both the classical (macroscopic) anisotropy as well the quantum (microscopic one) are exponentially suppressed, so that the resulting dynamics corresponds to an isotropic closed Robertson-Walker geometry.

Finally, there will be a conclusive chapter in which all the results obtained will be inserted and discussed critically.

Chapter 2

Quantum Cosmology: a brief introduction

In this chapter, I will first introduce the homogeneous and anisotropic cosmological models. Such models are included in the Bianchi classification. For the purposes of this thesis, I will analyze the properties of two of them: the Bianchi I model and the Bianchi IX model. Then, I will present the canonical quantization of the gravitational field with all its problems. After a brief historical background, I will introduce the ADM formalism in order to formulate a fundamental equation for the description of the dynamics of the Universe, the Wheeler-DerWitt equation. Next, I am going to show a particular approach that allows to gain insights on the problem and that is the logical extension of the idea of DeWitt, i.e. the Vilenkin approach. Finally, I will analyze a representation of quantum mechanics that is different from the Schrödinger one, the Polymer Quantum Mechanics.

2.1 Homogeneous Cosmological Models

We begin introducing the definition of homogeneity [47]: a space is homogeneous if its metric tensor allows an isometric group that maps the space in itself. Such a group is generated by the Killing vector fields which compose a Lie Algebra. We formulate this definition considering a group of transformations

$$x^{\mu} \rightarrow \bar{x}^{\mu} = f^{\mu}\left(x,\tau\right) \equiv f^{\mu}_{\tau}\left(x\right) \tag{2.1}$$

on a space Σ, where the τ are n independent parameters which characterize the group and we impose, also, that τ_0 corresponds to the identity $f^{\mu}_{\tau_0} = x^{\mu}$.

If we analyze now an infinitesimal transformation near the identity such that

$$\begin{aligned} x^{\mu} \rightarrow \bar{x}^{\mu} &= f^{\mu}\left(x,\tau_0+\delta\tau\right) \approx \\ &\approx f^{\mu}\left(x,\tau_0\right) + \left(\frac{\partial f^{\mu}}{\partial \tau^a}\right)\left(x,\tau_0\right)\delta\tau^a \equiv x^{\mu} + \xi^{\mu}_a\left(x\right)\delta\tau^a = \\ &= \left(1+\delta\tau^a\xi_a\right)x^{\mu} \ , \end{aligned} \tag{2.2}$$

where the n differential operators of the first order ξ_a are defined by $\xi_a = \xi^{\mu}_a\partial_{\mu}$ and correspond to the n vector fields with components ξ^{μ}_a, that are the generator fields.

In this way if we implement the transformation (2.2) on a generic point of the space Σ, it will be translated of $\delta x^\mu = \delta\tau^a \xi^\mu_a$ in the initial coordinates and so

$$\bar{x}^\mu \approx \left(1 + \delta\tau^a \xi_a\right) x^\mu \approx e^{\delta\tau^a \xi_a} x^\mu \ . \tag{2.3}$$

If the group is a Lie group, the generators create a Lie Algebra, i.e. a n-dimensional vector space where the ξ_a form a closed basis under the commutation operation

$$[\xi_a, \xi_b] = \xi_a\xi_b - \xi_b\xi_a = C^c_{ab}\xi_c \ , \tag{2.4}$$

where the C^c_{ab} are the structure constants of the group.

Let us consider a Lie group that acts on a variety Σ like the group of transformation (2.1) and define the orbit of x as

$$f_{\mathfrak{B}}(x) = \{f_\tau(x) \ | \ \tau \in \mathfrak{B}\} \ , \tag{2.5}$$

namely the set of all the points that can be reached by x via the transformation; we also define the isometry group in x as the subset of $\mathfrak{B}$ that let fixed x

$$\mathfrak{B}_x = \{f_\tau(x) = x \ | \ \tau \in \mathfrak{B}\} \ . \tag{2.6}$$

If we suppose $\mathfrak{B}_x = \{\tau_0\}$ and $f_{\mathfrak{B}}(x) = \Sigma$, every transformation of $\mathfrak{B}$ translate the point x and every point in Σ can be reached from x with a single transformation; since $\mathfrak{B}/\mathfrak{B}_x = \{\tau/\tau_0 \ | \ \tau \in \mathfrak{B}\}$, the group $\mathfrak{B}$ is isomorphic to the manifold Σ. As soon as we identify $\mathfrak{B}$ with Σ the metric tensor on Σ is invariant under the group $\mathfrak{B}$.

Let us consider the case of a *space-time* $(\mathbf{M}, g_{ij})$ whose metric is invariant under spatial isometries. This is called spatially homogeneous if it exists a family of *space-like* surfaces Σ_t such that for every couple $(p \ , \ q) \in \Sigma_t$ there is a single element $\tau : \mathbf{M} \to \mathbf{M}$ of a Lie group $\mathfrak{B}$ such that $\tau(p) = q$. For a spatially homogeneous space-time, it is necessary to consider only a representative group from every equivalence class of the Lie groups of tridimensional isometries. The classification of such groups takes its name from *Luigi Bianchi* and determines the various possible symmetries of the tridimensional spaces.

The metric in the homogeneous models have to assure that its properties are the same in every point of the space. Under the action of the isometry $\tau \ : \ x \to x'$ the spatial line element

$$dl^2 = h_{\alpha\beta}(t, x)\, dx^\alpha dx^\beta \ , \tag{2.7}$$

has to be invariant, i.e.

$$dl^2 = h_{\alpha\beta}(t, x')\, dx'^\alpha dx'^\beta \tag{2.8}$$

must be true with the spatial metric that has the same formulation in both the new and the old coordinates. The metric tensor of a homogeneous space-time is obtained choosing a dual vector basis preserved by the isometries.

In the general case of a tridimensional homogeneous non euclidean space, there are three invariant differential forms that we can write as $\omega^a = e^a_\alpha dx^\alpha$. We can then rewrite the line element as $dl^2 = \eta_{\alpha\beta}\left(e^a_\alpha dx^\alpha\right)\left(e^b_\beta dx^\beta\right)$ such that in the triadic representation the metric tensor is

$$h_{\alpha\beta}(t, x) = \eta_{\alpha\beta}(t)\, e^a_\alpha(x^\gamma)\, e^b_\beta(x^\gamma) \ , \tag{2.9}$$

with $\eta_{\alpha\beta}$ as a symmetric matrix dependent only on time. The invariance of the line element implies that

$$e^a_\alpha\left(x\right)dx^\alpha = e^a_\alpha\left(x'\right)dx'^\alpha \tag{2.10}$$

with the compact notation $x = x^\gamma$ and where the e^a_α are the same functions written respectively in terms of both the old and the new coordinates. The triad algebra enables to rewrite equation (2.10) in the form

$$\frac{\partial x'^\beta}{\partial x^\alpha} = e^\beta_a\left(x'\right)e^a_\alpha\left(x\right) \ . \tag{2.11}$$

This is a system of differential equations that define the change of variables in terms of the basis vector, the integrability of the system is given by the *Schwartz* condition

$$\frac{\partial^2 x'^\beta}{\partial x^\alpha \partial x^\gamma} = \frac{\partial^2 x'^\beta}{\partial x^\gamma \partial x^\alpha} \tag{2.12}$$

that explicitly implies

$$\left[\frac{\partial e^\beta_a\left(x'\right)}{\partial x'^\delta}e^\delta_b\left(x'\right) - \frac{\partial e^\beta_b\left(x'\right)}{\partial x'^\delta}e^\delta_a\left(x'\right)\right]e^b_\gamma\left(x\right)e^a_\alpha\left(x\right) = e^\beta_a\left(x'\right)\left[\frac{\partial e^a_\gamma\left(x\right)}{\partial x^\alpha} - \frac{\partial e^a_\alpha\left(x\right)}{\partial x^\gamma}\right] \tag{2.13}$$

Multiplying both sides by $e^\alpha_d\left(x\right)e^\gamma_c\left(x\right)e^f_\beta\left(x'\right)$ it is possible to demonstrate that

$$e^\alpha_a\frac{\partial e^\gamma_b}{\partial x^\alpha} - e^\beta_b\frac{\partial e^\gamma_a}{\partial x^\beta} = C^c_{ab}e^\gamma_c \ . \tag{2.14}$$

This expression states that the homogeneity condition reduces to a constraint for the 1-forms $\omega^a = e^a_\alpha dx^\alpha$ which have to satisfy the *Maurer-Cartan* equation

$$d\omega^a + \frac{1}{2}C^a_{bc}\omega^b \wedge \omega^c = 0 \ . \tag{2.15}$$

From the definition, the structure constants are anti-symmetric under the exchange of the lower indices and so the homogeneity can be written as the Jacobi cyclical identity

$$C^f_{ab}C^d_{cf} + C^f_{bc}C^d_{af} + C^f_{ca}C^d_{bf} = 0 \ . \tag{2.16}$$

Introducing the structure constants with two indices $C^c_{ab} = \epsilon_{abd}C^{dc}$, where ϵ_{abd} is the totally anti-symmetric tridimensional *Levi-Civita* tensor, the above equation (2.16) become

$$\epsilon_{bcd}C^{cd}C^{ba} = 0 \ . \tag{2.17}$$

Analyzing eq. (2.17), it is clear that the classification of all the possible homogeneous models reduces to the identification of all the non-equivalent sets of the structure constants of a tridimensional Lie group.

2.1.1 Minisuperspace and Bianchi Models

The idea of the Minisuperspace originates from the possibility to restrict the general problem of Quantum Gravity to the simple case of a highly symmetrical space-time, reducing the dynamics to a finite dimensional scheme and the quantization procedure to the natural Dirac prescription for the Universe wave-function. [48]

Type	a	n1	n2	n3
I	0	0	0	0
II	0	1	0	0
VII	0	1	1	0
VI	0	1	-1	0
IX	**0**	**1**	**1**	**1**
VIII	**0**	**1**	**1**	**-1**
V	1	0	0	0
IV	1	0	0	1
VII_a	a	0	1	1
III ($a = 1$) VI_a ($a \neq 1$)	a	0	1	-1

Figure 2.1. Overview Table of the Bianchi Models

The most relevant implementation, for the purpose of this Thesis, corresponds to the case of Homogeneous Universes, described by the Bianchi Models; those models represent Universes where all the space points are equivalent to each other, but the independent directions scale in time with different laws, creating a certain degree of anisotropy. It is worth noting that only three of the nine Bianchi Universes present the isotropic limit and so the anisotropy of such models is not only a purely dynamical factor, but it derives from an intrinsic geometrical reason.

The list of all the possible tridimensional Lie algebras was presented, for the first time, by *Luigi Bianchi* in 1897 so that every algebra exclusively determines the local properties of a $3-D$ group. A homogeneous space-time with its group of symmetries is a *Bianchi N Model* if its structure constants can be written as

$$C^{ab} = n^{ab} + \epsilon^{abc} a_c \ , \tag{2.18}$$

with $n^{ab} = n^{ba}$ e $a_a = C^b_{ba}$. Using this form, the Jacobi identity reduces to [47]

$$n^{ab} a_b = 0 \ , \tag{2.19}$$

and a Lie group is determined therefore by assigning a dual vector a_c and a symmetrical matrix n^{ab} that satisfy the constraint (2.19). Without loosing in generality we can impose $a_c = (a \ , \ 0 \ , \ 0 \ )$, for example with a global rotation of the triadic vectors, and redefine the symmetric matrix as a diagonal one $n^{ab} = \mathrm{diag}\,(n_1 \ , \ n_2 \ , \ n_3 \ )$, so that equation (2.19) reduces to $an_1 = 0$. In this way it is possible to identify, inside the Bianchi Models, two different groups:

- $a = 0$ Class A (6 models),
- $a \neq 0$ Class B (3 models) .

In Figure (2.1) it is indicated the list of all the possible choices of (a, n_1, n_2, n_3) that satisfy the constraint (2.19).

It is worth noting [47] that Bianchi I is isomorphic to the translation group on $\mathbb{R}^3$, for which the flat FRW model is a particular case when we restore the isotropy, Bianchi V contains the open FRW, while Bianchi IX, that holds $SO\,(3)$ as symmetry group, includes the closed FRW as a particular case.

The metric tensor can be easily written considering a basis of vectors ω^a preserved by the isometries. Remembering equation (2.9) the line element $4-D$ is in the form

$$ds^2 = N^2(t)\, dt^2 - \eta_{ab}(t)\, \omega^a \omega^b \ , \tag{2.20}$$

parametrized by the proper time, where the 1-forms ω^a satisfy the Maurer-Cartan equation. We can, now, write the Einstein equations for a homogeneous Universe. In the tetrad basis the equations reduce to a system of ODE (ordinary differential equations) that includes only functions of time [47]

$$\begin{aligned} R^0_0 &= \frac{\partial}{\partial t} K^a_a - K^b_a K^a_b = \kappa \left(T^0_0 - \frac{1}{2} T \right) \\ R^0_a &= K^c_b \left(C^b_{ca} - \delta^b_a C^d_{dc} \right) = \kappa T^0_a \\ R^a_b &= \frac{1}{\sqrt{\eta}} \frac{\partial}{\partial t} \left(\sqrt{\eta} K^a_b \right) - {}^3R^a_b = \kappa \left(T^a_b - \frac{1}{2} \delta^a_b T \right) \end{aligned} \tag{2.21}$$

in which the relation $K_{ab} = -\partial_t \eta_{ab}/2$ holds. The components of the Ricci tensor become

$${}^3R_{ab} = -\frac{1}{2} \left(C^{cd}_b C_{cda} + C^{cd}_b C_{dca} - \frac{1}{2} C^{cd}_b C_{acd} - C^c_{cd} C^d_{ab} + C^c_{cd} C^d_{ba} \right) \tag{2.22}$$

2.1.2 Bianchi I Model

Analyzing figure (2.1), the simplest model to study is Bianchi I, that corresponds to the case in which all the a and n_i are zeros, in the vacuum. The characteristics of such a model imply that the tridimensional Ricci tensor is identically null. Moreover, being the metric tensor independent of spatial coordinates, from the equations (2.21) we can see that even the $R_{0\alpha}$ are null. So the Einstein equations reduce to [47] :

$$\begin{aligned} \dot{K}^a_a + K^b_a K^b_a &= 0 \ , \\ \frac{1}{\sqrt{\eta}} \frac{\partial}{\partial t} \left(\sqrt{\eta} K^b_a \right) &= 0 \ . \end{aligned} \tag{2.23}$$

From the second equation we get the first conserved quantity

$$\sqrt{\eta} K^b_a = \zeta^b_a = \text{costante} \ , \tag{2.24}$$

whose contraction of a and b gives

$$K^a_a = \frac{\dot{\eta}}{2\eta} = \frac{\zeta^a_a}{\sqrt{\eta}} \ , \tag{2.25}$$

and finally

$$\eta = \left(\zeta^a_a \right)^2 t^2 \ . \tag{2.26}$$

Without loosing in generality, rescaling the coordinates x^α, we can impose

$$\zeta^a_a = 1 \ , \tag{2.27}$$

and substituting (2.24) in the first of equations (2.23) we get the relation between the constants ζ_a^b

$$\zeta_b^a \zeta_a^b = 1 \ . \tag{2.28}$$

Lowering the b index in the (2.24), we obtain a system of ODE in terms of η_{ab}

$$\dot{\eta}_{ab} = \frac{2}{t} \zeta_a^c \eta_{cb} \ . \tag{2.29}$$

The set of coefficients ζ_a^c can be considered the matrix associated to a certain linear transformation, reducible to a diagonal form, whose eigenvalues can be written as $(p_l, p_m, p_n) \in \mathbb{R}$ and the eigenvectors as $\mathbf{l}$, $\mathbf{m}$, $\mathbf{n}$. The solution of (2.29) can finally be put in the form

$$\eta_{ab} = t^{2p_l} l_a l_b + t^{2p_m} n_a n_b + t^{2p_n} m_a m_b \ . \tag{2.30}$$

If we choose the tridimensional basis and we call the coordinates x^1, x^2 and x^3, the spatial line element becomes [47]

$$dl^2 = t^{2p_l} \left(dx^1\right)^2 + t^{2p_m} \left(dx^2\right)^2 + t^{2p_n} \left(dx^3\right)^2 \ , \tag{2.31}$$

where the p_i are the so called *Kasner* indices that satisfy the relations

$$\begin{aligned} p_l + p_m + p_n &= 1 \ , \\ p_l^2 + p_m^2 + p_n^2 &= 1 \ , \end{aligned} \tag{2.32}$$

and so the solution is characterized by a unique independent parameter. Except for two particular cases, $(0, 0, 1)$ e $(-1/3, 2/3, 2/3)$, the Kasner indices are always different from each other and one is always negative while the other two are always positive.

Once ordered the indices in the following way

$$p_1 < p_2 < p_3 \ , \tag{2.33}$$

their existence domains are

$$-\frac{1}{3} \leq p_1 \leq 0 \ , \ 0 \leq p_2 \leq \frac{2}{3} \ , \ \frac{2}{3} \leq p_3 \leq 1 \ . \tag{2.34}$$

Such indices allows the following parametrization

$$p_1(u) = \frac{-u}{1 + u + u^2} \ , \ p_2(u) = \frac{1 + u}{1 + u + u^2} \ , \ p_3(u) = \frac{u(1 + u)}{1 + u + u^2} \ , \tag{2.35}$$

with the parameter u varying in the range $1 \leq u < \infty$. For the values of u that are inferior to 1 we can use the inversion property

$$p_1\left(\frac{1}{u}\right) = p_1(u) \ , \ p_2\left(\frac{1}{u}\right) = p_3(u) \ , \ p_3\left(\frac{1}{u}\right) = p_2(u) \ . \tag{2.36}$$

The line element, defined by (2.30), describes an anisotropic space where the volumes linearly increase with the time, while the linear distances grow in two dimensions and decrease along the third one. The metric has only a singularity that cannot be removed in $t = 0$ with the only exception of the case $(0, 0, 1)$ that corresponds to the standard Euclidean space.

2.1.3 Limitations of the Kasner Solution

Let us analyze, now, the limitations of the above Kasner Solution; this solution approximates correctly the cases in which the Ricci tensor ${}^3R_{ab}$ included in the Einstein equations is at least of the order of t^{-2} an therefore negligible; however, since one of the Kasner indices is negative there appear dominant terms with respect to the tensor order rendering the Kasner solution unstable near the initial singularity. We introduce three spatial vectors $e^a = \{l\left(x^\gamma\right), m\left(x^\gamma\right), n\left(x^\gamma\right)\}$ that satisfy the homogeneity constraint and that take the matrix $h_{\alpha\beta}$ in its diagonal form

$$h_{\alpha\beta} = a^2\left(t\right) l_\alpha l_\beta + b^2\left(t\right) m_\alpha m_\beta + c^2\left(t\right) n_\alpha n_\beta \ , \tag{2.37}$$

these are called Kasner vectors while the time dependent coefficients are the scale factors. As a consequence the Einstein equations in a synchronous system and for a generic homogeneous cosmological model in the vacuum take the form [47]

$$\begin{aligned} -R_l^l &= \frac{(\dot{a}bc)^{\cdot}}{abc} + \frac{1}{2a^2b^2c^2}\left[\lambda_l^2 a^4 - \left(\lambda_m b^2 - \lambda_n c^2\right)^2\right] = 0 \\ -R_m^m &= \frac{\left(a\dot{b}c\right)^{\cdot}}{abc} + \frac{1}{2a^2b^2c^2}\left[\lambda_m^2 b^4 - \left(\lambda_l a^2 - \lambda_n c^2\right)^2\right] = 0 \\ -R_l^l &= \frac{(ab\dot{c})^{\cdot}}{abc} + \frac{1}{2a^2b^2c^2}\left[\lambda_n^2 c^4 - \left(\lambda_l a^2 - \lambda_m b^2\right)^2\right] = 0 \\ -R_0^0 &= \frac{\ddot{a}}{a} + \frac{\ddot{b}}{b} + \frac{\ddot{c}}{c} = 0 \end{aligned} \tag{2.38}$$

in which the off-diagonal components are identically null because of the diagonal form of η_{ab}. Eventually, the 0α components can assume values different from zero if there is a matter term that causes the rotation of the Kasner axes; the constants λ_i respectively correspond to the structure constants with the equal indices introduced above.

If we use the notation

$$\alpha = \ln a \ , \ \beta = \ln b \ , \ \gamma = \ln c \tag{2.39}$$

and a new time variable defined by

$$dt = abc \ d\tau \ , \tag{2.40}$$

the system (2.38) becomes [47]

$$\begin{aligned} 2\alpha_{\tau\tau} &= \left(\lambda_m b^2 - \lambda_n c^2\right)^2 - \lambda_l^2 a^4 \\ 2\beta_{\tau\tau} &= \left(\lambda_l a^2 - \lambda_n c^2\right)^2 - \lambda_m^2 b^4 \\ 2\gamma_{\tau\tau} &= \left(\lambda_l a^2 - \lambda_m b^2\right)^2 - \lambda_n^2 c^4 \\ \frac{1}{2}\left(\alpha + \beta + \gamma\right)_{\tau\tau} &= \alpha_\tau \beta_\tau + \alpha_\tau \gamma_\tau + \beta_\tau \gamma_\tau \ . \end{aligned} \tag{2.41}$$

The Kasner regime described above is the solution that corresponds to a simultaneously cancellation of all the right hand sides of the system (2.41). However, this behavior cannot exist indefinitely for $t \to 0$ since near the singularity there is always at least one term on the RHS that becomes relevant.

2.1.4 Bianchi IX Universe and Taub Model

We introduce now a model more general than the Bianchi I model; the Bianchi IX Universe. This corresponds to set all the n_i to 1. We will study, for the purpose of this thesis, the solution of the system (2.38) using the standard *Belinskii*, *Khalatnikov* e *Lifshitz* approach [7, 8, 9, 10, 11]. For this model, the structure constants are $(\lambda = 1, 1, 1)$ and the equations (2.38) reduce to

$$\begin{aligned} 2\alpha_{\tau\tau} &= \left(b^2 - c^2\right)^2 - a^4 \\ 2\beta_{\tau\tau} &= \left(a^2 - c^2\right)^2 - b^4 \\ 2\gamma_{\tau\tau} &= \left(a^2 - b^2\right)^2 - c^4 \\ \frac{1}{2}\left(\alpha + \beta + \gamma\right)_{\tau\tau} &= \alpha_\tau\beta_\tau + \alpha_\tau\gamma_\tau + \beta_\tau\gamma_\tau \ . \end{aligned} \tag{2.42}$$

Let us consider the case in which the negative index corresponds to the function $a\,(t)$; the perturbation caused to the Kasner regime is given by the terms $\lambda_l^2 a^4$ while the others decrease with decreasing t; taking into account only the growing terms in the RHS of the (2.42) we get the system [48] [47]

$$\begin{aligned} \alpha_{\tau\tau} &= -\frac{1}{2}e^{4\alpha} \\ \beta_{\tau\tau} = \gamma_{\tau\tau} &= \frac{1}{2}e^{4\alpha} \end{aligned} \tag{2.43}$$

whose solutions describe the evolution of the metric from its initial definition (2.31). If we have initially

$$a \sim t^{p_1} \ , \ b \sim t^{p_2} \ , \ c \sim t^{p_3} \tag{2.44}$$

then

$$\begin{aligned} abc &= \Lambda t \\ \tau &= \frac{1}{\Lambda}\ln t + costante \end{aligned} \tag{2.45}$$

where Λ is constant, such that the initial conditions for the (2.43) can be written as

$$\alpha_\tau = \Lambda p_1 \ , \ \beta_\tau = \Lambda p_2 \ , \ \gamma_\tau = \Lambda p_3 \ , \ \text{per} \quad \tau \to \infty \ . \tag{2.46}$$

So the solution of the system becomes

$$\begin{aligned} a^2 &= \frac{2\Lambda|p_1|}{\cosh\left(2\Lambda\tau|p_1|\right)} \\ b^2 &= b_0^2 \exp\left[2\Lambda\tau\left(p_2 - |p_1|\right)\right]\cosh\left(2\Lambda\tau|p_1|\right) \\ c^2 &= c_0^2 \exp\left[2\Lambda\tau\left(p_3 - |p_1|\right)\right]\cosh\left(2\Lambda\tau|p_1|\right) \end{aligned} \tag{2.47}$$

We consider now the obtained solutions in the limit $\tau \to \infty$: towards the singularity they can be simplified as

$$\begin{aligned} a &\sim \exp\left[-\Lambda p_1\tau\right] \\ b &\sim \exp\left[\Lambda\left(p_2 + 2p_1\right)\tau\right] \\ c &\sim \exp\left[\Lambda\left(p_3 + 2p_1\right)\tau\right] \\ t &\sim \exp\left[\Lambda\left(1 + 2p_1\right)\tau\right] \end{aligned} \tag{2.48}$$

which, as function of t become

$$a \sim t^{p'_l} \ , \ b \sim t^{p'_m} \ , \ c \sim t^{p'_n} \ , \ abc = \Lambda' t \tag{2.49}$$

where we defined the $'$ variables in the following way

$$\begin{aligned} p'_l &= \frac{|p_1|}{1-2|p_1|} \ , \qquad p'_m = -\frac{2|p_1| - p_2}{1-2|p_1|} \ , \\ p'_n &= \frac{p_3 - 2|p_1|}{1-2|p_1|} \ , \qquad \Lambda' = (1-2|p_1|)\,\Lambda \ . \end{aligned} \tag{2.50}$$

Let us analyze the obtained results: the perturbation to the Kasner regime ensures that one Kasner epoch will be replaced by another one in such a way that the negative index goes from the direction **l** to the direction **m**. In this way the term that previously contributed to the perturbation now is damped and eventually becomes negligible, while one of the terms that before were negligible now grows to become the principal perturbation. Such index exchanges are formalized in the rules of the BKL map, with the bigger positive index that remains positive.

The following swaps are characterized by a series of *bounces*, with the negative index that shift from the l direction to the m one until the integer part of the initial value of u become null, i.e until $u > 1$. Then, thanks to the inversion rules above, we can transform $u < 1$ in $u > 1$ and we return to the situation in which one between p_l and p_m is negative while p_n is the smallest positive index, and so the next series of shifts will be between **l** and **n** or between **m** and **n**. In terms of the parameter u the map (2.50) takes the form

$$u' = \begin{cases} u-1, & \text{per} \quad u > 2 \\ \frac{1}{u-1}, & \text{per} \quad u < 2. \end{cases} \tag{2.51}$$

This phenomenon of growth and decrease of the various terms with the transition from one Kasner era to the next one is repeated an infinite number of times until the singularity. We now want to concentrate on the implication of the BKL map and its inversion properties.

We write the initial value of u as $u^0 = k^0 + x^0$ with k^0 and x^0 respectively the integer part and the fractional one of u. The continuous exchanges proceed until u becomes less than 1, i.e. for a number of times equal to k^0 Kasner eras. The new value of the parameter will be $u' = 1/x^0 > 1$, with the Kasner indices that transform as (2.36) and the new switches will be $l \to n$ or $m \to n$.

The evolution of the model towards the singularity consists in a succession of eras, in which the distances oscillate on two axes while decreasing along the third one, while the volumes always decrease (roughly) linearly with the synchronous time t. The order in which the switches between the axes take place and the lengths of the eras assume a stochastic behavior, and towards the singularity they tend to be thickened. The qualitative analysis does not change even if we insert a matter term in the equations.

In the Bianchi IX model, the dynamics of the Universe near the classical singularity can be described as a chaotic motion of the particle; more precisely, this particle impacts an infinite number of times against a pseudo-triangular potential barrier, on a bi-dimensional plane that describes the configuration space of the Universe dynamics. The Taub model consists in reducing the problem to the study of a $1-D$ particle that bumps into a potential wall with only one possible degree of freedom: this situation corresponds to choose a preferential direction in the Bianchi IX bi-dimensional configuration space, in particular we have chosen to cancel one of the anisotropic variables of the model [47], but the problem has triangular symmetry so one can choose arbitrarily the preferential direction.

2.2 Canonical and Polymer Quantizations of the Gravitational Field

2.2.1 Brief historical background

A little time after the formulation of the Quantum Field Theory (QFT), by Heisenberg, Pauli, Fock and Dirac, many scientists tried to implement it on fields different from the Electromagnetic one for which the theory was developed. In 1930, the Belgian physicist Léon Rosenfeld attempted to use it directly on the gravitational field but, from the beginning, he found out that there were some serious technical problems and tried to solve them with general methods; first thing he calculated the gravitational self-energy of a photon at the lowest perturbative order obtaining a quadratic divergence, confirming the divergent nature of the QFT already experienced in the calculation of the electromagnetic self-energy of an electron. Many read in his results a prediction that, from the very beginning, the quantum gravitodynamics was destined to be inextricably linked to the difficulties which are at the basis of the particles physics.

Throughout the vast excitement of the physics during the 30s, the problems linked to the *insane* nature of the QFT were often set aside; moreover it soon became clear that the quanta of the gravitational field (assuming their existence) could not give noticeable contributions beneath energies of the order of the Planck Energy, i.e. 10^{28} eV, and unfortunately this persuaded many researchers to give up on such a theory.

In 1950, the American physicist Bryce S. DeWitt, with his PhD thesis, retraced the path started by Rosenfeld, using a manifestly Lorentz-covariant and gauge invariant formulation; such a study was supported by the contemporary renormalization theories of Tomonaga, Schwinger and Feynman, and was due to the demonstration that the results of the Belgian scientist imply a mere renormalization of the charge rather than a finite mass for the photon. However, during his analysis, an unexpected difficulty appeared, caused by the fact that there were not one but two gauge groups at the same time (firstly the electromagnetic one and on the other hand the one associated to gravity) that do not combine in the form of a direct product, but instead they combine in the form of a *semidirect* product based on the authomorphisms of the electromagnetic gauge group under general transformations of the coordinates. This means that if we want to keep a fixed gauge, we have to implement on every coordinates transformation an electromagnetic gauge transformation; however the calculation was made at the first perturbative order, which includes only closed 1-loop Feynman diagrams and so, in this case, the problem can be easily solved.

Approximately in the same period of DeWitt, there was a more ambitious study carried out by the German physicist Peter Bergmann; although the renormalization technique obtained some important results in the quantum electrodynamics (QED), it was still under special surveillance because of the particular explicit manipulation of the divergences. Similar difficulties (even if more basic) still persisted in the classical particles theory, with only one exception: the interaction theory of point-particles with gravity; in 1938, Einstein, Infeld and Hoffmann demonstrated that the equations of motion of such particles were derived only from the equations of the gravitational field, without bringing up the divergent quantities or concepts like the *self-mass*, in addition this result was rapidly generalized to the case of electric charged particles and with the pledge of being applicable even to the case of particles with spin. The gravitational field, so, appeared as a classical regulator and Bergman inferred that it could be true even in the quantum theory; since that, in the work of Einstein, Infeld and Hoffmann, the fields were the basis and the particles were mere singularities of the fields themselves, the first duty of the German scientist was to quantize the gravitational field hoping that the commutation rules for the positions and their momenta would come out as corollaries.

The obstacles faced by Bergmann were enormous. First of all, the equations of motion depended strongly on the non-linearity of the Einstein equations and so it was mandatory to quantize the whole non-linearity of the gravitational field; then it was necessary to find a certain way of defining the positions and their conjugated momenta of the particles as function of only the field variables; on the other hand, it would eventually be required to include even the spin so that the calculation could be generalized to all the particles that obey the Dirac equation; finally, it was necessary to extract the Fermi statistics (for the particles) from the Bose one (followed by the gravitational field); moreover, he would have to be able to completely remove the asymmetry between the particles and the field in order to justify, as in QED, the creation of couples and the vacuum polarization. It is not surprising that, even nowadays, the objective of Bergmann is, like in the past, out of reach.

In order to reach his aim, Bergmann undertook the classical canonical way in search of a Hamiltonian; although this road, treating the time differently from the space, goes against the spirit of every relativistic theory, it seemed a good intuition for many reasons: firstly, because there wasn't an alternative method; secondly, the canonical approach allows for a fast way to observe some important properties of the theory; finally, at the time it seemed plausible that they could use the standard perturbative theory for some of the calculations.

However, Bergmann faced, from the very beginning, great difficulties, as Rosenfeld himself predicted, that were called "constraint problems" and they appeared in the following way: some of the variables of the field did not have a conjugated momentum, while the remaining conjugated momenta weren't dynamically independent, even the field equations were linearly dependent and few of them didn't include second derivative in time and so the Cauchy problem was more difficult to solve. All these problems were due to the existence of a group of general coordinates transformations as invariant group for the theory. Similar troubles were found even for the electromagnetic field and it was developed a method in order to treat them, but in the case of the gravitational field its implementation resulted much more complicated; a big problem was due to the fact that non all the relations between the momenta (see the constraints) are linear, moreover we should not forget that since the invariance group for the gravity is non-Abelian, the calculations, made in order to demonstrate that the commutators of the various constraints did not bring up inner inconsistencies, resulted longer and more difficult.

Bergmann and his team did a really great job in formulating specifically all the difficulties and solving them partially, while in the meantime an unexpected help came to them; in 1950 Dirac published the basis for a general Hamiltonian theory that had to be, in principle, applicable to every system described by an Action principle. Pirani and Schild rapidly understood the potential of this theory and implemented it on the gravitational field; unfortunately they chose to develop their theory in a parametric formalism in the hope of obtaining an evident covariance that the Dirac method would have otherwise destroyed; the complexity of the algebra prevented the calculation of all the constraints.

The theory spent many years in this incomplete state, but regained strength after the Relativity Jubilee in 1955 and the second international conference on the theory in 1957, a little step forward was made by DeWitt that showed how, using the Pirani-Schild formalism, the four so-called primary constraint could be rewritten as pure momenta thanks to a phase transformation. This meant that the gravity wavefunction did not depend on the metric's $g_{0\mu}$ components. Shortly after, Higgs demonstrated that the secondary (or dynamical) constraints were the generators of infinitesimal transformations for the spatial coordinates. This implied that the state has to be independent of the coordinates chosen on the space-like hypersurfaces $x^0 =$ constant and so they could not be taken as arbitrary functions of the metric's g_{ij} components. Dirac himself started to implement his method to the gravitational field and, following some simplifications and clarifications, it became clear that the fourth dynamical constraint was consistent with the others, and the theory for the first time gained the state "Technically completed". At the time, however, the scientists started to ask themselves "What is the meaning of all this?"

In the classical theory, the issue of the physical interpretation was easily solved by Arnowitt, Deser and Misner, which demonstrated how to use the canonical formalism in order to obtain a precise characterization of the gravitational radiation and its energy. In the quantum theory, instead, such an interpretation remained confusing for many years precisely because the scientists could not formalize the right questions, only in the 60s the priorities were highlighted, especially thanks to the patient research of Wheeler that was inspiring for many physicists, in particular for DeWitt.

The close cooperation between these two scientists gave to the literature a lot of contributions that are even nowadays largely used in the modern research in this field; it was, in particular, the necessity to study the structure of the manifold in which the wavefunction is defined that led to several interesting results, namely it gave a way to interpret all of the problems that, although not definitive, could be used in the past and even today. Their target was, initially, the case of finite Universes firstly because the issues are most critical and bizarre, and then because the case of infinite Universes is treated better with a manifestly covariant theory; although this theory reached the level of technical completeness thanks to the hard work of Feynman, it is quite different from the canonical theory and even now there is not a clear mathematical link between them even if they are complementary: the

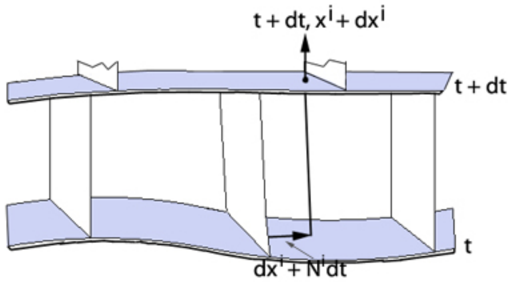


Figure 2.2. Example of a 3+1 Space Time

canonical formulation is needed for describing the quantum behavior of a 3-space as a geometrical object varying in time, while the covariant one describes the behavior of both real and virtual gravitons that propagate in it. [21]

Let us analyze how to formulate the issue of describing a tridimensional space as an object varying in time and this will lead to the natural birth of an important equation that is the basis of the majority of the modern quantum cosmology, the Wheeler-DeWitt equation.

2.2.2 ADM formulation

The study of the dynamics of the Universe in a quadrimensional space-time is always quite difficult, but there are a few prescriptions that allow to simplify the problem, one of such prescriptions is the subdivision of a 4-D space in a $3+1$ space-time obtained considering a family of hypersurfaces space-like. [42]

The simplest foliation one can imagine is the one shown in figure (2.2), in which the parameter that separate the surfaces is a "time" and the distance between two successive hypersurfaces is infinitesimal.

We start [31] requiring that our space-time variety is globally hyperbolic (i.e. it is composed by Cauchy hypersurfaces [1]) and so once fixed the initial conditions it is possible to describe the past and future evolution univocally. Every Cauchy hypersurface represents a picture of our universe, taken at a set value of the real parameter t which identify it uniquely. As a result we operate a space foliation of the kind $\mathcal{M} = \Sigma_t \otimes \mathbb{R}$, decomposing the 4-D variety $\mathcal{M}$ in a union of parallel 3-D subvarieties.

Such a foliation requires the introduction of a time-like vector n orthogonal to the surfaces Σ_t. Then, if we introduce also the 3-metric h_{ij} which characterize the geometry of the Σ_t, we can define two important quantities: the Lapse Function N and the Shift Vector N_i. Such functions specify, respectively, the proper time in the hypersurfaces, and the distance between the intersection of n^μ and Σ_{t+dt} and the position of x^i on Σ_{t+dt}. As we can observe from figure 2.2, the distance is redefined using the analogous of the Pitagora Theorem on curved spaces:

$$ds^2 = h_{ij}\left(dx^i + N^i dt\right)\left(dx^j + N^j dt\right) - (Ndt)^2 \ , \tag{2.52}$$

[1] **Cauchy Hypersurfaces**: Subset of the space-time intersected only by curves that are not space-like

where the metric tensor is the one of the 3-geometries, quite different from

$$ds^2 = {}^{(4)}g_{\alpha\beta}dx^\alpha dx^\beta \tag{2.53}$$

in which the metric tensor is the 4-D one. Comparing the two above expressions we can obtain the 4-metric from the tridimensional one in the following way [47]

$$\begin{vmatrix} {}^{(4)}g_{00} & {}^{(4)}g_{0k} \\ {}^{(4)}g_{i0} & {}^{(4)}g_{ik} \end{vmatrix} = \begin{vmatrix} (N_s N^s - N^2) & N_k \\ N_i & h_{ik} \end{vmatrix} \tag{2.54}$$

naturally the same can be done with the inverse metric.

The action of the gravity is the *Einstein-Hilbert* one and can be read as

$$S = -\frac{1}{2c\chi}\int d^4x\ \sqrt{-g}\ {}^{(4)}R \tag{2.55}$$

with ${}^{(4)}R$ the quadridimensional curvature scalar; it is possible to express it as function of the variables (N, N_i, h_{ij}) as:

$${}^{(4)}R = K^2 - K_{ij}K^{ij} - {}^{(3)}R \tag{2.56}$$

where K_{ij} is the extrinsic curvature, i.e. the curvature of Σ_t seen from a 4-D point of view, defined by

$$\begin{aligned} K_{ij} &\equiv \frac{1}{2N}\left({}^{(3)}\nabla_i N_j + {}^{(3)}\nabla_j N_i - \partial_t h_{ij}\right) \\ K &\equiv h_{ij}K^{ij} = Tr\left(K^{ij}\right)\ . \end{aligned} \tag{2.57}$$

We can rewrite the action (2.55) as

$$S = -\frac{1}{2c\chi}\int dt \int d^3x\ N\ \sqrt{h}\left[K^2 - K_{ij}K^{ij} - {}^{(3)}R\right]\ . \tag{2.58}$$

We can also calculate the conjugated momenta to N and N_i from the Lagrangian density $\mathcal{L}$ of the gravitational field:

$$\Pi = \frac{\delta\mathcal{L}}{\delta\left(\partial_t N\right)} = 0\ , \quad \Pi_i = \frac{\delta\mathcal{L}}{\delta\left(\partial_t N^i\right)} = 0\ . \tag{2.59}$$

The relations (2.59) are a consequence of the fact that the Lagrangian does not depend explicitly on the derivatives of N and N_i and so they are called Primary Constraint. In the same way we can obtain the conjugated momentum to the metric tensor h_{ij} as:

$$\Pi^{ij} = \frac{\delta\mathcal{L}}{\delta\left(\partial_t h_{ij}\right)} = \frac{1}{2c\chi}\sqrt{h}\left(Kh^{ij} - K^{ij}\right) \neq 0\ . \tag{2.60}$$

Using a Legendre transformation and the constraints (2.59), it is possible to rewrite the action in a more suitable form

$$S = \int dt \int d^3x\ \left\{\Pi^{ij}\partial_t h_{ij} - N\mathcal{H} - N^i\mathcal{H}_i\right\}\ , \tag{2.61}$$

where we defined

$$
\begin{aligned}
\mathcal{H} &\equiv G_{\alpha\beta\gamma\delta}\Pi^{\alpha\beta}\Pi^{\gamma\delta} - \frac{\sqrt{h}^3}{2\kappa} R \\
\mathcal{H}_\alpha &\equiv -2h_{\alpha\gamma}\nabla_b \Pi^{\gamma\beta} \\
G_{\alpha\beta\gamma\delta} &\equiv \frac{\kappa}{\sqrt{h}}\left(h_{\alpha\gamma}h_{\beta\delta} + h_{\alpha\delta}h_{\beta\gamma} - h_{\alpha\beta}h_{\gamma\delta}\right) \ .
\end{aligned}
\tag{2.62}
$$

The Lapse Function and the Shift Vector act in the action as Lagrange Multipliers, and so they do not affect the dynamics. Moreover, calculating the commutators with the Hamiltonian and imposing reasonable conditions, it is possible to observe that

$$
\begin{aligned}
\left[\Pi \ , \ H_{ADM}\right] &= -\mathcal{H} \approx 0 \ , \\
\left[\Pi_k \ , \ H_{ADM}\right] &= -\mathcal{H}_k \approx 0 \ ;
\end{aligned}
\tag{2.63}
$$

those make the SuperHamiltionian and the SuperMomentum second class constraints. In (2.63) we defined the ADM Hamiltonian that is simply the ordinary Hamiltonian solved in one of the inner variables. Being the ADM Hamiltonian a combination of first and second class constraints, we can state that even the latter is null, and this imposes an important constraint to the system, the Hamiltonian one.

Now all we have to do is to implement the Dirac prescription for the quantization of the constrained systems and define the physical states as the ones that are annihilated by the operators associated to the constraints [48]; since the conjugated momenta Π and Π_i are null, we can impose the following conditions on the wavefunction

$$
\begin{aligned}
-i\hbar\frac{\delta}{\delta N}\Psi\left(N, N^i, h_{ij}\right) &= 0 \ , \\
-i\hbar\frac{\delta}{\delta N^i}\Psi\left(N, N^i, h_{ij}\right) &= 0 \ ,
\end{aligned}
\tag{2.64}
$$

which can be easily solved taking a Universe wavefunction as a function only of the 3-metric and not of the variables that describe the slicing of the space-time. The SuperMomentum constraint, instead, can be seen as

$$
\hat{\mathcal{H}}_i\Psi = \mathcal{D}_i\left[\frac{\delta}{\delta h_{ij}}\Psi\left(N, N^i, h_{ij}\right)\right] = 0 \ , \tag{2.65}
$$

which is solved imposing that the wavefunction is a function only of the 3-geometries rather than one particular representation.

2.2.3 Hamiltonian formulation of the dynamics

We start considering the line element for a generic homogeneous space-time in the standard ADM formulation [47]

$$
ds^2 = N^2(t)\, dt^2 - h_{\alpha\beta}dx^\alpha dx^\beta \ , \tag{2.66}
$$

where

$$
h_{\alpha\beta} = e^{q_l} l_\alpha(x^\gamma)\, l_\beta(x^\gamma) + e^{q_m} m_\alpha(x^\gamma)\, m_\beta(x^\gamma) + e^{q_n} n_\alpha(x^\gamma)\, n_\beta(x^\gamma) \tag{2.67}
$$

with q_a $(a = l, m, n)$ depending only on time. For the Bianchi Models, moreover, it can be written even as function of the 1-forms imposing

$$h_{\alpha\beta}dx^{\alpha}dx^{\beta} = \eta_{\alpha\beta}\omega^{\alpha}\omega^{\beta} = e^{q_a}\delta_{ab}\omega^{a}\omega^{b} \ , \tag{2.68}$$

in such a way that for example for the Bianchi IX model we obtain [47]

$$\begin{aligned} \omega^1 &= \sin\psi\sin\theta d\phi + \cos\psi d\theta \\ \omega^2 &= -\cos\psi\sin\theta d\phi + \sin\psi d\theta \\ \omega^3 &= \cos\theta d\phi + d\psi \end{aligned} \tag{2.69}$$

where $\theta \in [0, \pi)$, $\phi \in [0, 2\pi)$ and $\psi \in [0, 4\pi)$ are the Euler angles. The Einstein-Hilbert action in the vacuum can be integrated on the spatial variables providing the factor

$$\int \omega^1 \wedge \omega^2 \wedge \omega^3 = \int \sin\theta d\phi \wedge d\theta \wedge d\psi = (4\pi)^2 \ . \tag{2.70}$$

It is worth noting that this is simply the surface of a tri-sphere of radius 2: the closed FRW, indeed, is a particular case of the Bianchi IX Model, for $q_a = q_b = q_c$. As a consequence, the evolution of the dynamics in vacuum of Bianchi IX is summed up by the variational principle

$$\delta S_B = \delta \int_{t_1}^{t_2} \mathcal{L}_B\left(q_a, \dot{q}_b\right) dt = 0 \ . \tag{2.71}$$

Here t_1 and t_2 define two fixed time values and the lagrangian $\mathcal{L}$ is described by

$$\mathcal{L}_B = -\frac{8\pi^2\sqrt{\eta}}{\kappa}\left[\frac{1}{2N}\left(\dot{q}_l\dot{q}_m + \dot{q}_l\dot{q}_n + \dot{q}_n\dot{q}_m\right) - N^3R\right] \ . \tag{2.72}$$

Defining more clearly the potential term [47] we obtain

$$\begin{aligned} \eta^3 R &= -\frac{1}{2}\left(\sum_a \lambda_a^2 e^{2q_a} - \sum_{a\neq b}\lambda_a\lambda_b e^{q_a+q_b}\right) \ , \\ \eta &= \det\left(\eta_{ab}\right) = \exp\left(\sum_a q_a\right) \ . \end{aligned} \tag{2.73}$$

From the Lagrangian formulation, the Hamiltonian is gained by a Legendre transformation, i.e. calculating the momenta p_a conjugated to the generalized coordinates q_a as [48] [47]

$$\begin{aligned} p_l &\equiv \frac{\partial\mathcal{L}}{\partial\dot{q}_l} = -\frac{4\pi^2}{\kappa}\frac{\sqrt{\eta}}{N}\left(\dot{q}_m + \dot{q}_n\right) \\ p_m &\equiv \frac{\partial\mathcal{L}}{\partial\dot{q}_m} = -\frac{4\pi^2}{\kappa}\frac{\sqrt{\eta}}{N}\left(\dot{q}_l + \dot{q}_n\right) \\ p_n &\equiv \frac{\partial\mathcal{L}}{\partial\dot{q}_n} = -\frac{4\pi^2}{\kappa}\frac{\sqrt{\eta}}{N}\left(\dot{q}_m + \dot{q}_l\right) \end{aligned} \tag{2.74}$$

and then taking into account the standard transformation

$$N\mathcal{H}_B = \sum_{a=l,m,n} p_a\dot{q}_a - \mathcal{L}_B \ , \tag{2.75}$$

where the $\dot{q}_a$ are obtained thanks to the equations (2.74). In this way we can derive the action

$$S_B = \int dt \left(p_a \dot{q}^a - N\mathcal{H}_B \right) \ , \tag{2.76}$$

with

$$\mathcal{H}_B = \frac{\kappa}{8\pi^2\sqrt{\eta}} \left[\sum_a \left(p_a\right)^2 - \frac{1}{2}\left(\sum_b p_b\right)^2 - \frac{64\pi^4}{\kappa^2}\eta^3 R \right] \ , \tag{2.77}$$

where $\mathcal{H}_B = 0$ is the constraint for those models.

We now introduce the so-called anisotropic parameters, defined by

$$Q_a \equiv \frac{q_a}{\sum_b q^b} \quad , \quad \sum_a Q_a = 1 \ . \tag{2.78}$$

These parameters allow us to read the last term on the RHS of (2.77) as a potential for the dynamics. In fact it can be rewritten as

$$\eta^3 R = -\frac{1}{2}\left(\sum_a \lambda_a^2 \eta^{2Q_a} - \sum_{b \neq c} \lambda_b \lambda_c \eta^{Q_b + Q_c} \right) \ . \tag{2.79}$$

The principal benefit of writing the potential as in (2.79) is when we study its properties in the asymptotic limit towards the cosmological singularity ($\eta \to 0$). Actually the second term on the RHS of equation (2.79) becomes negligible and the first one strongly dependent on the sign of the Q_a. As a consequence the potential can be represented as an infinitely deep box

$$-\eta^3 R = \sum_a \Theta_\infty \left(Q_a\right) \tag{2.80}$$

where

$$\Theta_\infty\left(x\right) = \begin{cases} +\infty, & \text{se}\, x < 0 \\ 0, & \text{se}\, x > 0 \ . \end{cases} \tag{2.81}$$

From equation (2.80) we can see how the Universe dynamics is similar to the one of a particle confined in the domain Π_Q, defined by the simultaneous positiveness of all the anisotropy parameters.

2.2.4 Wheeler-Dewitt equation

In order to continue the analysis of the canonical theory, it is necessary to introduce a specific representation for the quantum states; following the original approach of Wheeler and DeWitt we can use the so-called metric representation, in which the wavefunction Ψ depends only on the metric components and the momenta become differential operators

$$\Pi = -i\frac{\delta}{\delta N} \ , \ \Pi_i = -i\frac{\delta}{\delta N^i} \ , \ \Pi^{ij} = -i\frac{\delta}{\delta h_{ij}} \tag{2.82}$$

As above described, the first class constraints allow us to state that the wavefunction depends only on the tri-geometries and it will be labeled as $\Psi\left(h_{ij}\right)$. A method to express such a dependence is to impose that Ψ is a function of a numerable infinite set of variables, in particular all the constants that can be built from the Riemann tensor and its covariant derivatives multiplied by the topology of the tri-space.

Let us denote $\mathcal{M}$ the set of all the possible tri-geometries owned by a finite Universe, the first question to address is: "Is it possible to impose a topology on $\mathcal{M}$ that is useful and, at the same time, that holds a well defined physical meaning in the context of the Quantum Mechanics?" A possibility is to consider $\mathcal{M}$ as an infinite dimensional vector space in which the elements are discrete sets of the above invariants; in this case, the topology will be naturally defined by the Cartesian metric of such a space. But this method is not very useful since, even if we have to assign a metric (and so a pseudo-Riemanian structure) to $\mathcal{M}$, it does not grant us any concrete advantage, however it can be helpful in order to remember that $\mathcal{M}$ is not a simple set but a manifold which will be the domain of the wavefunction Ψ and its elements will be the tri-geometries.

We now want to describe the quantum dynamics of the gravitational field. As above said, all the dynamics is included, from a classical point of view, in the SuperHamiltonian constraint. In the same way, once implemented all the quantization procedure, all the informations on the system must necessarily be found in the quantum formulation of the same constraint, i.e.

$$\left(G_{ijkl}\frac{\delta}{\delta h_{ij}}\frac{\delta}{\delta h_{kl}} - \sqrt{h}\ {}^{(3)}R\right)\Psi\left(h_{ij}\right) = 0\ , \tag{2.83}$$

where

$$G_{ijkl} \equiv \frac{1}{2\sqrt{h}}\left(h_{ik}h_{jl} + h_{il}h_{jk} - h_{ij}h_{kl}\right)\ . \tag{2.84}$$

Equation (2.83) is known as the Wheeler-DeWitt equation and it is a fundamental relation for the quantum dynamics of the gravitational field.

There are, although, some things to highlight. First of all, a structure of a Hilbert space in the domain of the solutions of the constraints has yet to be identified. The major difficulties are the definition of a basis of the physical Hilbert space (the equation (2.83) is not linear) and the definition of an inner product. Another problem is that the equation holds a physical meaning only if we can regularize the product of the operators acting on the same point, this can be achieved by the definition of a triangulation of the spatial manifold and implementing the product only on the vertices of the triangles. This regularization allows to regularize the Wheeler-DeWitt and simplifies the potential term treatment. This approach is promising since it gives a more solid mathematical basis to the theory, but it is not yet sure that it could solve all the problems of the canonical quantization of the gravity.

Another big issue is the so-called "Frozen Formalism", in the ordinary quantum mechanics the Hamiltonian operator is the generator of the time-translation of the phase-space which leads to the Schrödinger equation, but, in the gravitation case, the Hamiltonian of the field is a linear combination of the SuperHamitonian and SuperMomentum constraints and so, under the Dirac scheme, it would annihilate the physical states

$$\hat{\mathcal{H}}\Psi = 0\ . \tag{2.85}$$

The last equation could be interpreted as a Schrödinger equation for a state independent of time and this means that there is no evolution for the states, and so there could not exist a quantum dynamics. The problem here is due to the different concept of the time in the two theories: for the quantum mechanics, time is an external parameter in which the system evolves, while, for the General Relativity, time is only a mere coordinate like the spatial ones and it is not observable (because the equations are invariant under general transformation of coordinates).

2.2.5 Vilenkin approach

Since the formulation of the Quantum Field Theory, many well-known physicists took on the challenge of quantizing the gravitational field, a lot of different approaches were tried but all of them showed a few problems often insurmountable. One of the most observed issues was the probabilistic interpretation of the Universe wavefunction; in fact, the quantum theory requires an external time in which the system evolves, but in General Relativity this cannot be possible since time is an inner variable and this fact causes enormous problems when we try to integrate the squared module of the wavefunction.

In this thesis, I chose a particular approach that suggests a viable solution to the above problem, the approach of Alexander Vilenkin. The Ukrainian theoretical physicist, now professor in the Tufts University (Massachusettes), in a paper published in 1989 [54] provided a rather linear and elegant procedure which allows to obtain a probabilistic interpretation of the Universe wavefunction consistent with the studies of Bohr from the beginning of the century.

He analyzed the simple case of a homogeneous minisuperspace where the variables are the tri-geometries (i.e. the tri-metric linked by diffeomorphisms), in addition he chose to use the ADM formulation. From the SuperHamiltonian constraint he derived the Wheeler-DeWitt equation (WDE) which is a generalized Klein-Gordon equation (KGE) in n dimensions and with a variable mass. This corresponded to a conserved current that ensured the conservation of the probability density. Such an analogy with the KGE naturally took to the well-known issue of the negative probabilities.

In order to avoid this problem, Vilenkin chose to divide the minisuperspace variables into two separate classes: semiclassical variables and quantum ones; the presence of the first class is fundamental in order to make the probability semidefinite positive. The results of the original paper are divided in two sections, in the first all the variables are classical, in the latter he included a set of quantum variables and compared the two dynamics; all the idea is based on three important assumptions:

1. WKB Approximation of the wavefunction:

$$\psi\left(h^{\alpha}\right)=A\left(h^{\alpha}\right)e^{\frac{i}{\hbar}S(h^{\alpha})}\phi\left(h^{\alpha},q_{\nu}\right)\ ; \tag{2.86}$$

   where A is the amplitude, S is the action of the system, h^{α} is a compact notation indicating all the semiclassical variables while q^{ν} denotes the quantum ones.

2. Adiabatic hypothesis: division between fast and slow variables [27];

3. Negligibility hypothesis: the effect of the quantum variables on the semiclassical ones is negligible [27].

For the purposes of the Vilenkin paper [54] the WDE is simply

$$\left(\nabla^2 - U - H_q\right)\psi = 0 \tag{2.87}$$

where the ∇ operator is defined with the covariant derivatives and in the studied case reduced to $g^{\alpha\beta}\partial_\alpha\partial_\beta$, H_q is the Hamiltonian related to the quantum variables of the system and the potential term U is of the order $\hbar^{-2}$; from this equation derives naturally the definition of the conserved current

$$j^\alpha = -\frac{i}{2}\hbar g^{\alpha\beta}\left(\psi^*\nabla_\beta\psi - \psi\nabla_\beta\psi^*\right) \ , \tag{2.88}$$

which satisfies $\nabla_\alpha j^\alpha = 0$.

Replacing equation (2.86) into (2.87), and deriving the various order in $\hbar$, he wrote the equations which describe the system. At the lowest order he obtained the Hamilton-Jacobi equation for the action S, while at the following order he gained both the equation for the amplitude A and, when there is at least one quantum variable, the Schrödinger equation for the ϕ. Now I will show how to practically derive those equations and I will try to explain their physical meaning, they will also be necessary for the purposes of my first original work that will be widely presented in the following.

Let us start with the case in which all the variables are semiclassical. This implies that equations (2.86) and (2.87) respectively reduce to

$$\begin{aligned} \psi\left(h^\alpha\right) &= A\left(h^\alpha\right)e^{\frac{i}{\hbar}S(h^\alpha)} \ , \\ \left(\nabla^2 - U\right)\psi &= 0 \ . \end{aligned} \tag{2.89}$$

and so we get the following equation

$$\left(\hbar^2 g^{\alpha\beta}\partial_\alpha\partial_\beta - U\right)Ae^{\frac{i}{\hbar}S} = 0 \tag{2.90}$$

that can be written explicitly as

$$\begin{aligned} \hbar^2 g^{\alpha\beta}\partial_\alpha\left[\left(\partial_\beta A\right)e^{\frac{i}{\hbar}S} + \frac{i}{\hbar}A\left(\partial_\beta S\right)e^{\frac{i}{\hbar}S}\right] - UAe^{\frac{i}{\hbar}S} = \\ \hbar^2 g^{\alpha\beta}\left[\left(\partial_\alpha\partial_\beta A\right)e^{\frac{i}{\hbar}S} + \frac{i}{\hbar}\left(\partial_\beta A\right)\left(\partial_\alpha S\right)e^{\frac{i}{\hbar}S} + \frac{i}{\hbar}\left(\partial_\alpha A\right)\left(\partial_\beta S\right)e^{\frac{i}{\hbar}S}\right] + \\ +\hbar^2 g^{\alpha\beta}\left[\frac{1}{\hbar}A\left(\partial_\alpha\partial_\beta S\right)e^{\frac{i}{\hbar}S} - \frac{1}{\hbar^2}A\left(\partial_\beta S\right)\left(\partial_\alpha S\right)e^{\frac{i}{\hbar}S}\right] - UAe^{\frac{i}{\hbar}S} = 0 \ . \end{aligned} \tag{2.91}$$

We now study the lowest order terms of the above equations. Those correspond to the Hamilton-Jacobi equation for the action S

$$g^{\alpha\beta}\left(\partial_\beta S\right)\left(\partial_\alpha S\right) + U = 0 \ . \tag{2.92}$$

If we consider the following perturbative order we get the equation for the amplitude A

$$i\hbar\left\{g^{\alpha\beta}\left[\left(\partial_\beta A\right)\left(\partial_\alpha S\right) + \left(\partial_\alpha A\right)\left(\partial_\beta S\right) + A\left(\partial_\alpha\partial_\beta S\right)\right]\right\} = 0 \ . \tag{2.93}$$

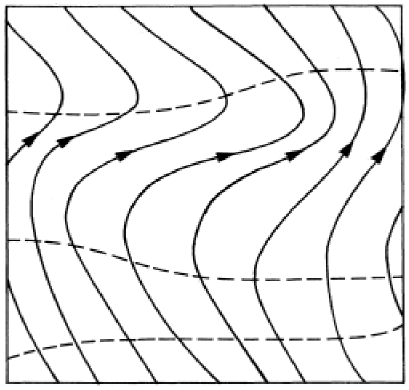


Figure 2.3. Space-like Hypersurfaces crossed only one time by the trajectories

From the definition of the current (2.88), instead, we get:

$$\begin{aligned} j^{\alpha} = & -\frac{i}{2}\hbar g^{\alpha\beta}\left\{\left(A^{\dagger}e^{-\frac{i}{\hbar}S}\right)\left[\left(\partial_{\beta}A\right)e^{\frac{i}{\hbar}S}+\frac{i}{\hbar}A\left(\partial_{\beta}S\right)e^{\frac{i}{\hbar}S}\right]\right\}+ \\ & +\frac{i}{2}\hbar g^{\alpha\beta}\left\{\left(Ae^{\frac{i}{\hbar}S}\right)\left[\left(\partial_{\beta}A^{\dagger}\right)e^{-\frac{i}{\hbar}S}-\frac{i}{\hbar}A^{\dagger}\left(\partial_{\beta}S\right)e^{-\frac{i}{\hbar}S}\right]\right\} \end{aligned} \tag{2.94}$$

which, at the lowest order, returns:

$$j^{\alpha} = |A|^{2}\left(\partial^{\alpha}S\right) \tag{2.95}$$

if we now differentiate the above current saturating the index α we get exactly the (2.93) and so we verify the existence of a conserved current.

The action S describes a family of classical trajectories, one for every point of the configuration space allowed by the reality condition of the action. The conjugated momentum, along the solution of the motion in every point h^{α} is $p_{\beta} = \partial_{\beta}S\left(h^{\alpha}\right)$, while the *velocity* is, from the Hamilton equations,

$$\dot{h}^{\alpha} = N\frac{\partial H}{\partial p_{\alpha}} = 2N\partial^{\alpha}S \propto p_{\alpha}\ . \tag{2.96}$$

Following the Vilenkin approach, we assume that the minisuperspace variables are chosen in such a way that $S\left(h\right)$ is a single value function[54] [55]; the probability distribution must be defined on $n-1$ dimension surfaces, in order to replicate the role of fixed time surfaces. Moreover, there is the possibility of choosing every family of surfaces, with the only requirement that they are crossed exactly once by the trajectories and in the same direction, as shown in figure (2.3).

Mathematically, this can be formulated as the condition that $\dot{h}^{\alpha}d\Sigma_{\alpha}$ has the same sign for every element of the surface. The choice of the sign is arbitrary and we can easily take it so that it satisfies $\dot{h}^{\alpha}d\Sigma_{\alpha} > 0$. The probability density is defined by $dP = j^{\alpha}d\Sigma_{\alpha}$ and for all the above discussion is semidefinite positive. In this way it is possible a normalization of the wavefunction so that $\int_{\mathfrak{V}} j^{\alpha}d\Sigma_{\alpha} = 1$ with $\mathfrak{V}$ representing all the space-time.

A suitable choice of the surfaces can be the one in which S is constant, being them orthogonal, by definition, to the family of trajectories; there is, also, the freedom to make a coordinates transformation in the superspace in order to choose $h_n = t$ as one of the coordinates. The conservation of the current $\partial_\alpha j^\alpha$ can be rewritten as

$$\frac{\partial \rho_0}{\partial t} + \partial_\alpha J^\alpha = 0 \ , \tag{2.97}$$

where $J^\alpha = \rho_0 \dot{h}^\alpha$ and the index α goes from 1 to $n-1$. In this case $\rho\left(h^\alpha, t\right)$ can be interpreted as the distribution function of an ensemble of classical Universes so that h^α characterizes the trajectories and ρ_0 is the probability density of the Universe evolving along the trajectory described by h^α.

If we consider the case in which the wavefunction is a superposition of many WKB terms, we observe that the interference terms are mediate to zero and so the results expressed above maintain their validity, once all the terms are taken into account.

In order to generalize this approach, let us consider a Universe with both semiclassical and quantum variables. To maintain a compact notation easy to understand, we will use the same one chosen by Vilenkin in its paper: the first half of the Greek alphabet will indicate the former while the other half of the Greek alphabet the latter.

We start again from the complete WDE

$$\left(H_0 - H_q\right)\psi = 0 \tag{2.98}$$

where H_0 is the part in which all the quantum variables and their conjugated momenta are neglected; we expand even the metric tensor in power of $\hbar$ and take only the zero order. Moreover, we assume that the mixed terms of the metric are negligible, in order to have a clear factorization of the wavefunction in semiclassical an quantum part. As before we start with a

$$\psi = A\left(h\right) e^{\frac{i}{\hbar}S} \phi\left(h, q\right) \equiv \psi_0 \phi \tag{2.99}$$

where the classical part satisfies the equation

$$H_0 \psi_0 = 0 \ . \tag{2.100}$$

Repeating the same steps of the earlier case, we find exactly the same equations for the action S and the amplitude A, while in this case we find even a third equation, at the first quantum order, which describes the purely quantum part of the system, let us see how:

$$\begin{aligned} &\left(\nabla_0^2 - U_0 - H_q\right) A e^{\frac{i}{\hbar}S}\phi = 0 \\ &\Rightarrow A e^{\frac{i}{\hbar}S} \nabla_0^2 \phi + 2\left[\left(\nabla_0 \ln A\right) e^{\frac{i}{\hbar}S} + iA\left(\nabla_0 S\right)\right] e^{\frac{i}{\hbar}S} \nabla_0 \phi - H_q A e^{\frac{i}{\hbar}S}\phi = 0 \\ &\Rightarrow 2i\left(\nabla_0 S\right)\nabla_0 \phi = H_q \phi \end{aligned} \tag{2.101}$$

where in the last line we exploited the adiabatic hypothesis in order to state that the variation of the quantum part of the wavefunction is way faster than its semiclassical counterpart. Being the term $\nabla_0 S$ proportional to the momentum and so to the velocity defined by (2.96) we obtain the differentiation in t that allows us to get the equation

$$i\frac{\partial\phi}{\partial t} = NH_q\phi \tag{2.102}$$

which is the Schrödinger equation for ϕ.

Applying the conservation law $\nabla_\alpha j^\alpha = 0$ in the case of a wavefunction like (2.99) we find the two principal terms in $\hbar$:

$$\begin{aligned} j^\alpha &= |\phi|^2|A|^2\nabla_0^\alpha S \equiv j_0^\alpha\rho_\phi \quad \text{for the classical variables} \\ j^\nu &= -\frac{i}{2}|A|^2\left(\phi^*\nabla^\nu\phi - \phi\nabla^\nu\phi^*\right) \equiv \frac{i}{2}|A|^2 j_\phi^\nu \quad \text{for the quantum variables} \end{aligned} \tag{2.103}$$

Using the conservation of the total current and the one relative to the only classical part, it is possible to find a continuity equation for the current

$$\frac{\partial\rho_\phi}{\partial t} + N\nabla_\nu j_\phi^\nu = 0 \ . \tag{2.104}$$

The probability distribution corresponding to the classical current can be written as

$$\rho\left(h,q,t\right) = \rho_0\left(h,t\right)\left|\phi\left(q,h\left(t\right),t\right)\right|^2 \tag{2.105}$$

If now we represent the surface element on the fixed time surfaces as $d\Sigma = d\Sigma_0 d\Omega_q$, where the term with the subscript 0 refers to the surface element defined by the classical variables, then the ρ_0 and the ϕ are normalized by

$$\begin{aligned} \int \rho_0 d\Sigma_0 &= 1 \ , \\ \int |\phi|^2 d\Omega_q &= 1 \ . \end{aligned} \tag{2.106}$$

We found again the standard interpretation of the wavefunction for a little subset of the Universe; if we assume that the starting wavefunction is a superposition of many WKB terms, it can be demonstrated, with the same logical steps, that the results are identical. There are not issues even if, during the evolution of the system, a few quantum variables become purely classical variables.

Until now we reported the calculations made by Vilenkin in his original paper in 1989 [54], explaining the more subtle steps.

The interpretation of the Universe wavefunction a la Vilenkin is approximated by its nature; it is only natural that the probability of a particular state of the Universe (or of a part of it) can be determined only approximately, with a precision level not exceeding the quality of the semiclassical approximation of the whole Universe. In this approach, even the unitarity is a sensitive concept and obviously the probabilities cannot add up to 1 with a better accuracy level than the one with whom they are defined. Anyway, the approximative nature of the reasoning is not necessarily a disadvantage. In fact, it is in excellent agreement with the standard interpretation of the quantum mechanics in which the classical measuring devices play a fundamental role.

2.2.6 Polymer Quantum Mechanics

Polymer Quantum Mechanics is a non-equivalent representation of the ordinary quantum mechanics, based on a modified version of the canonical commutation rules (CCR). In the following, we will clarify firstly what is the equivalence between different representations, then we will present the kinematics and the dynamics for the new model. The transition from the ordinary CCR to the Weyl ones will be showed for the case of a 1-D particle described by a couple of canonical variables (q, p).

Quantizing a system means switching from the Poisson Brackets

$$\{q, p\} = 1 \tag{2.107}$$

to the respective commutator between the operators associated to the classical canonical variables [53]

$$[\widehat{q}, \widehat{p}] = i\hbar\widehat{I} \ . \tag{2.108}$$

It is necessary to choose a Hilbert space and a polarization in order to redefine the quantum states. For the space, the choice is the space of the integrable squared functions, i.e. $\mathcal{H} = L^2(\mathbb{R}, d\mu)$; for the polarization, instead, the choice is the positions one, i.e. the q-polarization. The eigenvalue problem for the operator associated to the qs reduces to

$$\widehat{q}\,|q\rangle = q\,|q\rangle \ . \tag{2.109}$$

The basis kets are normalized to a Dirac Delta function

$$\langle q|q'\rangle = \delta\left(q - q'\right) \ . \tag{2.110}$$

Now that we have introduced all the fundamental elements, we can consider the projection onto a generic state

$$\langle q|\psi\rangle = \psi\left(q\right) \tag{2.111}$$

and even

$$\langle q|\widehat{q}|\psi\rangle = q\,\langle q|\psi\rangle = q\psi\left(q\right) \ . \tag{2.112}$$

Taking into account the CCR we can represent the operator associated to the ps as

$$\widehat{p} = -i\hbar\frac{d}{d\widehat{q}} + F\left(\widehat{q}\right) \tag{2.113}$$

with F generic; we can make a unitary transformation, which does not change the physics of the system, and get a definition of the momentum operator without the additional term, i.e.

$$\langle q|\widehat{p}|\psi\rangle = -i\hbar\frac{d}{dq}\psi\left(q\right) \ . \tag{2.114}$$

We get the following eigenvalue equation for the above operator

$$\widehat{p}\,|p\rangle = p\,|p\rangle \tag{2.115}$$

that projected on the basis $|q\rangle$ becomes

$$\langle q|\widehat{p}|p\rangle = p\,\langle q|p\rangle = -i\hbar\frac{d}{dq}\,\langle q|p\rangle \ , \tag{2.116}$$

where the last equality is a differential equation for $\langle q|p\rangle$ which admits a solution of the kind

$$\langle q|p\rangle = Ae^{\frac{iqp}{\hbar}} \quad , \quad p \in \mathbb{R} \ . \tag{2.117}$$

If we now change to the p-polarization and we follow the same steps we get a wavefunction and a representation of $\widehat{q}$

$$\langle p|\widehat{q}|\psi\rangle = i\hbar \frac{d}{dp}\psi\left(p\right) \ . \tag{2.118}$$

So, in summary we have

$$\begin{aligned} &\widehat{q}\psi\left(q\right) \to q\psi\left(q\right) \quad , \quad \widehat{p}\psi\left(q\right) \to -i\hbar\frac{d}{dq}\psi\left(q\right) \ , \ \text{basis}\,|q\rangle \ , \\ &\widehat{q}\psi\left(p\right) \to i\hbar\frac{d}{dp}\psi\left(p\right) \quad , \quad \widehat{p}\psi\left(p\right) \to p\psi\left(p\right) \quad , \ \text{basis}\,|p\rangle \ . \end{aligned} \tag{2.119}$$

We have just gone through the ordinary quantization procedure. Anyway, it can be possible that there is no differential operator associable to one of the canonical variables. This is the case of the theories which hold a reticular configuration of the space or the time. We then need another class of operators, i.e. the difference operators. Such objects are built thanks to the use of quotient operators, just like the derivative case; we can define two different kinds of quotient operators acting on adequate functional spaces [22]. If we take a test function $f\left[\mathbb{R}\right]$ we have

- the **additive** one

$$K^a f\left(x\right) = \frac{f\left(x+a\right) - f\left(x-a\right)}{\left(x+a\right) - \left(x-a\right)} = \frac{f\left(x+a\right) - f\left(x-a\right)}{2a} \qquad a \in \{\mathbb{R}\setminus\{0\}\} \ , \tag{2.120}$$

- the **multiplicative** one

$$K^s f\left(x\right) = \frac{f\left(sx\right) - f\left(s^{-1}x\right)}{sx - s^{-1}x} = \frac{1}{x}\frac{f\left(sx\right) - f\left(s^{-1}x\right)}{s - s^{-1}} \qquad s \in \{\mathbb{R}\setminus\{1\}\} \ . \tag{2.121}$$

If we consider the continuum limit $(a \to 0 \ , \ s \to 1)$ of the definitions (2.120) and (2.121) it is easy to observe that we get the ordinary definitions of differential operators.

Stone-von Neumann theorem

Let us analyze another important class of groups, the ones with a strongly continuous parameter; in order to give a definition of them, we introduce the self-adjoint operator and a real parameter t. We consider a family of unitary operators $\{U\left(t\right)\}$, such operators belong to a group with a strongly continuous parameter if the following two conditions are met

- $U\left(t+t'\right) = U\left(t\right)U\left(t'\right)$,
- $\lim_{t'\to t} U\left(t'\right) = U\left(t\right)$.

The Stone theorem states that, given an unitary representation U strongly continuous, it exists a **unique** self-adjoint operator A, called the generator of the group, such that

$$U(t) = e^{itA} \; . \tag{2.122}$$

For example, the family of the translation operators is a group with a strongly continuous parameter, and its generator is $A = -i\hbar \frac{d}{dx}$.

We introduce now unitary transformations that own as generators the operators associated to the canonical variables of the system. Let us consider the algebra generated by those operators

$$U(\alpha) = e^{\frac{i}{\hbar}\alpha\hat{q}} \quad , \quad V(\beta) = e^{\frac{i}{\hbar}\beta\hat{p}} \quad , \quad \alpha, \beta \in \mathbb{R} \tag{2.123}$$

where α and β are the parameters that characterize the transformation. It can be shown that, starting from such operators, one can obtain the Weyl commutation rules (WCR)

$$U(\alpha) V(\beta) = e^{\frac{i}{\hbar}\alpha\beta} V(\beta) U(\alpha) \; . \tag{2.124}$$

In general, a couple of unitary operators that acts on a fixed Hilbert space gives a Weyl representation if it satisfies the WCR.

A representation is *irreducible* if the Hilbert space holds an subspace invariant under the action of the null group. Two representations $(\{U(\alpha)\}, \{V(\beta)\})$ and $\left(\left\{U(\alpha)'\right\}, \left\{V(\beta)'\right\}\right)$ which act on two separate Hilbert spaces are *unitarily equivalents* only if it exists an unitary operator $W \; : \; \mathcal{H} \to \mathcal{H}'$ such that

$$WU(\alpha) W^* = U(\alpha)' \quad , \quad WV(\beta) W^* = V(\beta)' \quad , \; \forall \alpha, \beta \in \mathbb{R} \; . \tag{2.125}$$

Moreover, a representation is *regular* if the transformations

$$\alpha \to U(\alpha) \quad , \quad \beta \to V(\beta) \tag{2.126}$$

are continuous. We are now able to enunciate the following theorem

Stone-Von Neumann Theorem : *Every regular and irreducible representation of the CCR is unitarily equivalent to the Schrödinger representation*

Historically, this theorem was exploited in order to demonstrate the equivalence between the Schrödinger and the Heisenberg representations. We will observe, unfortunately, that the Polymer representation does not satisfy the regularity hypothesis and so can not be equivalent to the Schrödinger one.

Representations and polarization

The substantial difference between the Polymer representation and the Schrödinger one consists in the a priori choice of which variable is considered discrete. In the Schrödinger representation (see (2.119) for reference), the difference between the two polarizations is that the differential operator is associated either to the q variable (p-polarization) or to the p variable (q-polarization). If we choose to discretize the q variable in the Polymer paradigm, then in the p-polarization the operator $\hat{q}$ acts as a derivative with respect to p and it is not possible to define the momentum operator. In the q-polarization, instead, the operator $\hat{q}$ acts as a multiplier and it is not possible to define the operator $\hat{p}$ since the limit of the incremental ratio is not defined. So we need the difference operators introduced in (2.120). [23]

If in the Polymer representation we assign a discrete character to the p variable, the conclusions obtained are diametrically opposed. In the p-polarization the $\hat{p}$ operator acts as a multiplier and it is not possible to define the position operator. In the q-polarization, instead, the $\hat{p}$ operator acts as a derivative with respect to q and the position operator does not exist.

Kinematics

Let us understand now ho to redefine the kinematics in the Polymer paradigm, following [19]. We introduce a discrete set of kets $|\mu_i\rangle$, with $\mu_i \in \mathbb{R}$ and $i = 1, ..., N$, belonging to a certain Hilbert space $\mathcal{H}_{poly}$. The state of the system is described by a generic linear combination of the kets:

$$|\psi\rangle = \sum_{i=1}^{N} a_i \, |\mu_i\rangle \ . \tag{2.127}$$

The product of two kets is normalized to the Kronecker delta

$$\langle\nu|\mu\rangle = \delta_{\nu,\mu} \ , \tag{2.128}$$

as a consequence the product of two vectors $|\psi\rangle$ and $|\phi\rangle$ is:

$$\langle\psi|\phi\rangle = \sum_{i=1,j=1}^{N} \bar{b_j} a_i \, \langle\nu_j|\mu_i\rangle = \sum_{i=1}^{N} \bar{b_i} a_i \ . \tag{2.129}$$

Now we define two fundamental operators on this space: the **label** operator $\widehat{\varepsilon}$ and the **shift** operator$\widehat{s}(\lambda)$. They act in the following way:

$$\widehat{\varepsilon}\,|\mu\rangle = \mu\,|\mu\rangle \qquad \widehat{s}(\lambda)\,|\mu\rangle = |\mu+\lambda\rangle \ . \tag{2.130}$$

In order to associate physical operators to the abstract objects just introduced, in the following we will analyze a system with only one degree of freedom described by the phase space variables (q, p). We will make the physical choice of discretizing the position variable q and observe the differences between the states of the system obtained in both the representations.

P-polarization

We will first consider the p-polarization. The state projected into the basis vectors, in this case, is

$$\phi\,(p) = \langle p|\psi\rangle \ , \tag{2.131}$$

furthermore, we know that, as in the Schrödinger representation, the projection of the position vector in the momenta basis is

$$\phi_\mu\,(p) = \langle p|\mu\rangle = e^{-\frac{i}{\hbar}\mu p} \ . \tag{2.132}$$

By letting the operator $V(\lambda)$ act, introduced in the first part, on $\phi_\mu(p)$ we get

$$V(\lambda)\,\phi_\mu(p) = V(\lambda)\,e^{-\frac{i}{\hbar}\mu p} = e^{\frac{i}{\hbar}\lambda p}e^{-\frac{i}{\hbar}\mu p} = e^{\frac{i}{\hbar}(-\mu+\lambda)p} = \phi_{\mu+\lambda}(p)\ . \tag{2.133}$$

Remembering the definition given in 2.130, it is easy to identify the operator $V(\lambda)$ with the shift operator $\widehat{s}(\lambda)$.

Moreover, in this representation we identify the label operator with the position operator; let us show how it is a generator for the unitary transformation $U(\alpha)$:

$$\widehat{q}\phi_\mu(p) = i\hbar\frac{d}{dp}e^{-\frac{i}{\hbar}\mu p} = \mu e^{\frac{i}{\hbar}\mu p} = \mu\phi_\mu(p)\ . \tag{2.134}$$

From the definition of U in (2.123) we know that, given a generic φ_μ

$$\begin{aligned}\lim_{\alpha\to 0}\langle\varphi_\mu|U_a|\varphi_\mu\rangle = \lim_{\alpha\to 0}\langle\varphi_\mu|e^{i\alpha\widehat{q}}|\varphi_\mu\rangle = \lim_{\alpha\to 0}\langle\varphi_\mu|e^{i\alpha\mu}|\varphi_\mu\rangle =\\ = \lim_{\alpha\to 0}e^{i\alpha\mu}\langle\varphi_\mu|\varphi_\mu\rangle = e^{i\alpha\mu} = 1\ ,\end{aligned} \tag{2.135}$$

which means that it is a continuous relation. This ensures that it is possible to find an operator $\widehat{q}$. In particular, we have that

$$\widehat{q}\,|\mu\rangle = -i\lim_{\alpha\to 0}\alpha^{-1}\left(U(\alpha) - I\right)|\mu\rangle = \mu\,|\mu\rangle\ . \tag{2.136}$$

This shows how the $\widehat{q}$ operator is the generator of the transformations $U(\alpha)$.

In order to complete the scheme, we should demonstrate that the $\widehat{p}$ operator is the generator of the transformation $V(\lambda)$. Anyway, this is not possible because, even if we take an infinitesimal value for the parameter λ, two successive vectors $|\mu\rangle$ and $|\mu+\lambda\rangle$ are always orthogonal, i.e. remembering the identification of the $\widehat{V}$ operator with the shift operator

$$\langle\varphi_\mu|V_\lambda|\varphi_\mu\rangle = \langle\varphi_\mu|\widehat{s}(\lambda))|\varphi_\mu\rangle = \langle\varphi_\mu|\varphi_{\mu+\lambda}\rangle = \begin{cases}1, & \lambda = 0\\ 0, & \lambda \neq 0\end{cases} \tag{2.137}$$

This means that a transformation of the kind $\lambda \to \langle\mu|V_\lambda\mu\rangle$, as it happens in the case of the label operator, does not exist. Such a discontinuity violates the regularity hypothesis, it prevents the natural definition of the $\widehat{p}$ operator and so we can not use the Stone-Von Neumann theorem in this case.

Essentially, the Polymer representation is non-equivalent to the Schrödinger representation. Let us observe how in this scheme the normalization given by (2.128) is correct. In order to do so, we should define a measure $d\mu$ in the space in which we defined the $\phi_\mu(p)$. What we can demonstrate is that the space $\mathcal{H}_{poly}$ is isomorphic to the space

$$\mathcal{H}_{poly,p} = L^2\left(\mathbb{R}_b, d\mu_H\right) \tag{2.138}$$

where $\mathbb{R}_b$ is the Bohr compactification of the real line and $d\mu_H$ is the Haar measure. Once introduced those elements, we can redefine the inner product as

$$\begin{aligned}\langle\psi_\nu(p)\,|\psi_\lambda(p)\rangle = \int_{\mathbb{R}_b} d\mu_H\bar{\psi}_\nu(p)\,\psi_\lambda(p) = \lim_{L\to\infty}\frac{1}{2L}\int_{-L}^{L}dp\bar{\psi}_\nu(p)\,\psi_\lambda(p) =\\ \lim_{L\to\infty}\frac{1}{2L}\int_{-L}^{L}dpe^{\frac{i}{\hbar}\nu p}e^{-\frac{i}{\hbar}\lambda p}\ .\end{aligned} \tag{2.139}$$

From this, we can note that the normalization with the Dirac delta function, given by 2.128, is accurate. In fact

$$\langle \psi_\nu | \psi_\lambda \rangle = \lim_{L \to \infty} \frac{1}{2L} \int_{-L}^{L} dp e^{-\frac{i}{\hbar}\nu p} e^{\frac{i}{\hbar}\lambda p} = \begin{cases} 1, & \nu = \lambda \\ 0, & \nu \neq \lambda \end{cases} \tag{2.140}$$

Q-polarization

Let us analyze the same system but in the position representation. In this case the wavefunction depends on the q variable

$$\phi(q) = \langle q | \psi \rangle \ . \tag{2.141}$$

This time the projection of the state vector $|\mu\rangle$ on the basis vectors is realized with the vectors $|q\rangle$. It is obtained simply inserting a completeness relation

$$\begin{gathered} \phi\left(q\right)_\mu = \langle q | \mu \rangle = \langle q | \int_{\Re_b} d\mu_H \, |p\rangle \, \langle p | \mu \rangle = \int_{\Re_b} d\mu_H \, \langle q | p \rangle \, e^{\frac{i}{\hbar}\mu p} = \\ \int_{\Re_b} d\mu_H e^{-\frac{i}{\hbar}pq} e^{\frac{i}{\hbar}\mu p} = \delta_{q,\mu} \ . \end{gathered} \tag{2.142}$$

Let us study what are the changes in the label and shift operators in this polarization. We expect that they could be represented in the opposite way, but maintaining the same characteristics. We notice that, as in the previous case, the $\widehat{p}$ operator does not exist because the derivative of the Kronecker delta is not defined. In fact, being in the position representation, we get $\widehat{p} \to -i/\frac{d}{dq}$.

So

$$\widehat{p}\phi_\mu\left(q\right) = -i\hbar \frac{d}{dq}\delta_{q,\mu} \tag{2.143}$$

is an inconsistent operation. Moreover, the identification of the V operator with the shift one maintains its validity

$$V\left(\lambda\right)\phi\left(q\right) = \phi\left(q + \lambda\right) \tag{2.144}$$

and the $\widehat{q}$ operator acts as multiplication operator for the basis vectors:

$$\widehat{q}\phi_\mu\left(q\right) = \mu\phi_\mu\left(q\right) \ . \tag{2.145}$$

As in the previous case it is possible to define a Hilbert Space

$$\mathcal{H}_{poly,x} = L^2\left(\mathbb{R}_d, d\mu_c\right) \tag{2.146}$$

and an inner product normalized to the Kronecker delta

$$\langle \psi_\nu\left(q\right) | \psi_\lambda\left(q\right) \rangle = \delta_{\mu,\lambda} \tag{2.147}$$

As we have seen in both the representations, it is impossible to define a differential operator as the limit of the incremental ratio. This is a direct consequence of the physical choice of assigning to the spatial variable q a discrete character. There is no reason we cannot, naturally for different physics problems, choose the momentum variable as discrete. In that case, we could have reproduced exactly all the above calculations, obtaining that in both polarizations the position operator $\widehat{q}$ does not exist.

Dynamics

In order to grant a dynamics to the studied model, we ought to know the Hamiltonian properties of the system. Let us take the simplest possible case of a 1-D free particle with mass m inside a potential $V(q)$. Classically we get

$$H = \frac{p^2}{2m} + V(q) \tag{2.148}$$

whose quantum counterpart is given by

$$\widehat{H} = \frac{\widehat{p^2}}{2m} + V(\widehat{q}) \ . \tag{2.149}$$

We immediately notice that, even for the simplest system, in the Polymer case there is not a direct quantum implementation because of the presence of both $\widehat{p}$ and $\widehat{q}$ operators in $\widehat{H}$. How can we solve the problem of the non-existence of one of the two operators? The idea behind every quantization of the Polymer kind consists in the approximation of the terms corresponding to the non-existing operator and in the identification of adequate and well defined quantum operators for its implementation. We choose to characterize the q as a discrete variable, and so the p cannot be promoted to differential operator, as in the ordinary case, and we approximate the kinetic term $\frac{p^2}{2m}$ in such a way that its quantum counterpart is well defined. The standard procedure consists in the definition of a subspace $\mathcal{H}_{\gamma_a}$ of $\mathcal{H}_{poly}$ which includes all the existent vectors on the lattice of all the equidistant points defined by

$$\gamma_a = \{q \in \mathbb{R} | q = na, \forall n \in \mathbb{Z}\} \tag{2.150}$$

where the parameter a is a length and it is the distance between two successive points.

As a consequence, the basis vectors are of the kind $|\mu_n\rangle$ (where $\mu_n = na$) and the states are all in the form

$$|\psi\rangle = \sum_n b_n |\mu_n\rangle \ . \tag{2.151}$$

Let us see how to approximate the kinetic term. In the section (2.2.6) we saw how the operator $\widehat{V}(\lambda))$, in both the representations, is defined as the shift operator. Given its validity, we can use it to implement at the quantum level the approximation of the kinetic term. Recalling the action of the shift operator defined in (2.130) and requiring that such operation does not take the vectors outside of the lattice, it is only natural to identify the parameter λ with a. So the action of V on a state vector is

$$\widehat{V}(a) |\mu_n\rangle = |\mu_n + a\rangle = |\mu_{n+1}\rangle \ . \tag{2.152}$$

This is the basis of the approximation of every polynomial function of p. In fact we get that, for $p \ll \frac{\hbar}{a}$,

$$p \simeq \frac{\hbar}{a} \sin\left(\frac{ap}{\hbar}\right) = \frac{\hbar}{2ia}\left(e^{\frac{i}{\hbar}ap} - e^{-\frac{i}{\hbar}ap}\right) \ . \tag{2.153}$$

Now we can define an alternative version of the p operator. It depends on the scale a that we chose and acts on the vectors in a multiplicative way:

$$\widehat{p}_a |\mu_n\rangle = \frac{\hbar}{2ia} [V(a) - V(-a)] |\mu_n\rangle = \frac{i\hbar}{2a} (|\mu_{n-1}\rangle - |\mu_{n+1}\rangle) \ . \tag{2.154}$$

Similarly, we can define the alternative version of the operator associated to p^2. Always for $p \ll \frac{\hbar}{a}$, even it acts in a multiplicative way:

$$p^2 \simeq \frac{2\hbar^2}{a^2} \left[1 - \cos\left(\frac{ap}{\hbar}\right)\right] = \frac{2\hbar^2}{a^2} \left[1 - e^{\frac{i}{\hbar}ap} - e^{-\frac{i}{\hbar}ap}\right] \ . \tag{2.155}$$

So

$$\widehat{p}_a^2 |\mu_n\rangle = \frac{\hbar^2}{a^2} [2 - V(a) - V(-a)] |\mu_n\rangle = \frac{\hbar^2}{a^2} [2 |\mu_n\rangle - |\mu_{n+1}\rangle - |\mu_{n-1}\rangle] \tag{2.156}$$

We are now able to give a proper definition of the Hamiltonian operator in this Hilbert subspace $\mathcal{H}_{\gamma_a}$:

$$\widehat{H}_a = \frac{1}{2m} \widehat{p}_a^2 + V(\widehat{q}) \ . \tag{2.157}$$

Free Particle

A particular case that could be useful for the following is the free particle case. Let us analyze the system in the momenta polarizations. The classical Hamiltonian, for small enough momenta, reduces to

$$H \simeq \frac{\hbar^2}{ma^2} \left[1 - \cos\left(\frac{ap}{\hbar}\right)\right] \ . \tag{2.158}$$

For all we said in the section (2.2.6), in this approximation is possible to implement a quantization procedure. We write the quantum version of the above equation and we solve the eigenvalue problem. Given a wavefunction $\psi(p)$:

$$\widehat{H}_a \psi(p) = E_a \psi(p) \longrightarrow \left[\frac{\hbar^2}{ma^2} \left(1 - \cos\left(\frac{ap}{\hbar}\right)\right) - E_a\right] \psi(p) = 0 \ . \tag{2.159}$$

The energy spectrum takes the form

$$E_a = \frac{\hbar^2}{ma^2} \left[1 - \cos\left(\frac{ap}{\hbar}\right)\right] \leq \frac{2\hbar^2}{ma^2} = E_a^{max} \tag{2.160}$$

from which we can deduce that, for every chosen scale, our system has always a finite spectrum. Naturally, we can see how the energy spectrum we got tends, for $a \to 0$, to the one typical of a quantum particle in the Schrödinger representation. In fact, the spectrum assumes the form

$$E_a = \frac{\hbar^2}{ma^2} \left[1 - \cos\left(\frac{ap}{\hbar}\right)\right] \xrightarrow[a \to 0]{} \frac{p^2}{2m} \tag{2.161}$$

while the superior limit of the spectrum becomes

$$E_a^{max} = \frac{2\hbar^2}{ma^2} \xrightarrow[a \to 0]{} \infty \ . \tag{2.162}$$

Let us analyze now the form of the eigenfunctions. In this representation, we can easily verify that the solution for the eigenfunctions $\psi(p)$ is in the form

$$\psi(p) = A\delta(p - P_a) + B\delta(p + P_a) \tag{2.163}$$

where

$$P_a = \frac{\hbar}{a} \arccos\left(1 - \frac{ma^2}{\hbar^2} E_a\right) . \tag{2.164}$$

With an inverse Fourier transform we can obtain the eigenfunctions in the q-polarization. Considering the discrete structure assigned to the q variable (we considered only the points included in the lattice γ_a), the eigenfunctions of p that preserve this structure are all of the form $e^{\frac{i}{\hbar}anp}, n \in \mathbb{Z}$. Such functions have a period of $\frac{2\pi\hbar}{a}$ and, in terms of the inner product, this results in calculating the integral on the momenta only in the range $p \in \left(-\frac{\pi\hbar}{a}, \frac{\pi\hbar}{a}\right)$

$$\begin{aligned} \psi(q) &= \frac{1}{\sqrt{2\pi}} \int_{-\frac{\pi\hbar}{a}}^{\frac{\pi\hbar}{a}} \psi(p)\, e^{\frac{i}{\hbar}pq} = \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\frac{\pi\hbar}{a}}^{\frac{\pi\hbar}{a}} \left[A\delta(p - P_a) + B\delta(p + P_a)\right] e^{\frac{i}{\hbar}pq} = \\ &= \frac{\sqrt{2\pi}\hbar}{a} \left(Ae^{\frac{iqP_a}{\hbar}} + Be^{-\frac{iqP_a}{\hbar}}\right) . \end{aligned} \tag{2.165}$$

If the system is such that the momenta are comparable to the value $\frac{\pi\hbar}{a}$, then we expect that the approximation will be very rough and very different from the standard case, in both classical and quantum dynamics. On the other hand, if we stay always inside the region where the approximation holds, we can be near enough to the standard case.

Particle in a box

Another relevant example is the well-known particle in the box. The physical system consists in a particle confined along a segment of length $L = Na, N \in \mathbb{N}$. In this case the potential $V(q) = V(na)$ is in the form

$$V(q) = \begin{cases} \infty, & x > L, x < 0 \\ 0, & 0 < x < L \end{cases} \tag{2.166}$$

Basically, the particle behaves as a free particle inside the box and it can not trespass the border due to the infinite potential wall. This results in some boundary conditions for the wavefunction found in (2.165):

$$\psi(0) = \psi(L) = 0 . \tag{2.167}$$

Let us take the (2.165) and impose the conditions (2.167)

$$\begin{aligned} &\psi(0) = \frac{\sqrt{2\pi}\hbar}{a}(A + B) = 0 \longrightarrow A = -B \\ &\psi(L) = \frac{\sqrt{2\pi}\hbar}{a} A\left(e^{\frac{iLP_a}{\hbar}} - e^{-\frac{iLP_a}{\hbar}}\right) = \frac{\sqrt{2\pi}/}{a} A \sin\left(\frac{LP_a}{\hbar}\right) = 0 \rightarrow \\ &\quad \rightarrow LP_a = n\pi\hbar \quad n \in \mathcal{Z} \end{aligned} \tag{2.168}$$

In the end, the eigenfunctions results in the form

$$\psi\left(q\right)=\frac{2\sqrt{2\pi}\hbar}{a}A\sin\left(\frac{n\pi q}{L}\right)\ , \tag{2.169}$$

we can calculate the energy spectrum simply considering the boundary conditions for the (2.160). We obtain a discrete and limited spectrum:

$$E_{a,n}=\frac{\hbar^2}{ma^2}\left[1-\cos\left(\frac{an\pi}{L}\right)\right]\ . \tag{2.170}$$

If we take the limit for $a\rightarrow 0$ of the above spectrum

$$\lim_{a\rightarrow 0}E_{a,n}=\lim_{a\rightarrow 0}\frac{\hbar^2}{ma^2}\left[1-\cos\left(\frac{an\pi}{L}\right)\right]=\frac{\pi^2n^2\hbar^2}{2mL^2} \tag{2.171}$$

we get exactly the same infinite spectrum of the standard particle in the box.

2.3 Open Issues in Quantum Cosmology

2.3.1 Bounce Cosmology and Cyclic Universe

One of the most recent and appreciated developments of Modern Cosmology is the existence of a Big Bounce for the Planckian evolution of the isotropic universe. Despite some theoretical shortcomings, like the problem of entropy, the idea of a cyclic (closed) Universe, oscillating between a Big Bounce and a turning point, seemed to Einstein and other theoreticians a very pleasant alternative to the Big Bang singularity. In this respect, the results obtained by Ashtekar and his collaborators are a very encouraging issue in favor of this cyclical idea.

The isotropic Big Bounce has been derived implementing the ideas and formalism of Loop Quantum Gravity (mainly due to Ashtekar, Smolin and Rovelli). This canonical approach to the quantization of the gravitational field has the great merit of starting from a continuous description of the spacetime manifold, nonetheless recovering the discrete structure of the space, in terms of discrete spectra of the geometrical operators, like areas and volumes. The kinematical sector of Loop Quantum Gravity resembles a non-Abelian gauge theory and it allows the extension to the gravitational field of the so-called Wilson loops approach for strongly coupled Yang-Mills theories. However, the dynamical implementation of the super-Hamiltonian quantum constraint contains a certain level of ambiguity, e.g. the non-unitary equivalence of theories corresponding to different values of the Immirzi parameter, entering the canonical variables definition.

The application of Loop Quantum Gravity to the minisuperspace of a homogeneous cosmological model, expectedly implies a non-singular behavior of the quantum Universe, as a direct consequence of the cut-off scale imposed on the Universe volume, by the minimal (taken Planckian) value of its operator spectrum. Indeed, the Friedmann-Robertson-Walker geometry acquires in Loop Quantum Cosmology a non-singular behavior as described in terms of a free massless scalar field (the kinetic term of the inflaton field) playing the role of a relational time. The semiclassical picture of this non-singular Universe can be restated in the form of a maximal critical energy density for the asymptotic approach to the initial instant.

This cut-off on the maximal available temperature of the primordial Universe does not affect the theory of the Hot Big Bounce, because its scale is much greater than the physical regions of interest for the Standard Cosmological Model predictions like inflation, baryogenesis and nucleosynthesis. In this new scenario, the idea of a cyclical Universe takes new vigor and is substantiated by a precise quantum and semiclassical scenario. Although the Big Bounce theory is a promising perspective and deserving many attempts to extend its applicability to more general cosmological models (up to the generic quantum Universe), nevertheless its derivation is affected by some open issues. In fact, the restriction of the Loop Quantum Gravity theory to the minisuperspace has the non-trivial implication to replace the non-Abelian SU(2) by an Abelian U(1) symmetry, unable to ensure the discreteness of the volume spectrum.

The possibility to recover the Big Bounce from the minisuperspace dynamics relies on the introduction by hands of the space discreteness as a natural, but not direct, consequence of the full theory equipment. These shortcomings of imposing the symmetries of the isotropic model before quantizing its dynamics prevent the Big Bounce to be self-consistently derived, but do not seem able to affect the impact of this issue on the modern idea of a primordial Universe.

In my research group many authors addressed the problem of the removal of the initial singularity (see for reference [5, 34]). In particular, in [5] there are some noteworthy ideas. They studied the Taub cosmology, a particular case of the Bianchi IX model, with a Polymer quantization prescription; this was one of the first attempt to analyze the Early Universe with this kind of quantization procedure. They decided to implement the Polymer Representation only to the anisotropic variable and they demonstrated that in this way the singularity cannot be removed but the work is nevertheless a fascinating one.

My first work [14] is the natural extension of this study, we implemented the Polymer Quantum Mechanics on all the variables, both semiclassical and quantum ones. For my research we decided to adopt the Vilenkin approach [54] in order to retrieve a wavefunction of the Universe with a well defined probability density. We found that the Taub cosmology is a singularity-free Universe and that the evolution of the volume of the Universe is confined between a series of big bounces and maximum volume turning points, this suggests that this model is cyclical. All of this will be better explained in (3).

2.3.2 The isotropization Mechanism

In quantum cosmology the Universe is described by a single wave function Ψ providing puzzling interpretations as soon as the differences with respect to ordinary quantum mechanics are addressed [54, 24]. Quantum cosmology is defined up to the following two assumptions. (i) The analyzed model is the Universe as a whole and thus there is no longer an a priori splitting between classical and quantum worlds. No external measurement crutch is available and an internal one cannot play the observer-like role because of the extreme conditions a primordial Universe is subjected to. (ii) In General Relativity, time is an arbitrary label and clocks, being parts of the Universe, are also described by the wave function Ψ.

Time is thus included in the configuration space and the integral of $|\Psi|^2$ over the whole minisuperspace diverges as in quantum mechanics when the time coordinate is included in the configuration-space element. As a result, the standard interpretation of quantum mechanics (the Copenhagen interpretation) does not work in quantum cosmology. On a given (space-time) background structure only, observations can take place in the sense of ordinary quantum theory.

In [6] a wave function of a generic inhomogeneous Universe, which has a clear probabilistic interpretation, has been obtained. It can be meaningfully interpreted because of a separation between semiclassical degrees of freedom, in the Wentzel-Kramers-Brillouin (WKB) sense, and quantum ones. In particular, the quantum dynamics of weak anisotropies (the physical degrees of freedom of the Universe) is traced with respect to the isotropic scale factor which plays an observer-like role as soon as the Universe expands sufficiently. A generic inhomogeneous cosmological model, describing a Universe in which any specific symmetry has been removed, represents a generic cosmological solution of the Einstein field equations [11]. Belinski-Khalatnikov-Lifshitz (BKL) showed that such a geometry evolves asymptotically to the singularity as an ensemble, one for each causal horizon, of independent Bianchi IX homogeneous Universes [43]. This model represents the best description we have of the (classical) physics near a spacelike cosmological singularity.

The main result of their paper is that the wave function of the Universe is spread over all values of anisotropies near the cosmological singularity, but it is asymptotically peaked around the isotropic configuration. The closed Friedmann-Robertson-Walker (FRW) cosmological model is then the naturally privileged state as soon as a sufficiently large volume of the Universe is taken into account. A semiclassical isotropization mechanism for the Universe is thus predicted. This model can be regarded as a concrete implementation, to a physically interesting cosmological problem, of the semiclassical approach to quantum cosmology [54]. An isotropization mechanism is in fact necessary to explain the transition between a very early Universe and the observed one. The isotropic FRW model can accurately describes the evolution of the Universe until decoupling time [31].

On the other hand, the description of its primordial stages requires more general models. It is thus fundamental to recover a mechanism which can match these two cosmological epochs. Although many efforts have been made inside classical theory [30, 18] (especially by the use of the inflation field), no quasi-classical (or purely quantum) isotropization mechanism has not yet been developed in detail.

The authors of my research group [6] demonstrated that when the Universe moves away from the cosmological singularity, the probability density to find it is asymptotically peaked (as a Dirac δ-distribution) around the closed FRW configuration. Near the singularity all values of the anisotropies are almost equally favored from a probabilistic point of view. On the other hand, as the volume of the Universe grows, the isotropic state becomes the most probable state of the Universe. The key feature of such a result relies on the fact that the isotropic scalar factor has been considered as an intrinsic variable with respect to the anisotropies. It has been treated semiclassically (WKB) while the two physical degrees of freedom of the Universe have been described as quantum variables . In this way, a positive semidefinite probability density can be constructed for the wave function of the quantum subsystem of the Universe.

Their pioneering work inspired us to further develop the research and with our paper [15] we have shown that, even if the Universe is in a corner-configuration, it is possible to retrieve an isotropization mechanism that leads the Bianchi IX model towards an isotropic Universe. This will be fully covered in chapter (4).

Chapter 3

WKB approximation for the Polymer quantization of the Taub Model

In this Chapter we develop a suitable technical algorithm to implement a separation of the Minisuperspace configurational variables into quasi-classical and purely quantum degrees of freedom, in the framework of a Polymer quantum Mechanics reformulation of the canonical dynamics. We then implement this technique to a Taub Universe, in the presence of a free massless scalar field. In particular, we identify the quasi-classical variables in the Universe volume and a suitable function of the scalar field, while the purely quantum degree of freedom corresponds to the Universe anisotropy. We demonstrate that the Taub cosmology is associated to a cyclical Universe, oscillating between a minimum and maximum volume turning points, respectively. The pure quantum Universe anisotropy has always a finite value.

3.1 Introduction

One of the most puzzling shortcomings of the Universe representation in modern Cosmology is the presence of an initial singularity, predicted by the Einstein equation, but undoubtedly it is an unphysical ultraviolet divergence to be somehow regularized [47, 31, 56].

Various non-singular cosmological models can be constructed on a classical and quantum level, see for instance [17] but the emergence of a Bounce Cosmology can be attributed to the implementation of Loop Quantum Gravity on a cosmological setting, see [4]. When a metric approach is considered, the most natural way to deal with a singularity-free cosmological model, relies on the implementation of a Polymer Quantum Mechanics approach to the Minisuperspace [19, 4]. This approach is, de facto, a discretization procedure of the considered configurational variables (in cosmology they are Universe scale factors), which turn out to live on a graph and can have only a discrete spectrum, for a picture of the literature in merit, see [48, 5, 34, 19].

From the side of the quantum physics of space-time, an highly non-trivial question concerns the absence of a parametric (external) time variable, when the canonical method is implemented [26, 51, 46, 38].

Among many different proposal to construct a suitable clock in quantum gravity [32], it stands the WKB approach proposed in [54], see also [28]. The proposed scenario relies on a Born-Oppenheimer approximation, in which some Minisuperspace variables behaves slowly and are quasi-classical degrees of freedom, becoming a good clock for the fully quantum and rapidly changing variables. In other words, the time dependence of the wave function of the quantum part is recovered by its dependence on the quasi-classical variables, in turn linked to the coordinate time.

The present work explores the possibility to deal with a cosmological model in which the singularity is regularized via a Polymer Quantum Mechanics approach and a time dependence of the Universe wave function is defined via a Born-Oppenheimer decomposition of the quantum dynamics. The non trivial technical question we address here is to reconcile the momentum representation of the quantum dynamics, mandatory for a Polymer quantization, as developed in [19] for the continuum limit and the WKB scheme, thought in the coordinate representation. The crucial point is that the potential term emerging in the Minisuperspace model is, in general, non quadratic in the configurational variables, like instead in general is the Kinetic part of the Hamiltonian in the momenta. To overcome this difficulty, we introduce a suitable and general algorithm and then we implement it in the particular and important case of a Taub Cosmological model [40, 47].

The classical Taub solution links a non-singular expanded universe to a singular point of the space-time curvature, as it naturally arises because it is nothing more than a Bianchi IX model with two equal cosmic scale factors (the spatial geometry is the same of a closed Robertson-Walker geometry).

The cosmological model resulting from our regularization is a very intriguing paradigm: we get an evolution quantum picture, whose description corresponds to a (non-singular) cyclical Universe.

Our study of the Taub cosmology in the presence of a scalar field is performed using Misner-Chitrè-like variables [25]. The quasi-classical variables are identified in the scalar field and in the one that is most directly linked to the Universe volume, actually in the adopted variables the isotropic metric component and the anisotropies are somehow mixed together. The quantum degree of freedom is identified in the relic anisotropy coordinate of the Taub model, a suitable redefinition of the variables is also necessary during the technical derivation.

The resulting evolution (Schrödinger) equation for this anisotropy variable has, in the spirit of the analysis here presented, two main physical implications: i) the Taub model is reduced to a cyclical Universe, evolving between a minimum and a maximum value of the Universe variables, offering an intriguing paradigm for the physical implementation of a cosmological history: clearly the maximum volume turning point is expected to live in a classical domain of the Universe dynamics, while the Bounce turning point has a pure quantum character , in the sense of a Polymer regularization; ii) the Universe anisotropy is always finite in value as a result of the singularity regularization and its specific value in the Bounce turning point depends on the initial conditions of the system, but in principle, it can be restricted to small enough values to make the Bounce dynamics unaffected by their behavior, i.e. the applicability of the Born-Oppenheimer approximation is ensured in the spirit of the analysis provided in [1].

All of this is inserted in [14] that is undergoing the refereeing procedure.

3.2 The generalization of the Vilenkin Approach

In this paragraph I will extend the study of Vilenkin [54] to the case of a totally general homogeneous universe. We will start from the Wheeler-De Witt equation in the momenta base that is written as:

$$\left[g^{\alpha\beta}\left(\frac{\partial S}{\partial p_\gamma}\right)p_\alpha p_\beta - U\left(\frac{\partial S}{\partial p_\gamma}\right) - H_q\right]\psi\left(p\right) = 0 \tag{3.1}$$

and the Action S is in the ADM form and the wave function will be:

$$\psi\left(p\right) = A\left(p\right)e^{\frac{i}{\hbar}S(p)}\phi\left(p,q\right) \ . \tag{3.2}$$

The first step to achieve the generalized approach is to introduce a generalization of the Derivative operator [39] that will greatly help in the following. Let us start from the simplest cases:

$$\begin{aligned} D_p^\mu\left[p^\nu\right] &= \frac{\Gamma\left(\nu+1\right)}{\Gamma\left(\nu-\mu+1\right)}p^{\nu-\mu} \\ D_p^\mu\left[e^p\right] &= D_p^\mu\left[\sum_{k=0}^{\infty}\frac{p^k}{k!}\right] = \sum_{k=0}^{\infty}\frac{p^{k-\mu}}{\Gamma\left(k+1-\mu\right)} \equiv E_\mu^p \ ; \end{aligned} \tag{3.3}$$

where E_μ^p is the generalized exponential function defined by:

$$\begin{aligned} E_\mu^{ap} &\equiv p^\mu e^{ap}\gamma^*\left(\mu,ap\right) \ , \\ \gamma^*\left(\mu,ap\right) &\equiv e^{-ap}\sum_{j=0}^{\infty}\frac{\left(ap\right)^j}{\Gamma\left(\mu+j+1\right)} \ . \end{aligned} \tag{3.4}$$

let us further advance and introduce the case of a grade-n polynomial as the exponent

$$D_p^\mu\left[e^{ap}\right] = D_p^\mu\left[\sum_{k=0}^{\infty}\frac{\left(ap\right)^k}{k!}\right] = a^\mu\sum_{k=0}^{\infty}\frac{\left(ap\right)^{k-\mu}}{\Gamma\left(k+1-\mu\right)} \equiv a^\mu E_\mu^{ap} \tag{3.5}$$

let us define another function for the purpose of this paper

$$Ln_\mu\left[E_\mu^{ap}\right] \equiv ap \ . \tag{3.6}$$

When everything is taken into account it must be said that as soon as we put a generic function in the place of the exponential of a polynomial, all the maths starts to decade because the initial definition has a lot of problems that are solved only in the case of polynomial functions. In the following this generalized derivative will be often used because we will only consider functions that are related to polynomial.

3.2.1 Ordinary Case

The Hamilton-Jacobi equation is described by the first order expansion of the Wheeler-DeWitt equation. In order to obtain it, it's necessary to expand the exponential in its power series and take only the right order terms. We get:

$$\psi\left(p\right)=A\left(p\right)\left[1+\frac{i}{\hbar}S\left(p\right)-\frac{1}{2\hbar^{2}}S^{2}\right]\phi\left(p,q\right) \tag{3.7}$$

and so the WDE becomes at the lowest order:

$$\begin{aligned}g^{\alpha\beta}\left(\frac{\partial S}{\partial p_{\gamma}}\right)p_{\alpha}p_{\beta}A\left(p\right)\left(-\frac{1}{2\hbar^{2}}S^{2}\right)\phi\left(p,q\right)+\\ -U\left(\frac{\partial S}{\partial p_{\gamma}}\right)A\left(p\right)\phi\left(p,q\right)=0\ ;\end{aligned} \tag{3.8}$$

with the due simplifications and introducing the notation $\left(\frac{\partial}{\partial p_{\gamma}}\right)\equiv\left(\partial_{\gamma}\right)$ we obtain

$$g^{\alpha\beta}\left(\frac{\partial S}{\partial p_{\gamma}}\right)p_{\alpha}p_{\beta}\frac{S^{2}}{\hbar^{2}}+2U\left(\frac{\partial S}{\partial p_{\gamma}}\right)=0\ . \tag{3.9}$$

that reproduce exactly the Hamilton-Jacobi equation of the classical case once we identify $\left(\frac{\partial S}{\partial p_{\gamma}}\right)$ with h^{γ}.

At the next order we get two separate equations given that, as in the case analyzed by Vilenkin, we can exploit the adiabatic approximation. let us start analyzing first the equation for the amplitude A and then the one for the quantum wavefunction. Studying the general case, we don't have the explicit forms of the metric and the potential term, and so we can't let them act directly on the wavefunction; what we can do is, instead, multiply by the identity both of the terms defining

$$\mathbb{I}=\left(i\hbar\partial_{\gamma}\right)^{-1}\left(i\hbar\partial_{\gamma}\right)\ . \tag{3.10}$$

The desired equation can be obtained at the next order of the expansion in $\hbar$. Multiplying by the identity defined above and having the exotic derivative acting only on the amplitude while the normal one acts on the exponential term we obtain:

$$g^{\alpha\beta}p_{\alpha}p_{\beta}\left[\left(\partial^{-1}A\right)\left(\partial\ e^{\frac{i}{\hbar}S}\right)\right]\phi-U\left[\left(\partial A\right)\left(\partial^{-1}e^{\frac{i}{\hbar}S}\right)\right]\phi=0 \tag{3.11}$$

Those are not the only terms at the right order so we multiply again the equation by the identity and we get:

$$\begin{aligned}ig^{\alpha\beta}p_{\alpha}p_{\beta}\left\{\left[2\partial^{-1}\left(\partial\partial^{-1}A\right)\left(\partial S\right)\right]+\left[\left(\partial^{-2}A\right)\left(\partial^{2}S\right)\right]\right\}e^{\frac{i}{\hbar}S}+\\ -U\hbar\left[2\left(\partial A\right)\left(\partial^{-1}e^{\frac{i}{\hbar}S}\right)\right]=0\end{aligned} \tag{3.12}$$

And this is the equation for the amplitude $A\left(p\right)$.

Now we analyze the equation for the pure quantum wavefunction. As in the above case, we multiply the initial equation by the identity, but this time the important part, in order to obtain the Schrödinger equation, is when the exotic derivative acts on the exponential and the normal one acts on the quantum term; before we approach the real calculation it's opportune expanding the action in its power series: $S(p) = \sum_{k=0}^{\infty} c_k(t)\, p^k(t)$.

let us start applying the exotic derivative on the exponential using the definition:

$$\begin{aligned}
(i\hbar\partial_\gamma)^{-1} e^{\frac{i}{\hbar}\sum_{k=0}^{\infty} c_k p^k} &= (i\hbar\partial_\gamma)^{-1} \prod_{k=0}^{\infty}\sum_{j=0}^{\infty}\left[\frac{\left(\frac{i}{\hbar}c_k p^k\right)^j}{j!}\right] = \\
&= \frac{1}{i\hbar}\left\{\frac{1}{\sum_{k=1}^{\infty}\left[\frac{i}{\hbar}c_k k\right]}\prod_{k=0}^{\infty}\sum_{j=0}^{\infty}\frac{\left(\frac{i}{\hbar}c_k p^k\right)^{j+1}}{\Gamma(j+2)}\right\} = \\
&= \frac{1}{i\hbar\mathfrak{C}}\prod_{k=0}^{\infty} E_{-1}^{\frac{i}{\hbar}c_k p^k} ,
\end{aligned} \tag{3.13}$$

where Γ is the Euler Gamma Function, for the sake of notation I have defined $\mathfrak{C} = \sum_{k=1}^{\infty}\frac{i}{\hbar}c_k$ and I have introduced the generalized exponential function defined above in (3.4). The equation

$$\hat{H}_0\left(\partial^{-1}e^{\frac{i}{\hbar}S}\right)(\partial\phi) = \hat{H}_q e^{\frac{i}{\hbar}S}\phi \tag{3.14}$$

becomes, exploiting (3.13),

$$\hat{H}_0\frac{1}{\mathfrak{C}}\prod_{k=0}^{\infty}E_{-1}^{\frac{i}{\hbar}c_k p^k}(\partial_\gamma\phi) = \hat{H}_q e^{\frac{i}{\hbar}\sum_{k=0}^{\infty}c_k p^k}\phi , \tag{3.15}$$

where $\hat{H}_0$ is the classical part of the WD. We highlight in particular the property of one of the terms in equation (3.15):

$$\frac{\frac{1}{\mathfrak{C}}\prod_{k=0}^{\infty}E_{-1}^{\frac{i}{\hbar}c_k p^k}}{e^{\frac{i}{\hbar}\sum_{k=0}^{\infty}c_k p^k}} = \frac{F(p)}{F'(p)} = \frac{1}{\partial_\gamma Ln_{-1}[F(p)]} \tag{3.16}$$

and so we obtain:

$$\hat{H}_0\frac{1}{\partial_\gamma Ln_{-1}[F(p)]}(\partial_\gamma\phi) = \hat{H}_q\phi . \tag{3.17}$$

We can rewrite the p-derivative of the logarithm as its time derivative times $\frac{\partial t}{\partial p_\gamma}$, thanks to the properties of the differentials, and it ensures that it's possible to obtain the time derivative even of the quantum terms. let us see how it can be done

$$\hat{H}_0\frac{1}{\partial_t Ln_{-1}[F(p)]\,\partial_\gamma t}(\partial_\gamma\phi) = \hat{H}_q\phi . \tag{3.18}$$

The time derivative of the logarithm, $\partial_t Ln_{-1}[F(p)]$ can be written as $\frac{i}{\hbar}\mathfrak{D}$ and so we obtain the equation:

$$\frac{1}{\frac{i\mathfrak{D}}{\hbar}}\left(\frac{\partial p_\gamma}{\partial t}\frac{\partial\phi}{\partial p_\gamma}\right) = \hat{H}_0^{-1}\hat{H}_q\phi . \tag{3.19}$$

We can take all the temporal dependence of the above equation and define a new time derivative in τ in order to get

$$-i\hbar\frac{1}{\mathfrak{D}}\left(\frac{\partial\phi}{\partial t}\right)=\hat{H}_0{}^{-1}\hat{H}_q\phi\ , \tag{3.20}$$

if we define τ such that

$$\frac{\partial}{\partial\tau}\equiv\frac{1}{\mathfrak{D}}\left(\frac{\partial}{\partial t}\right) \tag{3.21}$$

and after we take all the other terms to the second member we obtain:

$$-i\hbar\frac{\partial\phi}{\partial\tau}=\hat{H}_1\phi \tag{3.22}$$

that is the desired Schrödinger's equation for the quantum wavefunction. In equation (3.22) I have defined

$$\hat{H}_1\equiv\hat{H}_0^{-1}\hat{H}_q$$

3.2.2 Polymer Case

As seen in the section about the Polymer quantum mechanics, imposing a Polymer quantization means assuming a discrete structure for some of the variables of the phase space. The consequence of this fact is that it's not possible to associate to the conjugated variables quantum differentials operators as in the ordinary case. The Polymer paradigm, to solve this problem, consists in the substitution $p\to\frac{1}{\mu}\sin(\mu p)$. As a consequence, the Polymer version of the WD equation is:

$$\left[\frac{\hbar^2}{\mu^2}g^{\hat{\alpha}\beta}\sin\left(\frac{\mu p_\alpha}{\hbar}\right)\sin\left(\frac{\mu p_\beta}{\hbar}\right)-U-H_q\right]\psi=0\ . \tag{3.23}$$

Expanding it at the lowest order and using the power series of the exponential we find the Hamilton-Jacobi equation for the Polymer case:

$$\begin{aligned}&-\frac{\hbar^2}{\mu^2}g^{\hat{\alpha}\beta}\sin\left(\frac{\mu p_\alpha}{\hbar}\right)\sin\left(\frac{\mu p_\beta}{\hbar}\right)\frac{AS^2\phi}{2\hbar^2}-UA\phi=0\\ &\Rightarrow\frac{1}{\mu^2}g^{\hat{\alpha}\beta}\sin\left(\frac{\mu p_\alpha}{\hbar}\right)\sin\left(\frac{\mu p_\beta}{\hbar}\right)S^2+2U=0\ .\end{aligned} \tag{3.24}$$

As seen above at the next order we find two separate equations because of the adiabatic approximation. In order to find those equations we will use the same method of the last section with the identity defined by

$$\mathbb{I}=\left(i\hbar\partial_{\gamma Pol}\right)^{-1}\left(i\hbar\partial_{\gamma Pol}\right)\ .$$

Using the same notation of the last section we get:

$$\begin{aligned}&\frac{\hbar^2}{\mu^2}g^{\hat{\alpha}\beta}\sin\left(\frac{\mu p_\alpha}{\hbar}\right)\sin\left(\frac{\mu p_\beta}{\hbar}\right)\phi-U\mathbb{I}\psi=0\quad\Rightarrow\\ &\frac{\hbar^2}{\mu^2}g^{\hat{\alpha}\beta}\sin\left(\frac{\mu p_\alpha}{\hbar}\right)\sin\left(\frac{\mu p_\beta}{\hbar}\right)\mathbb{I}\left(\partial_{Pol}^{-1}A\right)\left(\partial_{Pol}E_+\right)\phi-U\mathbb{I}\left[\left(\partial_{Pol}A\right)\left(\partial_{Pol}^{-1}E_+\right)\right]\phi=0\\ &\Rightarrow\frac{\hbar^2}{\mu^2}g^{\hat{\alpha}\beta}\sin\left(\frac{\mu p_\alpha}{\hbar}\right)\sin\left(\frac{\mu p_\beta}{\hbar}\right)\left(\partial_{Pol}^{-1}\right)\left(\partial_{Pol}\right)\left[\left(\partial_{Pol}^{-1}A\right)\left(\partial_{Pol}E_+\right)\right]\phi-\\ &U\left(\partial_{Pol}^{-1}\right)\left(\partial_{Pol}\right)\left[\left(\partial_{Pol}A\right)\left(\partial_{Pol}^{-1}E_+\right)\right]\phi=0\ .\end{aligned} \tag{3.25}$$

If we write explicitly the known terms we obtain:

$$\begin{aligned}&\frac{i\hbar}{\mu^2}g^{\hat{\alpha}\beta}\sin\left(\frac{\mu p_\alpha}{\hbar}\right)\sin\left(\frac{\mu p_\beta}{\hbar}\right)\left[2\left(\partial_{Pol}^{-1}A\right)\left(\partial_{Pol}S\right)+\left(\partial_{Pol}^{-2}A\right)\left(\partial_{Pol}^{2}S\right)\right]E_+\\&-U\hbar\left[2\left(\partial_{Pol}A\right)\left(\partial_{Pol}^{-1}E_+\right)\right]=0\end{aligned} \tag{3.26}$$

This is the equation for the Polymer amplitude A.

Although the calculation made till now demonstrates that the equations that we obtain in both the representations are the same taking into account the correction introduced by the passage from one to the other, let us see what happen to the quantum wavefunction. The method is exactly the same of the last section since $f\left[\sin\left(p\right)\right]\equiv f\left(p\right)$. The equation

$$\hat{H}_{0_{Pol}}\left(\partial_{Pol}^{-1}e^{\frac{i}{\hbar}S}\right)\left(\partial_{Pol}\phi\right)=\hat{H}_{q_{Pol}}e^{\frac{i}{\hbar}S}\phi \tag{3.27}$$

becomes, exploiting (3.13),

$$\hat{H}_{0_{Pol}}\frac{1}{\mathfrak{C}}\prod_{k=0}^{\infty}E_{-1}^{\frac{i}{\hbar}c_kp^k}\left(\partial_\gamma\phi\right)=\hat{H}_{q_{Pol}}e^{\frac{i}{\hbar}\sum_{k=0}^{\infty}c_kp^k}\phi\ , \tag{3.28}$$

where with $\hat{H}_{0_{Pol}}$ has been indicated the classical part of the WD in the Polymer representation. In this particular case the generalized exponential function contains all the Polymer correction and it is substantially different from the ordinary one. We highlight, even in this case, the property of one of the terms in equation (3.28):

$$\frac{\frac{1}{\mathfrak{C}}\prod_{k=0}^{\infty}E_{-1}^{\frac{i}{\hbar}c_kp^k}}{e^{\frac{i}{\hbar}\sum_{k=0}^{\infty}c_kp^k}}=\frac{F\left(p\right)}{F'\left(p\right)}=\frac{1}{\partial_\gamma Ln_{-1}\left[F\left(p\right)\right]} \tag{3.29}$$

and so we get:

$$\hat{H}_{0_{Pol}}\frac{1}{\partial_\gamma Ln_{-1}\left[F\left(p\right)\right]}\left(\partial_\gamma\phi\right)=\hat{H}_{q_{Pol}}\phi\ . \tag{3.30}$$

Taking into account the properties of the differentials, we can rewrite the p-derivative of the logarithm as the time derivative of the logarithm times $\frac{\partial t}{\partial p_\gamma}$

$$\hat{H}_{0_{Pol}}\frac{1}{\partial_t Ln_{-1}\left[F\left(p\right)\right]\partial_\gamma t}\left(\partial_\gamma\phi\right)=\hat{H}_{q_{Pol}}\phi\ . \tag{3.31}$$

The time derivative of the logarithm, $\partial_t Ln_{-1}\left[F\left(p\right)\right]$ can be written as $\frac{i}{\hbar}\mathfrak{D}_{Pol}$ and so we get the equation:

$$\frac{1}{\frac{i\mathfrak{D}_{Pol}}{\hbar}}\left(\frac{\partial p_\gamma}{\partial t}\frac{\partial\phi}{\partial p_\gamma}\right)=\hat{H}_{0_{Pol}}^{-1}\hat{H}_{q_{Pol}}\phi\ . \tag{3.32}$$

We can take all the temporal dependence of the above equation and define a new time derivative in τ in order to get

$$-i\hbar\frac{1}{\mathfrak{D}_{Pol}}\left(\frac{\partial\phi}{\partial t}\right)=\hat{H}_{0_{Pol}}^{-1}\hat{H}_{q_{Pol}}\phi\ , \tag{3.33}$$

if we define τ_{Pol} such that

$$\frac{\partial}{\partial \tau_{Pol}} \equiv \frac{1}{\mathfrak{D}_{Pol}} \left(\frac{\partial}{\partial t} \right) \tag{3.34}$$

and after we take all the other terms to the second member we obtain:

$$- i\hbar \frac{\partial \phi}{\partial \tau_{Pol}} = \hat{H}_{1_{Pol}} \phi \ , \tag{3.35}$$

where

$$\hat{H}_{1_{Pol}} \equiv \hat{H}^{-1}_{0_{Pol}} \hat{H}_{q_{Pol}}$$

.

The equation above is the desired Schrödinger equation and it's equivalent to the ordinary case. Clearly both in the time variable and in the terms of the Hamiltonian there is the Polymer correction, but formally they are the same.

3.2.3 Conserved Current

We analyze now the probability current defined from the WDE in order to obtain the continuity equation that allow us to replicate the Vilenkin approach. We start from $\psi(p) = A(p) e^{\frac{i}{\hbar} S(p)} \phi(p,q)$ and its complex conjugated $\psi^*(p) = A^\dagger(p) e^{-\frac{i}{\hbar} S(p)} \phi^*(p,q)$. Imposing the Hamiltonian constraint we can formally find $p_\alpha = f(h^\alpha)$ along the equation of motion. Furthermore it is possible to use the Hamilton equations to find the analytical expressions for $\dot{p}$ and $\dot{h}$. The definition of the probability current is:

$$J^\delta = \frac{i}{2} \hbar p_\alpha p_\beta \hat{g}^{\alpha\beta} \left(\frac{\partial}{\partial p_\delta} \right)^{-1} \left(\frac{\partial}{\partial p_\gamma} \right)^{-1} \left[\psi^* \partial_\gamma \psi - \partial_\gamma \psi^* \psi \right] \tag{3.36}$$

We differentiate the above equation to obtain:

$$\begin{aligned}
&\partial_\delta J^\delta = \\
&\frac{i}{2} \hbar p_\alpha p_\beta \hat{g}^{\alpha\beta} \left[\left(\partial_\gamma^{-1} \psi^* \right) (\partial_\gamma \psi) - (\partial_\gamma \psi^*) \left(\partial_\gamma^{-1} \psi \right) - \psi^* \psi + \psi^* \psi - \psi^* \psi + \psi^* \psi - \psi^* \psi + \psi^* \psi \right] \\
&+ \frac{i}{2} \hbar \partial_\delta \left(p_\alpha p_\beta \hat{g}^{\alpha\beta} \right) \partial_\delta^{-1} \left[\left(\partial_\gamma^{-1} \psi^* \right) (\partial_\gamma \psi) - (\partial_\gamma \psi^*) \left(\partial_\gamma^{-1} \psi \right) \right] \\
&+ \frac{i}{2} \hbar p_\alpha p_\beta \hat{g}^{\alpha\beta} \partial_\delta^{-1} \left\{ \partial_\delta \left[\left(\partial_\gamma^{-1} \psi^* \right) (\partial_\gamma \psi) - (\partial_\gamma \psi^*) \left(\partial_\gamma^{-1} \psi \right) \right] \right\} + \\
&+ \frac{i}{2} \hbar p_\alpha p_\beta \hat{g}^{\alpha\beta} \partial_\delta^{-1} \partial_\gamma^{-1} \left[(\partial_\delta \psi^*) (\partial_\gamma \psi) - (\partial_\gamma \psi^*) (\partial_\delta \psi) + \psi^* (\partial_\delta \partial_\gamma \psi) - (\partial_\delta \partial_\gamma \psi^*) \psi \right] \ ;
\end{aligned} \tag{3.37}$$

with the due simplifications and defining

$$\Lambda \equiv \left[\left(\partial_\gamma^{-1} \psi^* \right) (\partial_\gamma \psi) - (\partial_\gamma \psi^*) \left(\partial_\gamma^{-1} \psi \right) \right] \tag{3.38}$$

we obtain the following equation:

$$\begin{aligned}
&\partial_\delta J^\delta = \\
&\frac{i}{2}\hbar p_\alpha p_\beta \hat{g}^{\alpha\beta}\left[4\Lambda + \left(\partial_\delta^{-1}\partial_\gamma^{-1}\psi^*\right)(\partial_\delta\partial_\gamma\psi) - (\partial_\delta\partial_\gamma\psi^*)\left(\partial_\delta^{-1}\partial_\gamma^{-1}\psi\right)\right] + \\
&\frac{i}{2}\hbar p_\alpha p_\beta \hat{g}^{\alpha\beta}\left[\left(\partial_\delta\partial_\gamma^{-1}\psi^*\right)\left(\partial_\delta^{-1}\partial_\gamma\psi\right) - \left(\partial_\delta^{-1}\partial_\gamma\psi^*\right)\left(\partial_\delta\partial_\gamma^{-1}\psi\right)\right] + \\
&\frac{i}{2}\hbar^2\partial_\delta\left(p_\alpha p_\beta \hat{g}^{\alpha\beta}\right)\partial_\delta^{-1}\Lambda \ .
\end{aligned} \tag{3.39}$$

The last two terms within the square brackets of the above equation are null for the properties of the generalized derivative while the last line of the right hand side reproduce exactly the equation of motion and so it's null.

From the analysis of the term in Λ it is evident that the only terms at the right order in $(\hbar)$ are:

$$\begin{aligned}
&\Lambda = i\left(\partial_\gamma^{-1}|A|^2\right)(\partial_\gamma S)\,|\phi|^2 + \\
&+|A|^2\left(\partial_\gamma^{-1}E_-\right)E_+\phi^*(\partial_\gamma\phi) - |A|^2E_-\left(\partial_\gamma^{-1}E_+\right)(\partial_\gamma\phi^*)\phi \ ,
\end{aligned} \tag{3.40}$$

with the notation $E_\pm \equiv e^{\pm\frac{i}{\hbar}S}$. A property very important of the generalized derivative is, as in the ordinary one, the Leibniz law, that applied in this case gives the relation

$$\left(\partial_\gamma^{-1}E_-\right)E_+ + E_-\left(\partial_\gamma^{-1}E_+\right) = D_p^{-1}(E_-E_+) = D_p^{-1}(1) = p \tag{3.41}$$

and so it is possible to express one term of the left hand side as a function of the other, in order to maintain the initial ordering we choose the relation $E_-\left(\partial_\gamma^{-1}E_+\right) = p - \left(\partial_\gamma^{-1}E_-\right)E_+$ and we get

$$\Lambda = i\left(\partial_\gamma^{-1}|A|^2\right)(\partial_\gamma S)\,|\phi|^2 + |A|^2\left(\partial_\gamma^{-1}E_-\right)E_+\left(\partial_\gamma|\phi|^2\right) \tag{3.42}$$

the term that contains p is of a different order and so it can be neglected.

As for the second term on the right hand side of the first line of the equation (3.39) the only term of the right order is $i\left(\partial_\delta^{-1}\partial_\gamma^{-1}|A|^2\right)(\partial_\delta\partial_\gamma S)\,|\phi|^2$. At the end we can say that the dominant terms of the equation (3.39) reduce to:

$$\begin{aligned}
\partial_\delta J^\delta = i&\left[\left(\partial_\gamma^{-1}|A|^2\right)(\partial_\gamma S)|\phi|^2 + \left(\partial_\delta^{-1}\partial_\gamma^{-1}|A|^2\right)(\partial_\delta\partial_\gamma S)|\phi|^2\right] + \\
&+|A|^2\left(\partial_\gamma^{-1}E_-\right)E_+\left(\partial_\gamma|\phi|^2\right) \ .
\end{aligned} \tag{3.43}$$

Those are the equations (3.12) and (3.14) for the Universe wavefunction and for its complex conjugate derived before. Considering their definitions the term on the right hand side it's identically null and so even in the case of this study there is a conserved probability current. This demonstration is valid for both Standard and Polymer Quantum mechanics once taken the correct assumptions.

3.3 Application to the Taub Model

In this section I will applicate the results of the previous sections to the Taub Model (one of the particular cases of Bianchi IX model), the result will be a quantum wavefunction for the Universe that will allow us to infer the behavior of the Early Universe.

Although usually the best choice for this kind of study are the Misner Variables $(\alpha, \beta_+, \beta_-)$ for their immediate physical interpretation: α is related to the volume of the Universe, while the β are related to the two physical degree of freedom of the Gravitational Field, for the following discussion I chose another set of variables more complicate and with a not immediate physical sense, the Misner-Chitrè variables. They enable us to study the dynamics of the system in the so-called *Poincaré Half Plane* that eliminate the dynamics of the potential's wall. In particular the two set of variables have the following relations [49]:

$$\begin{aligned} \alpha - \alpha_0 &= -e^{\tau} \frac{1 + u + u^2 + v^2}{\sqrt{3}v} \\ \beta_+ &= e^{\tau} \frac{-1 + 2u + 2u^2 + 2v^2}{2\sqrt{3}v} \\ \phi &= e^{\tau} \frac{-1 - 2u}{2v} \ . \end{aligned} \tag{3.44}$$

In order to make the Vilenkin Approach works it's necessary to insert a term of matter, for the purpose of this study I chose the Scalar Field.

The dynamics of this model near the singularity reduces to the one of a particle that hit continuously the walls of a pseudo-triangular box [43] [44]; the cosmological singularity is reached when the trajectory ends in one of the corner of the box. This model consists in taking one preferential direction in the β-plane, and so only one of the walls of the Bianchi IX Universe that the particle hits only one time and then goes directly in the opposite corner. This means that the Misner β_- is identically null and so the Misner-Chitrè u is always a constant and equal to $-1/2$, implying that the conjugate momentum p_u is always zero.

In the chosen variables the Super-Hamiltonian constraint $\mathcal{H} = 0$ leads to a WD equation without all the terms in p_u. In this case the metric assumes the simple form

$$ds^2 = \frac{\epsilon}{v^2} \left[du^2 + dv^2 \right] \ . \tag{3.45}$$

In order to make the math easier we change again variables, introducing

$$\begin{aligned} v &= \rho \sin(2\delta) \\ u &= \rho \cos(2\delta) \ , \end{aligned} \tag{3.46}$$

with $0 < \rho < \infty$ and $0 < \delta < \pi$. If we insert them in the metric it's simple to verify that (3.45) becomes

$$ds^2 = \epsilon \left[\frac{d\rho^2}{\rho^2 \sin^2(2\delta)} + \frac{8 d\delta^2}{\sin^2(2\delta)} \right] \ . \tag{3.47}$$

If now we define $dx = d\rho/\rho$ e $d\theta = d\delta/\sin(2\delta)$ and integrate them we find two variables with the same limits of the Misner-Chitrè ones

$$\begin{aligned} x &= \log|\rho| \quad , \quad -\infty < x < \infty \\ \theta &= \frac{1}{2}\log|\tan(\delta)| \quad , \quad -\infty < \theta < \infty \; ; \end{aligned} \tag{3.48}$$

with a few calculations it's possible to rewrite the term $\sin^2(2\delta)$ present in (3.47) as a function of the new variable θ only as

$$\begin{aligned} \boxed{\sin^2(2\delta)} &= 4\sin^2(\delta)\cos^2(\delta) = \\ 4\sin^2\left[\arctan\left(e^{2\theta}\right)\right]&\cos^2\left[\arctan\left(e^{2\theta}\right)\right] = \\ 4\frac{e^{4\theta}}{e^{4\theta}+1}\frac{1}{e^{4\theta}+1} &= \boxed{\frac{2}{1+\cosh(4\theta)}} \end{aligned} \tag{3.49}$$

where I used the formula $\sin^2[\arctan(x)] = \frac{x^2}{x^2+1}$ and the definition of the hyperbolic cosine. With these substitutions the metric becomes

$$ds^2 = \epsilon\left[\frac{2d\rho^2}{1+\cosh(4\theta)} + 8d\theta^2\right] \; , \tag{3.50}$$

we can choose a gauge and we decided to use the condition $H' = \theta H$ and so the Hamiltonian of the system becomes

$$H = \theta\left[-p_\tau^2 - \frac{p_\theta^2}{8} + \cosh^2(2\theta)\, p_x^2\right] \; . \tag{3.51}$$

3.3.1 Ordinary Case

let us analyze this Hamiltonian (3.51) in order to get the equations for the dynamics of the system, we derive them via the Ehrenfest Theorem as

$$\begin{aligned} \langle \dot{p_\theta} \rangle &= \frac{1}{i\hbar}\langle [p_\theta, H]\rangle = p_\tau^2 + \frac{p_\theta^2}{8} \\ \langle \dot{\tau} \rangle &= \frac{1}{i\hbar}\langle [\tau, H]\rangle = -2\theta p_\tau \\ \langle \dot{\theta} \rangle &= \frac{1}{i\hbar}\langle [\theta, H]\rangle = -\frac{\theta p_\theta}{4} \\ \langle \dot{x} \rangle &= \frac{1}{i\hbar}\langle [x, H]\rangle = 2\theta\cosh^2(2\theta)\, p_x \end{aligned} \tag{3.52}$$

The Hamiltonian (3.51) doesn't depend explicitly on τ and x and so their momenta are constant of motion. Those are the equations that describe the dynamics of the Universe.

Now I will adapt the Vilenkin approach to the Taub Universe. First of all I will use a wavefunction in the form $\psi(p_\tau, p_\theta, p_x) = A(p_\tau, p_\theta)\, e^{\frac{i}{\hbar}S}\chi(p_\tau, p_\theta, p_x)$ where $S(p_\tau, p_\theta)$ is the Action of the system. If we take the lowest order of the Hamiltonian constraint $H\psi = 0$ we find the Hamilton-Jacobi equation for the system as in (3.9):

$$p_\tau^2 S\, \mathrm{d}S - \frac{\hbar^2 p_\theta\, \mathrm{d}p_\theta}{4} = 0 \; ; \tag{3.53}$$

as seen in the previous section we derive the equations for the Amplitude of the wavefunction and the Schrödinger equation for the dynamics of the quantum variables respectively as:

$$-\frac{i}{\hbar}p_\tau^2 A\frac{\partial S}{\partial p_\theta}+\frac{p_\theta^2}{8}\frac{\partial A}{\partial p_\theta}=0 \tag{3.54}$$

$$i\hbar\frac{\partial \chi}{\partial t}=p_x^2\chi \tag{3.55}$$

Putting together equations (3.53) and (3.54) we get the amplitude of the Universe wavefuntion as $A=A_0 e^{-4i\frac{p_\tau}{p_\theta}}$ and this completely characterize the classical part of the probability density defined above.

The variable t, that appears in (3.55), is a time-variable defined by $\frac{\partial}{\partial t}\equiv\frac{1}{\frac{\partial S}{\partial p_\theta}\cosh^2(2\theta)}\frac{\partial}{\partial z}$ and z is the Vilenkin time defined by $\frac{\mathrm{d}}{\mathrm{d}z}\equiv\dot{p_\tau}\frac{\partial}{\partial p_\tau}+\dot{p_\theta}\frac{\partial}{\partial p_\theta}$. If we consider a quantum part of the Universe wavefunction in the form $\chi=e^{\frac{i}{\hbar}Et}\phi(p_\theta,p_x)$ and we put it in (3.55) we can solve it and we find

$$\begin{aligned}
E&=\frac{p_x^2}{2}\\
\phi(p_x)&=C_1\delta(p_x-p_{E,x})+C_2\delta(p_x+p_{E,x})\\
\phi(x)&=\frac{1}{\sqrt{2\pi}}e^{-ip_{E,x}x}\left(C_1+C_2e^{2ip_{E,x}x}\right)\quad.
\end{aligned}\tag{3.56}$$

3.3.2 Polymer Case

let us go back to the Hamiltonian (3.51) and use the Polymer Quantum Dynamics instead of the classical one. If we want the Hamilton equations we must remember that in this case the canonical commutator is $[\hat{x}_i,\hat{p}_i]=i\hbar\cos(\mu p_i)$. The Wheeler-De Witt equation in this case is in the form:

$$\begin{aligned}
&\theta\left\{-\frac{1}{\mu^2}\sin^2(\mu p_\tau)-\frac{1}{8\mu^2}\sin^2(\mu p_\theta)\right\}\Psi+\\
&\quad+\theta\left\{\frac{\cosh^2(2\theta)}{\mu^2}\sin^2(\mu p_x)\right\}\Psi=0
\end{aligned}\tag{3.57}$$

With the same calculations of the previous section we find the equations for the dynamics of the particle Universe

$$\begin{aligned}
\langle\dot{p_\theta}\rangle&=\frac{1}{\mu^2}\sin^2(\mu p_\tau)+\frac{1}{8\mu^2}\sin^2(\mu p_\theta)\\
\langle\dot{\tau}\rangle&=\frac{\theta}{\mu}\sin(2\mu p_\tau)\\
\langle\dot{\theta}\rangle&=\frac{\theta}{4\mu}\sin(2\mu p_\theta)\\
\langle\dot{x}\rangle&=\frac{2\theta\cosh^2(2\theta)}{\mu}\sin(2\mu p_x)\quad.
\end{aligned}\tag{3.58}$$

As in the previous section, even in this case the other two momenta are constant of motion. Those are the equations that describe the dynamics of the Early Universe.

Now we use the Vilenkin approach in this case, from equation (3.57) we can derive the Hamilton-Jacobi equation, the equation for the amplitude of the wavefunction and the Schrödinger equation for the quantum variables respectively

$$\frac{1}{\mu^2}\sin^2(\mu p_\tau)\, S\, \mathrm{d}S - \frac{\hbar^2}{4\mu^2}\sin(\mu p_\theta)\cos(\mu p_\theta)\, \mathrm{d}p_\theta = 0 \tag{3.59}$$

$$\frac{iA\sin^2(\mu p_\tau)}{\hbar}\frac{\partial S}{\partial p_\theta} + \frac{\sin^2(\mu p_\theta)}{8}\frac{\partial A}{\partial p_\theta} = 0 \tag{3.60}$$

$$i\hbar\frac{\partial \chi}{\partial t_{pol}} = \frac{[1-\cos(\mu p_x)]\,\chi}{\mu^2} \tag{3.61}$$

Using together equations (3.59) and (3.60) we get the amplitude of the Universe wavefuntion as $A = A_0 e^{-4i\frac{\sin(\mu p_\tau)}{\sin(\mu p_\theta)}}$ and this completely characterize the classical part of the probability density defined above.

The variable t_{pol}, that appears in (3.61), is a time-variable defined by $\frac{\partial}{\partial t_{pol}} \equiv \frac{\sin(\mu p_\tau)}{\hbar\cos(\mu p_\theta)\cosh^2(2\theta)}\frac{\partial}{\partial z_{pol}}$ where z_{pol} is the Vilenkin time in the Polymer representation. If we consider a quantum part of the Universe wavefunction in the form $\chi = e^{\frac{i}{\hbar}kt_{pol}}\phi(p_\theta, p_x)$ and we put it in (3.61) we can solve it and we find

$$\begin{aligned} k = k(\mu) &= \frac{1}{\mu^2}[1-\cos(\mu p_x)] \le k_{max} = \frac{2}{\mu^2} \\ \phi_{k,\mu}(p_x) &= C_1\delta(p_x - p_{k,\mu}) + C_2\delta(p_x + p_{k,\mu}) \\ \phi_{k,\mu}(x) &= \frac{1}{\sqrt{2\pi}}e^{-ip_{k,\mu}x}\left(C_1 + C_2 e^{2ip_{k,\mu}x}\right) . \end{aligned} \tag{3.62}$$

We can notice that those are the same results of the previous section once taken into account the Polymer modifications, moreover we can also notice that the eigenvalue here has an upper limit and this will be very important in the dynamics of the Universe.

3.4 Discussion of the results

We now analyze the equations that we found in the previous section, in particular the Hamilton equations (3.52) and (3.58) obtained in the two different cases. If we integrate those systems we obtain the following equations for the volume of the Universe τ, the scalar field θ and its momenta p_θ

$$\begin{aligned} \langle p_\theta \rangle &= 2\sqrt{2}p_\tau \tan(J) \\ \langle \theta \rangle &= C_2\cos^{2.}(J) \\ \langle \tau \rangle &= C_3 + \frac{4\sqrt{2}C_2}{3}\cos^{3.}(J)\csc(J)\, \cdot \\ &\cdot\ {}_2F_1\left[\frac{1}{2},\frac{3}{2},\frac{5}{2},\cos^{2.}(J)\right]\sin(J) \ . \end{aligned} \tag{3.63}$$

Those are the equation for the ordinary case in which we defined $J = \frac{1}{4}\left(p_\tau z + 8\sqrt{2}C_1\right)$, the dynamics of the volume of the Universe will be plotted in Fig (3.1) while the equation for the anisotropy x is numerically solved and we will show its dynamics in Fig (3.2). The Universe starts at a point with finite volume, evolves towards the potential wall and then goes straight into the singularity without the possibility to evade it. The anisotropies, instead, explode near the singularity and are practically null near the wall.

For the Polymer case there are no analytical solutions of the system (3.58), all the equations are numerically integrated and their dynamics will be plotted in Fig (3.3) and Fig (3.4) (solid line).

The plots shown in figure (3.3) and (3.4) allow us to state that the Taub model can be reduced to a singularity-free model with a cyclical behavior in both volume and anisotropies. In the four plots it's possible to highlight the main differences between the two representations, in the ordinary case the singularity is unavoidable, while in the Polymer approach there is a periodic behavior of the Universe variables, and so the singularity is regularized.

If we take the general solution of the Schrödinger equation (3.62) with the boundary conditions due to the Taub Cosmological Model, that in our variables it can be shown that read as $\phi(x_0) \equiv \phi(\infty) \equiv 0$ (where we defined $x_0 = \log\left(\frac{1}{\sqrt{2}}\right)$), the wave function of the Universe becomes

$$\Psi = \frac{C_1}{\sqrt{2\pi}} e^{\frac{i}{\hbar}kz}\left[e^{ipx} - e^{ip(x_0-x)}\right] \tag{3.64}$$

With this we can now construct a Gaussian packet and study its dynamics, the first step is to define the packet as

$$\Xi = \int_0^{k_{\mathrm{Max}}} \exp\left[-\frac{(k-k_0)^2}{2\sigma^2}\right] \Psi \, \mathrm{d}k \tag{3.65}$$

then we numerically evaluate this integral at different times in order to obtain a dynamics of the Gaussian packet, in figure (3.4) we have shown the results of our analysis and we have even compared the evolution of the Gaussian packet with the dynamics of the mean value of the quantum anisotropy that we got with the Ehrenfest theorem.

From the plot it can be seen that the two trajectories coincide up to the Bounce-turning-points, then the packet dynamics reveals a series of turning point like the volume variable and we can even see a correspondence between the behavior of the two variables. In those points the variance, calculated via the distribution theory, on the Ehrenfest equation for the anisotropy is comparable to the mean value and so we can say that in the bounce-turning-points of this model, the Ehrenfest theorem cannot be applied straightforwardly, i.e. the packet dynamics shows the correct evolution of the anisotropy variable. Thus we can conclude that in our approach the true singularity of the Taub Model is regularized with the Polymer Quantization within the Vilenkin approach.

In figure (3.5) we have shown the dynamics of the other Universe variables, while for the momentum conjugated to the scalar field we can state that in the Polymer case it gains an oscillatory behavior between a minimum and a maximum turning point, for the scalar field the difference between the two representations is only a time-shift, in particular we can observe a delay induced by the Polymer Quantum Mechanics.

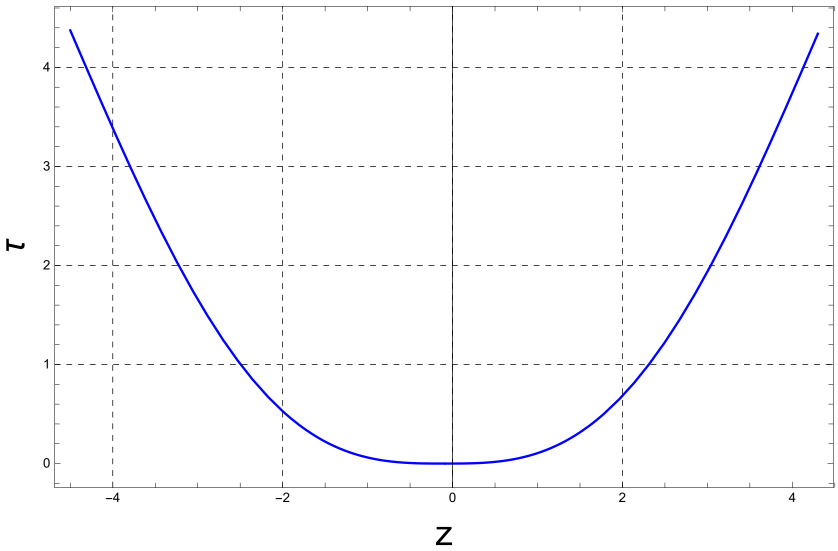


Figure 3.1. Dynamics of the volume of the Universe in the Vilenkin time variable z defined above. The Universe starts at finite volume, reach the potential barrier (z=0) and then goes toward the singularity of the model ($z = \infty$).

The reason we concentrate our attention on the Taub cosmology in the presence of a massless scalar field consists both of the presence of the necessary Minisuperspace degrees of freedom and because the WKB construction of a Schrödinger evolution for the real quantum variables naturally apply for the Universe anisotropy degree of freedom. More specifically, on one hand, the possibility to deal with two quasi-classical variables and a purely quantum one, allows to fully implement the scheme introduced in [54] and, on the other hand, the polymer regularized anisotropy variable (we will see that its value no longer diverges, as in standard evolution) is a phase space sample very appropriate to the concept of "smallness" of the quantum system also invoked in [54].

Furthermore, the Taub cosmology has a non-trivial meaning for the physics of the early Universe. It corresponds to a Bianchi IX model with two scale factor equal to each other and, it is well-known, that the Bianchi dynamics in the "corner" of the spatial curvature induced potential [15, 48] closely resembles small oscillations around a Taub configuration. Thus the generality of the Bianchi IX cosmology, versus a generic inhomogeneous cosmological model [47] justifies the interest for the present analysis. Finally, implementing the polymer paradigm within a WKB decomposition of the Minisuperspace dynamics, we are trying to clarifying the behavior of the anisotropy degree of freedom when a Big-Bounce emerges. The case of a vacuum Taub cosmology, when the polymer quantum mechanics is implemented on the anisotropy dynamics only, was analyzed in [5], showing how the cosmological singularity is not removed, but only probabilistic weakened. The merit of such an investigation consists in clarifying that the emergence of a bouncing cosmology requires that the polymer reformulation also involves the Universe volume. In this respect, the present analysis is the conceptual continuation of the study in [5]. We

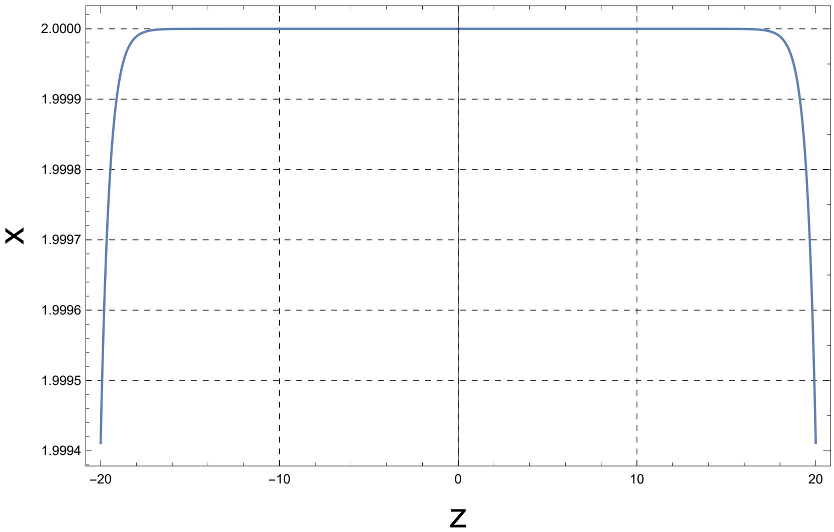


Figure 3.2. Dynamics of the anisotropies of the universe in the Vilenkin time variable z defined above. The Universe starts with a finite degree of anisotropy, it then reaches a constant value near the potential wall (z=0) and then explodes in the singularity of the model ($z = \infty$).

include in the quantum dynamics a massless scalar field in order to deal with a relational time variable giving a material nature [32].

When we face the description of the anisotropy degree of freedom as a pure quantum variable, we adopt the quasi-classical representation for both the Universe volume and the scalar field. However, following the analysis in [54], we are able to identify, in the end, the label time coordinate along the space-time slicing, with a suitable function of the volume and the massless scalar field, by using a gauge fixing. All the variable are approached in the polymer formulation and therefore we are able to infer a bouncing cosmology, with the very important feature that the anisotropy degree of freedom is now really "small” in the sense of the WKB analysis requirement, see also [1] for a more precise characterization of this concept.

By means of some non-trivial technicalities, like a suitable re-definition of the Misner-Chitrè-like variables here adopted, we finally demonstrate that the Taub cosmology is a good candidate, in the present paradigm, for describing a cyclical anisotropic Universe, always remaining not to far form the Robertson-Walker geometry.

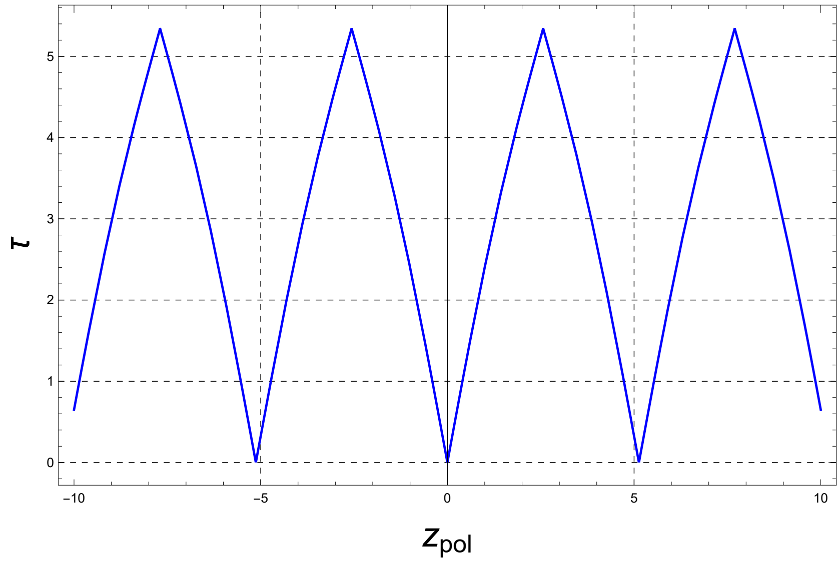


Figure 3.3. Dynamics of the volume of the universe in the Vilenkin time variable z_{pol} defined above. The Universe starts with a finite volume, it then reaches a series of turning points.

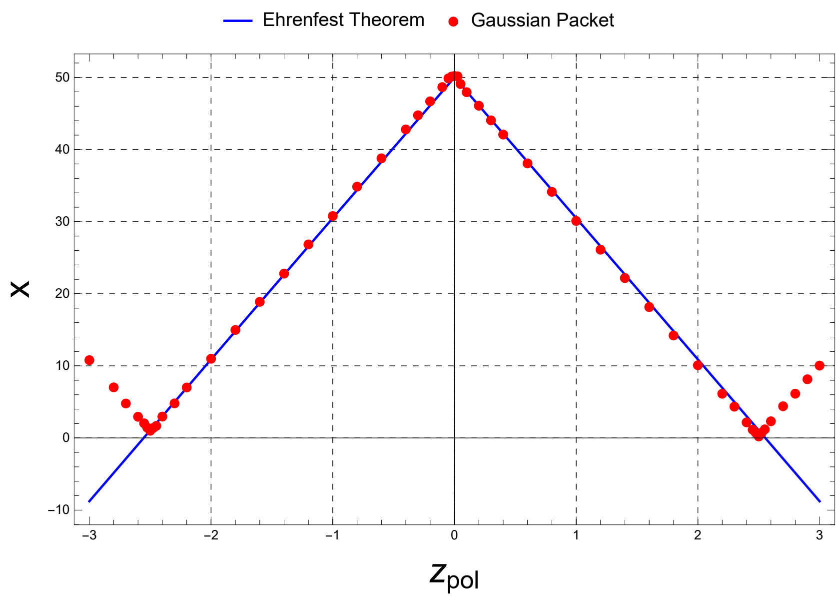
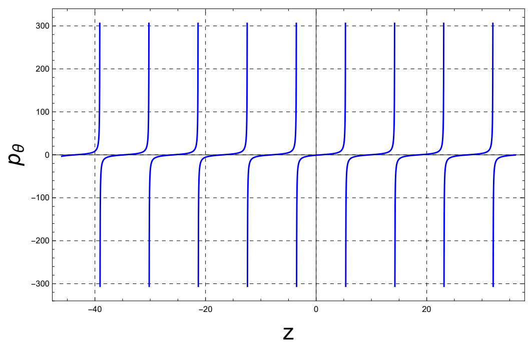
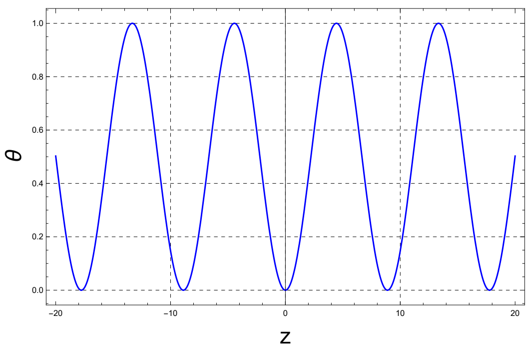


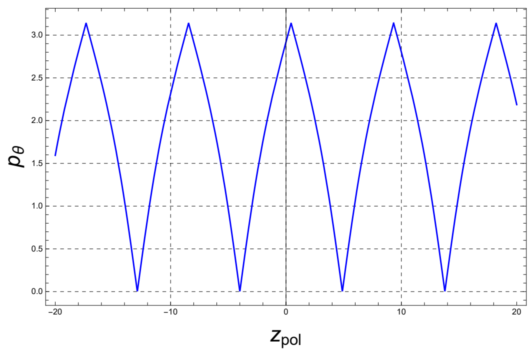
Figure 3.4. Dynamics of a Gaussian packet build from the solution of the Schrödinger equation in the Vilenkin time variable compared to the dynamics obtained with the Ehrenfest Theorem.



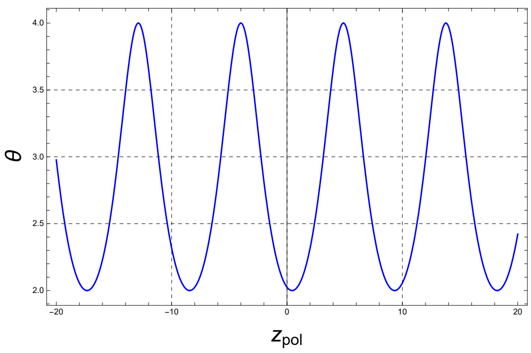
(a) Dynamics of the momentum conjugated to the scalar field in the ordinary case



(b) Dynamics of the scalar field in the ordinary case



(c) Dynamics of the momentum conjugated to the scalar field in the polymer case



(d) Dynamics of the scalar field in the polymer case

Figure 3.5. Dynamics of the other two variables in both standard and polymer case

Chapter 4

Quantum dynamics of the corner of the Bianchi IX model in WKB approximation

In this Chapter we will analyze the Bianchi IX Universe dynamics within the corner region associated to the potential term which the spatial curvature induces in the minisuperspace. We investigate the dynamics in terms of WKB scenario : the isotropic Misner variable (α) and one of the two anisotropic variables (β_+) are treated as semi-classical, while the remaining anisotropy (β_-) is described on a pure quantum level. The quantum dynamics always reduces to the one of a time-dependent Schrödinger equation for a harmonic potential with a time dependent frequency.

The study is done in the vacuum and in the presence of a massless scalar field ϕ and a cosmological constant term Λ. The vacuum case is treated in the limits of a collapsing and an expanding Universe, while the dynamics in presence of ϕ and Λ is studied only for $t \to \infty$. In both analyses the quantum dynamics of the anisotropy variable β_- suggests a suppression of the quantum anisotropy associated. In the vacuum case the corner configuration becomes an attractor for the dynamics and the evolution resembles that of a Taub cosmology in the limit of a non-singular initial Universe. This suggests that if the Bianchi dynamics enters deeply enough in the potential corner the initial singularity is removed and a Taub picture emerges. The case when ϕ is present well mimics the de-Sitter phase of an inflationary Universe. Here we show that both the classical and quantum anisotropies are exponentially suppressed, so that the resulting dynamics corresponds to an isotropic closed Robertson-Walker geometry.

4.1 Introduction

The Bianchi IX model [11, 2, 47] has a relevant role in the study of the cosmological dynamics since, despite its spatial homogeneity, it possesses typical features of the generic cosmological solution [9, 29, 45], like a chaotic time evolution of the cosmic scale factors near the cosmological singularity [25, 47]. In the Hamiltonian representation, the Bianchi IX dynamics can be reduced to that of a two-dimensional point-particle in a time-dependent potential [2, 42]. The chaotic features of the model correspond to an infinite sequence of bounces of the point particle against the potential walls, which in the representation based on the so-called Misner-Chitrè-like variables can be shown to induce an ergodic evolution, having also a significant degree of stochasticity [16, 42, 25].

Approaching the cosmological singularity, the potential term of the Bianchi IX dynamics resembles an infinite well having the morphology of an equilateral triangle, as shown in Fig.4.1.

The three open corners which appear in the vertices of such a triangular configuration correspond to the non-singular Taub cosmology [40], which defines the limit when the Bianchi dynamics is associated to two equal scale factors of the three possible independent ones.

It was shown [25] (see also the original literature therein) that, during its evolution toward the initial singularity, there is always a situation where the point-particle is deeply inside one of the corners and two of the scale factors rapidly oscillate. In [11] the authors defined this regime as "small oscillation". It is a well-known result [47] that the Bianchi IX universe, after spending a long time in this regime, escapes from it to restore the standard dynamics in the central region of the potential well. Furthermore, the probability that small oscillations take place again is strongly suppressed.

In the present analysis we study the situation in which the Bianchi IX dynamics is trapped in a corner of the potential, but the oscillating small degree of anisotropy, is in a quantum regime.

In particular, we consider the corner configuration for which $\beta_+ \to \infty$ and $|\beta_-| \ll 1$ (which corresponds to the corner to the far right in Fig. 4.1), given this is the simplest case to be addressed. Indeed, the potential level surfaces for a fixed value of the variable α are invariant under a $\pi/3$ rotation and it is clear that, choosing a different "corner", a re-definition of the coordinates β_+ and β_-, trough a $\pi/3$ rotation in their plane, would restore the same picture we are considering here.

The paradigm we are addressing corresponds to the WKB proposal of Vilenkin [54] for the interpretation of the wave function of a small quantum subsystem of the minisuperspace. The idea is that a part of the primordial Universe has reached a quasi-classical limit and can therefore play the role of a clock for the small quantum subsystem.

Here we consider the volume α, the macroscopic anisotropy β_+ and ϕ when present as semi-classical variables, while the small anisotropy variable β_- as quantum variable. We consider β_- to be the quantum variable because its dynamics is somehow trapped in the corner phase space. In [1] it has been shown that the Vilenkin picture can be applied to a quantum subset only if, in agreement to the Vilenkin hypotheses, the region of the phase space concerning that subset is "small". Therefore, considering the variable β_+ as a quantum coordinate, in the considered corner configuration, would have no clear physical justification, since its classical dynamics covers a much larger phase space than it is available to β_-. The same it's true for the variable α and the scalar field ϕ.

The analysis in which both β_+ and β_- are simultaneously treated as quantum variable must be referred to a quasi-isotropic Universe. In this case both the anisotropic variables are close to the origin of their plane. For an implementation of this scenario in the case of Bianchi IX Universe see [6]. The same quasi-isotropic scenario, in the case of a Taub has been discussed in [20].

The Bianchi IX dynamics in the corner is studied in two different cases: Bianchi IX in the vacuum, and also in presence of a massless scalar field ϕ and a cosmological constant Λ. The latter is interesting since it mimics an inflationary-like scenario.

In both scenarios, it has been shown that the small quantum degrees of freedom are naturally suppressed by the Universe's exponential expansion during the de-Sitter phase.

In the vacuum case we distinguish two different situations corresponding to the expanding or collapsing behavior of the Universe respectively. When the volume expands and the classical anisotropy β_+ increases, the standard deviation of the probability distribution associated to the small quantum anisotropy β_- is damped to zero and the Universe asymptotically approaches a Taub cosmological model [40]. As a result, if the point-Universe enters sufficiently into the corner, this configuration becomes an attractor and the quantum anisotropy is increasingly damped.

If we consider this picture in the direction of a collapsing Universe instead, we get that the frequency of the harmonic oscillator associated to the quantum anisotropy takes a constant value. Therefore, the classical component of the Universe takes the form of a Taub Universe, possessing a small fluctuating additional anisotropy. It is known [40] that the Taub model has a singularity in the future, but a non-singular finite Universe volume in the past. Thus if we start with a point Universe entering the corner backward in time, thought as the past of the considered framework, the approach to the initial singularity would be stopped.

In this respect, differently from the pure classical behavior (see [11, 47]), in a WKB scenario **a la Vilenkin**, where the small anisotropy is thought as a quantum degree of freedom, the existence of the initial singularity could be removed. The backward extension of a Mixmaster dynamics [2] sooner or later would deeply enters the corner and the limiting initial configuration of the Universe would be a finite volume Universe, endowed with a small stationary distribution for the relic quantum anisotropy. This conjecture could offer a more general paradigm if we recall that the Bianchi IX model is the prototype for the generic cosmological solution [9, 47].

When ϕ and Λ are included in the dynamics, we consider the limit of an asymptotic exponentially expanding Universe, according to a de-Sitter phase of an inflationary paradigm. We show that both the classical macroscopic anisotropy, and the small quantum one are exponentially suppressed as the volume expands. In other words, we are implementing a new dynamical scheme for the isotropization of the Bianchi IX dynamics. This issue completes the analysis in [6], where the depicted scenario corresponds to the case of two small quantum anisotropies, i.e. the case when the point-particle is close to the potential center.

The present study seems to be of more cosmological interests since we expect, due to the time reversibility of the Einsteinian dynamics, that also in the expanding picture the Bianchi IX Universe spends long time in the corner configuration. This consideration makes plausible that, on one hand the small anisotropy degree of freedom is in a quantum regime, and on the other hand, the cosmological constant term has time to grow, and therefore the de-Sitter phase has time to start.

All of this is included in the paper [15] that has just been published in PRD.

4.2 Hamiltonian Formulation of the Mixmaster model

The importance of the Hamiltonian formulation of the Mixmaster model, obtained following the ADM method [47], relies on the fact that it shows how it is possible to reduce the dynamics of the Bianchi IX model to the dynamic of a two-dimensional point particle performing an infinite series of bounces inside a potential well.
In this paper we adopt natural units: $\hbar = c = 1$.

The line element for this model is

$$ds^2 = N^2(t)dt^2 - e^{q_a}\delta_{ab}\omega^a\omega^b \tag{4.1}$$

where ω^i are 1-form depending on the Euler angles $\theta \in [0,\pi]$, $\phi \in [0,2\pi]$, $\psi \in [0,4\pi)$

$$\begin{aligned} \omega^1 &= \sin\psi\sin\theta d\phi + \cos\psi d\theta \\ \omega^2 &= -\cos\psi\sin\theta d\phi + \sin\psi d\theta \\ \omega^3 &= \cos\theta d\phi + d\psi \end{aligned} \tag{4.2}$$

and N is the lapse function.
Following the computation presented in [47], we obtain the action

$$S_B = \int dt(p_a\dot{q}^a - N\mathcal{H}_B) \tag{4.3}$$

where p_a are the conjugate momenta to the generalized coordinates q^a,

$$p_a \equiv \frac{\partial\mathcal{L}}{\partial\dot{q}^a} \tag{4.4}$$

and the *Hamiltonian density* can be written as

$$\mathcal{H}_B = \frac{k}{8\pi^2\sqrt{\eta}}\left[\sum_a (p_a)^2 - \frac{1}{2}\left(\sum_b p_b\right)^2 - \frac{64\pi^4}{k^2}\eta\ {}^3R\right] \tag{4.5}$$

where

$$\eta\ {}^3R = -\frac{1}{2}\left(\sum_a \lambda_a^2 e^{2q_a} - \sum_{a\neq b}\lambda_a\lambda_b e^{q_a+q_b}\right) \tag{4.6}$$

can be interpreted as the potential for the dynamics.

To obtain a Hamiltonian that resembles the one of a point-particle, it is necessary to diagonalize the kinetic part introducing the following variables:

$$\begin{cases} q_1 = 2(\alpha + \beta_+ + \sqrt{3}\beta_-) \\ q_2 = 2(\alpha + \beta_+ - \sqrt{3}\beta_-) \\ q_3 = 2(\alpha - 2\beta_+) \end{cases} \tag{4.7}$$

where α, $\beta_\pm$ are the *Misner variables*, introduced by Misner in [2]: α describes the volume of the Universe, $\beta_\pm$ describe the anisotropy degrees of freedom.

The introduction of the Misner variables allows us to write the super-Hamiltonian constraint for the Bianchi IX Universe in the ADM formalism [2] as

$$\begin{aligned}\mathcal{H}_{IX} = &\frac{Nk}{3(8\pi)^2}e^{-3\alpha}(-p_\alpha^2+p_+^2+p_-^2+p_\phi^2)+\\ &+\frac{Nk}{3(8\pi)^2}e^{-3\alpha}\left[\frac{3(4\pi)^4}{k^2}e^{4\alpha}V_{IX}(\beta_-,\beta_+)+\Lambda e^{6\alpha}\right]=0\end{aligned} \tag{4.8}$$

where $(p_\alpha,\, p_\pm)$ are the conjugate momenta to $(\alpha,\, \beta_\pm)$ and we added a classical scalar field ϕ and the cosmological constant Λ in order to obtain an inflationary scenario.
$V_{IX}(\beta_-,\beta_+)$ is the potential of the Bianchi IX model and is given by

$$\begin{aligned}V_{IX}(\beta_-,\beta_+) =& e^{-8\beta_+} - 4e^{-2\beta_+}\cosh(2\sqrt{3}\beta_-)+\\ &+2e^{4\beta_+}[\cosh(4\sqrt{3}\beta_-)-1].\end{aligned} \tag{4.9}$$

As seen from Fig.(4.1) this function has the symmetry of an equilateral triangle with steep exponential walls and three open angles.

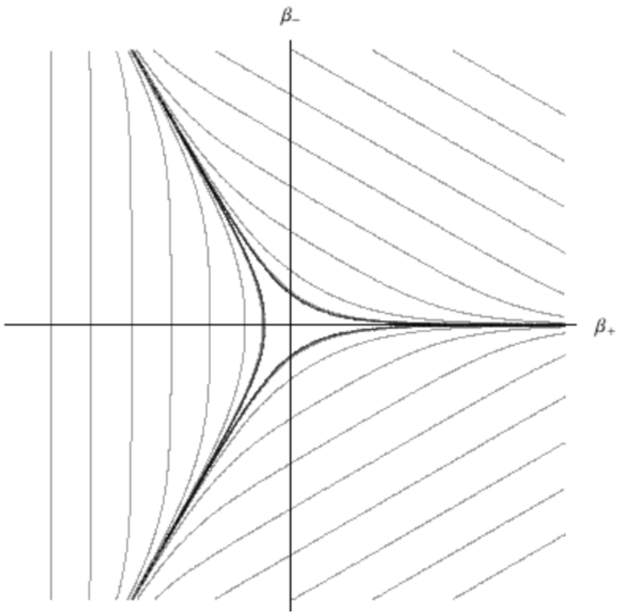


Figure 4.1. Equipotential lines for the Bianchi IX potential (4.9) in the plane (β_+,β_-). [47]

The expressions for the potential 4.9 for large values of $|\beta_+|$ and small $|\beta_-|$ are:

$$V_{IX} \propto \begin{cases} e^{-8\beta_+}, & \beta_+\to-\infty, |\beta_-|\ll 1\\ 48\beta_-^2 e^{4\beta_+}, & \beta_+\to+\infty, |\beta_-|\ll 1\end{cases} \tag{4.10}$$

while close to the origin, for $\beta_\pm = 0$,

$$V_{IX} \propto (\beta_+^2+\beta_-^2). \tag{4.11}$$

The Hamiltonian approach provides the following equations of motion

$$\dot{\alpha} = N\frac{\partial \mathcal{H}_{IX}}{\partial p_\alpha}, \qquad \dot{p}_\alpha = -N\frac{\partial \mathcal{H}_{IX}}{\partial \alpha}, \tag{4.12}$$

$$\dot{\beta}_\pm = N\frac{\partial \mathcal{H}_{IX}}{\partial p_\pm}, \qquad \dot{p}_\pm = -N\frac{\partial \mathcal{H}_{IX}}{\partial \beta_\pm}. \tag{4.13}$$

The Universe evolution at this point is described as the motion of a *point-like particle* governed by (4.10) and (4.11) and is characterized by a sequence of bounces against the potential wall, when the system evolves towards the singularity [47, 48].

4.3 Quantum behavior of the Mixmaster model

In this section we are going to briefly introduce the *Wheeler-DeWitt equation* (WDW) and to show how it is used in [54] in order to obtain an interpretation of the wave function of the Universe.

The WDW equation describes the quantum behavior of the Universe and it can be seen as the quantum version of the super-Hamiltonian constraint (4.8).

To canonically quantize a system, the required commutation relation is

$$[\widehat{q}_a, \widehat{p}_b] = i\delta_{ab} \tag{4.14}$$

which is satisfied for $\widehat{p}_a = -i\partial_a$.

Therefore, imposing the constraint equation (4.8) and replacing the canonical variables with their operators in order to select the physically allowed states, we obtain the WDW equation

$$\widehat{\mathcal{H}}\Psi = (\nabla^2 - V)\Psi = 0 \tag{4.15}$$

where Ψ is the *wave function of the Universe*, which provides information about the physical state of the Universe.

It is important to notice that in the general formulation of the WDW equation, Ψ is defined on a *superspace*, intended as the infinite dimensional space of all the possible three-metric where the wave function is defined, while in the present paper it is defined on a *mini-superspace*; this is obtained restricting the number of degrees of freedom of the metric to a finite number by imposing symmetries. This simplification is possible since we are focusing on homogeneous models where only three degrees of freedom (the three different scale factors) are allowed.

With this in mind, we can finally write the WDW equation for the Bianchi IX model

$$\begin{aligned} \widehat{\mathcal{H}}_{IX}\Psi &= \frac{Nk}{3(8\pi)^2}e^{-3\alpha}[\partial_\alpha^2 - \partial_+^2 - \partial_-^2 - \partial_\phi^2]\Psi + \\ &+ \frac{Nk}{3(8\pi)^2}e^{-3\alpha}\left[\frac{3(4\pi)^4}{k^2}e^{4\alpha}V_{IX} + \Lambda e^{6\alpha}\right]\Psi = 0 \end{aligned} \tag{4.16}$$

where $\Psi = \Psi(\alpha, \beta_+, \beta_-, \phi)$.

4.3.1 Resolution of the Schrödinger equation

The quantum probability distribution for the wave function of the universe, as show in the probability density definition, is given by $|\chi|^2$. This can be computed solving the Schrödinger equation.

Substituting $\mathcal{H}_q$ explicitly with its expression, the Shrodinger equation becomes

$$i\frac{d\chi}{d\tau} = \left(p_-^2 + 16e^{4(\alpha+\beta_+)}\beta_-^2\right)\chi \tag{4.17}$$

which can be viewed as the Schrödinger equation of a harmonic oscillator with time-dependent frequency and unitary mass if we impose $\omega^2(\tau) \equiv 16e^{4(\alpha+\beta_+)}$ and redefine the time variable $\tau' = 2\tau$. In the following we will use τ instead than τ' for simplicity.

In [35, 36, 37] the authors developed a method to obtain eigenvectors and eigenvalues for this particular Schrödinger equation using the invariant method. As summarized in [50] the general solution of an equation of the form (4.17) is given by:

$$\chi = \sum_n c_n e^{i\alpha_n(\tau)}\phi_n(\beta_-,\tau) = \sum_n c_n\chi_n(\beta_-,\tau) \tag{4.18}$$

where c_n are numerical coefficients that weight the different χ_n,

$$\alpha_n(\tau) = -(n+\frac{1}{2})\int_0^\tau \frac{1}{\rho^2}d\tau' \tag{4.19}$$

$$\chi_n(\beta_-,\tau) = \Omega_n \exp\left[\frac{i}{2}\left(\frac{\dot\rho}{\rho} + \frac{i}{\rho^2}\right)\beta_-^2]\mathcal{H}_n(\frac{\beta_-}{\rho})\right] \tag{4.20}$$

where $\Omega_n = \left[\frac{1}{(\pi)^{1/2}n!2^n\rho}\right]^{1/2}$ and ρ is a c-number quantity satisfying

$$\rho'' + \omega^2(\tau)\rho - \frac{1}{\rho^3} = 0 \tag{4.21}$$

where the $'$ indicates a differentiation respect to the time variable ρ depends to, which is τ.

It is usually complicated to solve (4.21) analytically, but in [36] the authors developed a method that allows us to have the explicit expression of the ρ as a linear combination of $f(\tau)$ and $g(\tau)$, linear solutions of

$$\frac{\partial^2 q}{\partial\tau^2} + \omega^2(\tau)q = 0. \tag{4.22}$$

4.3.2 Bianchi IX in the vacuum

As first part of our work we study the dynamical evolution of the Mixmaster model in the simplest case: the vacuum. In this case the Hamiltonian (4.8) is simply

$$\mathcal{H} = e^{-3\alpha}K(-p_\alpha^2 + p_+^2 + p_-^2 + \mathcal{V}) \tag{4.23}$$

where K is a numerical coefficient.
The quantum part of the Hamiltonian $\mathcal{H}_q$ is given by

$$\mathcal{H}_q = -p_-^2 + \omega^2(\tau) = \left(p_-^2 + 16e^{4(\alpha+\beta_+)}\beta_-^2\right) \tag{4.24}$$

as already stated in (4.17).

To compute the solution of (4.17) we need to write $\omega^2(\tau)$ explicitly as a function of τ. This can be done starting from (4.12), (4.13) and (4.8) . In particular

$$\dot{\alpha} = \frac{\partial \alpha}{\partial t} = \frac{\partial \mathcal{H}_0}{\partial p_\alpha} = -2p_\alpha k e^{-3\alpha} \tag{4.25}$$

$$\dot{p}_\alpha = \frac{\partial p_\alpha}{\partial t} = -\frac{\partial \mathcal{H}_0}{\partial \alpha} = -3\mathcal{H} = 0 \tag{4.26}$$

where $\mathcal{H}_0 = e^{-3\alpha} k(-p_\alpha^2 + p_+^2)$.

Integrating (4.25) through separation of variables, and using the result of (4.26), which states that p_α has a constant value, we get

$$e^{3\alpha} = 6|p_\alpha|Kt \tag{4.27}$$

which gives

$$\alpha(t) = \frac{1}{3}\log 6|p_\alpha|K + \frac{1}{3}\log t \tag{4.28}$$

It is worth noticing that, in the calculation above we used the absolute value of p_α; looking at (4.25) we see that $\dot{\alpha}$, which denotes how the volume of the Universe changes with time, has the opposite sign of p_α. Since our study is based on an expanding Universe and therefore we need $\dot{\alpha} > 0$, we impose $p_\alpha < 0$.
Using (4.28) in the new time variable definition we obtain

$$\tau(t) = \frac{1}{6|p_\alpha|}\log t \tag{4.29}$$

that can be substitute it in (4.28) to give

$$\alpha(\tau) = \frac{1}{3}\log 6|p_\alpha|K + 2|p_\alpha|\tau. \tag{4.30}$$

Given (4.29), and the asymptotic behavior of the synchronous time variable t, $0 < t < \infty$, we have that $-\infty < \tau < \infty$.

As mentioned in the introduction , for the study of the vacuum , we decided to characterize two different situations: the dynamical evolution of the Bianchi IX model in an expanding and in a collapsing Universe.

Bianchi IX in the vacuum: expanding Universe

In this section we consider the dynamical evolution when the semi-classical anisotropy variable β_+ increases in the direction of an expanding Universe, that means $\dot{\beta}_+(t) > 0$.
To find the explicit expression for $\beta_+(t)$ and consequently for $\beta_+(\tau)$, we follow the same arguments presented in the computation of $\alpha(t)$.

In particular from (4.13)

$$\dot{\beta}_+(t) = \frac{\partial \mathcal{H}_0}{\partial p_+} = 2p_+ K e^{-3\alpha}$$
$$\beta_+(t) = \frac{1}{3}\frac{p_+}{|p_\alpha|}\log t + \beta_0 \tag{4.31}$$

$$\dot{p_+} = -\frac{\partial \mathcal{H}_0}{\partial \beta_+} = 0 \ \rightarrow \ p_+ = const. \tag{4.32}$$

The ratio $p_+/|p_\alpha|$ can be simplified using the Hamilton-Jacobi equation

$$\left(\frac{\partial S}{\partial \alpha}\right)^2 - \left(\frac{\partial S}{\partial \beta_+}\right)^2 = 0 \rightarrow p_\alpha = \pm p_+ \tag{4.33}$$

and taking into account that we are interested in studying what happens for $t \rightarrow \infty$ (hence $\dot{\alpha} > 0$) and deeply inside the corner, therefore for $\dot{\beta_+} > 0$: this translates in the condition $p_+ > 0$.

Substituting (4.30) and (4.29) into (4.31) we obtain

$$\beta_+(\tau) = \beta_0 + 2|p_\alpha|\tau \tag{4.34}$$

The frequency of the harmonic oscillator becomes

$$\begin{aligned}\omega^2(\tau) &= 16e^{4(\alpha(\tau)+\beta_+(\tau))} \\ &= 16e^{4(\alpha_0+\beta_0)}e^{16|p_\alpha|\tau} \propto Ce^{k\tau},\end{aligned} \tag{4.35}$$

with k and C constants.
The solution of equation (4.17), with $\alpha(\tau)$ and $\beta(\tau)$ given in (4.30) and (4.34), can be obtained solving (4.22) to find $\rho(\tau)$. The 2 independent solutions are :

$$f(\tau) = J_0\left[\frac{2\sqrt{C}\sqrt{e^{k\tau}}}{k}\right] \tag{4.36}$$

$$g(\tau) = N_0\left[\frac{2\sqrt{C}\sqrt{e^{k\tau}}}{k}\right] \tag{4.37}$$

where J_0 and N_0 represent the Bessel functions of the first and the second kind.

Combining them together we obtain

$$\rho(\tau) = \frac{\pi}{2k}\sqrt{J_0^2\left[\frac{2\sqrt{C}\sqrt{e^{k\tau}}}{k}\right] + \frac{64k^2N_0^2\left[\frac{2\sqrt{C}\sqrt{e^{k\tau}}}{k}\right]}{\pi^2} + \frac{8\sqrt{3}kJ_0\left[\frac{2\sqrt{C}\sqrt{e^{k\tau}}}{k}\right]N_0\left[\frac{2\sqrt{C}\sqrt{e^{k\tau}}}{k}\right]}{\pi}} \tag{4.38}$$

Substituting (4.38) into (4.18) and defining its conjugate, we can finally compute numerically the probability distribution for the quantum part of the Universe wave function, namely

$$|\chi\left(\tau, \beta_-\right)|^2 = \sum_n c_n\chi_n\left(\sum_m c_m\chi_m\right)^* \tag{4.39}$$

The coefficients c_n are given by

$$c_n = \int \chi_0 \chi_n^* d\beta_- \tag{4.40}$$

where $\chi_0 = \chi_n(\tau_0)$ and it has been chosen such that $|\chi_0|^2$ has a gaussian shape peaked around $\beta_- = 0$.
We plot $|\chi|^2$ as a function of the quantum anisotropic variable β_- for different times t in Fig.4.2.

To conclude the study of the probability density of the wave function of the Universe, we calculate the probability density of the semiclassical variables, $|A(\alpha, \beta_+)|^2$, by variable separation.
In particular, $A(\alpha, \beta_+) = A_1(\alpha)A_2(\beta_+)$ and results:

$$A(\alpha, \beta_+) = e^{\frac{W}{p_\alpha}(\alpha+\beta_+)} \tag{4.41}$$

where W is a constant.

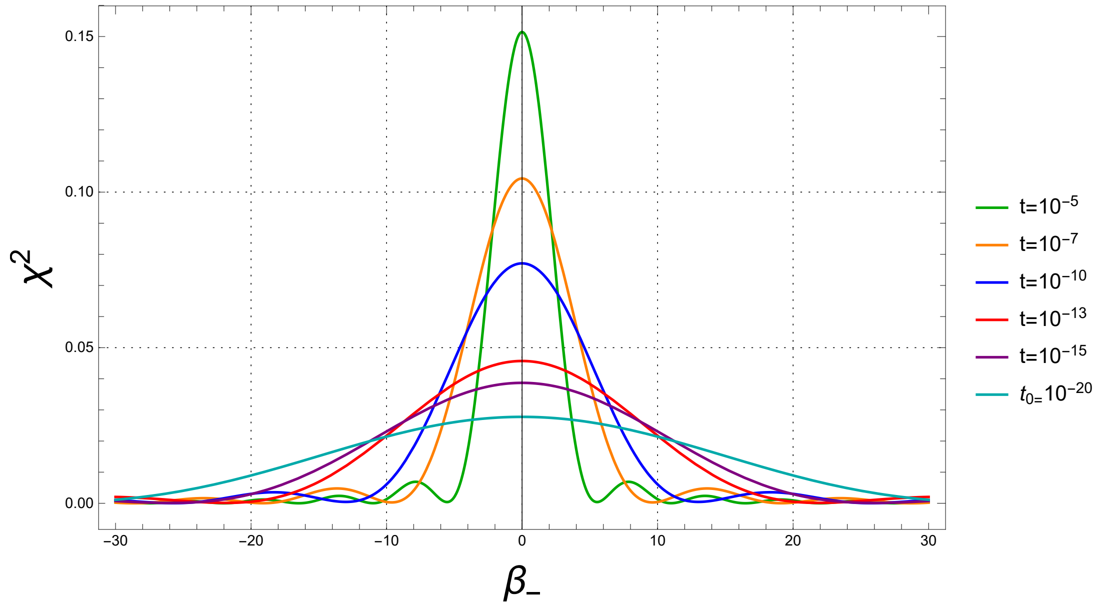


Figure 4.2. Probability density function for different values of the synchronous time variable for Bianchi IX in the vacuum in the case $\beta_+ = 2|p_\alpha|\tau$, for an expanding Universe.

Bianchi IX in the vacuum: collapsing Universe

In this section we consider the dynamical evolution when β_+ decreases for $t \to \infty$, since we are interested in changes in the $|\chi|^2$ in the direction of a collapsing Universe. The equations of motion and the Hamilton-Jacobi equation do not change compared to those of the previous case (4.31) and (4.33).

However, the initial assumption in this case is that $\dot{\beta}_+ < 0$, which translates in $p_+ < 0$. Therefore the semi-classical anisotropic variable becomes:

$$\beta_+(\tau) = \beta_0 - 2|p_\alpha|\tau \tag{4.42}$$

and the frequency $\omega^2(\tau)$ reads as

$$\omega^2(\tau) = 16e^{4(\alpha(\tau)+\beta_+(\tau))} = 16e^{4\beta_0} \tag{4.43}$$

which is a constant.

The solution of (4.21) can be computed as in [37] and it results:

$$\rho(\tau) = \frac{1}{\sqrt{\omega(\tau)}} = \frac{e^{-\beta_0}}{2}. \tag{4.44}$$

The eigenfunctions χ_n, which depend on time through $\rho(\tau)$, are constant as well; hence the probability density distribution $|\chi|^2$ is defined simply by choosing its shape at the initial time. Therefore, as the point-Universe moves towards the time singularity, it moves deeply inside the corner ($\dot{\beta}_+ < 0$), while the probability density $|\chi|^2$ remains constant.
In this case, given that $p_\alpha = p_+$

$$A(\alpha, \beta_+) = e^{\frac{W}{p_\alpha}(\alpha - \beta_+)} \tag{4.45}$$

where W, as before, is a constant.

4.3.3 Bianchi IX model in presence of cosmological constant and scalar field

Finally we study the Bianchi IX model in the presence of a cosmological constant Λ and a scalar field ϕ, in order to mimic the inflationary scenario. In this case the Hamiltonian takes the form

$$\mathcal{H} = e^{-3\alpha}K(-p_\alpha^2 + p_+^2 + p_-^2 + p_\phi^2 + \mathcal{V} + \Lambda e^{6\alpha}). \tag{4.46}$$

$\mathcal{H}_q$ does not change respect to the previous case, while $\mathcal{H}_0 = e^{-3\alpha}K(-p_\alpha^2 + p_+^2 + p_\phi^2 + \Lambda e^{6\alpha})$.
In this case equations (2.92) and continuity equation give the following probability distribution for the semi-classical component of the wavefunction of the Universe:

$$A\left(\alpha, \beta_+, \phi\right) = A_1(\alpha)A_2(\beta_+)A_3(\phi)$$

where

$$A_1(\alpha) = \frac{Exp\left[\frac{C_1 \tanh^{-1}\frac{\sqrt{p_+^2+p_\phi^2+\Lambda e^{6\alpha}}}{\sqrt{p_+^2+p_\phi^2}}}{6\sqrt{p_+^2+p_\phi^2}}\right]}{(p_+^2 + p_\phi^2 + \Lambda e^{6\alpha})^{1/4}}$$

$$A_2(\beta_+) = Exp\left[\frac{C_2}{2p_+}\beta_+\right]$$

$$A_3(\phi) = Exp\left[-\frac{C_1 + C_2}{2p_\phi}\phi\right] \tag{4.47}$$

with C_1 and C_2 constants. Following the same steps of the previous subsection (4.3.2) we can write the full expression for $\tau(t)$, $\alpha(\tau)$ and $\beta_+(\tau)$

$$\begin{aligned}
\tau(t) &= \frac{1}{6\sqrt{p_+^2 + p_\phi^2}} \log\left\{\tanh\left[\frac{1}{2}\left(6Kt\sqrt{\Lambda} + J\right)\right]\right\} \\
\alpha(\tau) &= \frac{1}{3}\log\left\{\frac{\sqrt{(p_+^2 + p_\phi^2)}}{\sqrt{\Lambda}} \sinh\left[2\tanh^{-1}\left(e^{6\tau\sqrt{p_+^2+p_\phi^2}}\right)\right]\right\} \\
\beta_+(\tau) &= \beta_0 + 2p_+\tau
\end{aligned} \tag{4.48}$$

and their asymptotic behavior

$$\begin{aligned}
-\infty &< \tau < 0 \\
-\infty &< \alpha < \infty \\
-\infty &< \beta_+ < \beta_0
\end{aligned} \tag{4.49}$$

Given the complexity of the analytic expression of the time and the Misner variables, it was not possible to solve (4.21) analytically, therefore we computed $|\chi|^2$ numerically for different values of t.
The plots obtained are shown in Fig (4.3).

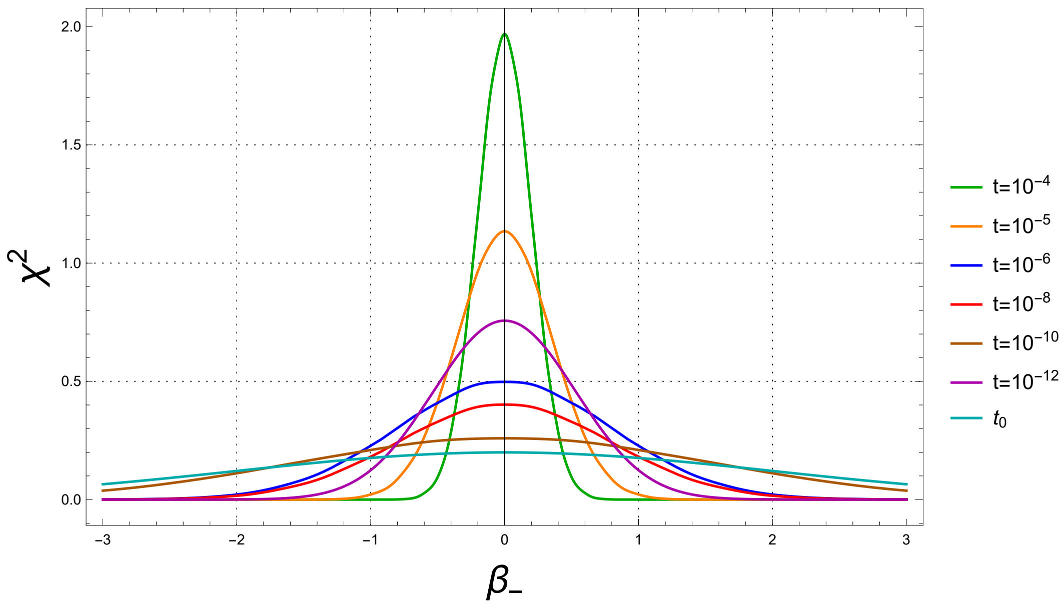


Figure 4.3. Probability density of the quantum subsystem for different values of the time variable in the case of an expanding volume.

It is worth mentioning that, we realized different plots changing the numerical values of Λ and the standard deviation σ of $|\chi_0|^2$. The results did not change respect to those proposed in Fig.(4.3).

4.4 Discussion of the results

Here we are going to discuss the results obtained above. It is worth reminding that in both cases the initial conditions were such that $\beta_+ \gg 1$ and $|\beta_-| \ll 1$.

Here we found that once we give the initial condition on the quantum anisotropy β_-, namely $\chi_n(\tau_0)$, if we evaluate the dynamics of a Gaussian packet initially peaked in $\beta_- = 0$, we obtain that as β_+ grows in time (meaning that the Universe moves deeper in the corner) the packet tends to peak even more around the value $\beta_- = 0$. This can be observed in Fig.(4.2).
We can conclude that the corner of the potential is an attractor for the point-particle Universe; once the Universe enters, it cannot escape any more. This situation resembles the case of the Taub Model (a particular case of the Bianchi IX model where β_- is set to zero), which is a singularity-free model. Therefore the result obtained can be seen as a first step in order to remove the Mixmaster's singularity.

From the analysis of the wave packet behavior we see that, as far as, the point-Universe enters deeply in the corner, in correspondence to an expanding Universe, the small quantum anisotropy is damped to zero, as described by the temporal profile of its standard deviation, see Fig.(4.2). Firstly we are going to analyze the subsection (4.3.2). Here we found that, when we evaluate the dynamics of a Gaussian packet initially peaked in $\beta_- = 0$, namely $\chi_n(\tau_0)$, as β_+ grows in time (meaning that the Universe moves deeper in the corner), the packet tends to peak even more around the value $\beta_- = 0$.

This can be observed in Fig.(4.2). As a consequence the corner becomes an attractor for the global system dynamics in the proposed representation and the Universe approaches on a very good level a Taub cosmological model.

On the contrary, when the point-Universe enters the corner in a backward picture in time, so that the volume is collapsing, the standard deviation of the small quantum anisotropy remains constant, as a consequence of the constant character of the harmonic oscillator frequency. In this case the backward evolution of the Universe would correspond to a Taub Universe, which is no longer a singular cosmology in the past, endowed with a small fluctuating anisotropy degree of freedom, in addition to the macroscopical classical one.

This picture becomes intriguing if the following scenario is addressed. When we follow, like in [11], the backward dynamics of a classical Bianchi IX model, we know that it, soon or later, will deeply enter the corner. If the variable β_- becomes so "small" that it is required a quantum treatment for its evolution, we can apply the above backward picture and the singularity in the past would be removed, due to the emergence of a Taub model.
Clearly a phenomenological implementation for this suggestive scenario, in the past history of our Universe, would require a characterization of the available initial conditions on the cosmological problem and a more detailed understanding of the time reversibility of the proposed dynamical framework.
Finally we analyze the results of section (4.3.3) summarized in Fig (4.3).

In this case we can conclude that there is not a precise trend of the probability density evolution in time, but as the Universe evolves in time, the variable β_+ leans to a constant value and the variable β_- tends to peak around the value $\beta_- = 0$; thus the presence of the cosmological constant tends to isotropize the Universe.

Conclusions

In the first proposed work, we developed a technical algorithm to implement the WKB approach to the quantum Minisuperspace dynamics [54] within the Polymer representation of quantum mechanics [19]. One of the difficulties of the analysis above consisted in the necessity to deal with the momenta representation of the quantum dynamics, the only viable for the Polymer quantization procedure, as approached in the continuum limit. The point is that the potential term of the Minisuperspace Hamiltonian is, in general, not quadratic in the Minisuperspace variable, like the kinetic part is in the momenta.

We proposed a procedure to construct the semi-classical WKB limit in the momentum representation, which is, in principle, applicable to any Minisuperspace system. Such an algorithm has the aim to implement the concept of a cut-off on the quantum dynamics of the Universe, by separating the dynamics into a quasi-classical evolution of a set of configurational variables, e.g. the Universe volume, and those ones rapidly evolving in a fully quantum picture of the dynamics. According to the original idea proposed in [54], we arrived to define a Schrödinger-like equation for the quantum subsystem, allowing a consistent probabilistic interpretation of the wavefunction.

Then, we applied the general procedure constructed above, to the particular case of a Taub cosmology, as described in the framework of Misner-Chitrè -like variables. We considered as quasi-classical variables the most closely resembling the Universe volume and a suitable function of the free massless scalar field included in the dynamics. As purely quantum variable, we adopted that one most closely resembling the Universe anisotropy.

As a result, we got a consistent cosmological picture, describing a cyclical Universe in which a quantum anisotropy is regularized, i.e. its amplitude is always finite. The obtained cosmological paradigm is of significant interest in view of constructing a realistic global (quantum and classical) dynamics of the Universe, being characterized by a regular minimum volume turning point (the Big-Bounce), where the possibility for an interpretation of the anisotropy wavefunction can be coherently pursued. Furthermore, such a resulting model has a maximum volume turning point, living in the pure classical region of the dynamics for all configurational coordinates and allowing for the emergence of cyclical closed Universe dynamics, slightly generalizing the positive curved Robertson-Walker geometry, but removing the singular point in which the Big-Bang takes place for the Standard Cosmological Model [47, 31, 56].

In the second work, we analyzed the Bianchi IX cosmology in vacuum and when a massless scalar field ϕ and a cosmological constant term Λ are present. We limited our attention to the situation in which the point-Universe is trapped in a corner of the scalar curvature potential. The adopted dynamical scheme corresponded to deal with a WKB decoupling of the quasi-classical degrees of freedom, the Misner variables α and β_+ and ϕ when present, from a microscopic fully quantum degree of freedom, the small anisotropy variable β_-.

In both cases, we had to solve a time dependent Schrödinger equation with a quadratic potential, which resembled the equation of a harmonic oscillator with time-dependent frequency. We demonstrated that, both with and without matter, the solution of this equation suggests that the small quantum anisotropy β_- is strongly suppressed via the dynamics of the quasi-classical variables, .

In the vacuum case we observed that, if we considered the situation when the point-Universe entered the corner with an expanding Universe, we found a suppression of the the quantum variable β_-, as its standard deviation decayed in time. We concluded that the corner of the potential was an attractor for the point-particle Universe; once the Universe enters, it cannot escape any more.

Following this analysis, we also studied the limit in which the system entered in the corner when it approached the cosmological singularity. Here the constant character of the variance associated to the anisotropic variable had a very deep meaning on the whole structure of the Bianchi IX dynamics.

When $\beta_- \simeq 0$, the resulting cosmology is indistinguishable from a Taub Universe, which is not a singular model in the limit $\alpha \to -\infty$. Since the emergence of a long regime of the classical Bianchi IX dynamics within the a corner has been convincing established [47], if the proposed picture is applicable, i.e. the smallness of the β_- values justifies its quantum treatment, then the singular behavior of the Bianchi IX Universe could be removed.

This result, in view of the prototype character of the Bianchi IX cosmology versus the generic cosmological solution [9, 25], could have a deep implication on the notion of the cosmological singularity as a general property of the Einstein equations, under cosmological hypotheses.

Finally in the last section (4.3.3), the study of the Bianchi IX dynamics, performed in the presence of ϕ and Λ, is developed in expanding picture, i.e. for $\alpha \to \infty$. The aim of this analysis was to mimic the behavior of the Bianchi IX Universe if the de-Sitter phase, which is associated to the inflationary paradigm for the primordial Universe, takes place when a corner evolution is performed by the point-Universe.

In this case, we have shown that, in the limit of applicability of the WKB proposed scheme, the Universe naturally isotropizes since the classical anisotropy degree of freedom β_+ is suppressed via the natural exponential decay emerging from the Hamilton dynamics, while the fully quantum variable, i.e. β_-, is characterized by a decaying standard deviation. In other words, if we start with a Gaussian distribution for β_-, its natural evolution in the future is towards a Dirac delta-function around the zero value. Thus, this study offers a new paradigm for the Bianchi IX cosmology isotropization, based on the idea that the de-Sitter phase is associated with a corner regime of the model.

To conclude, this study generalizes and completes the results discussed in [6], where the Bianchi IX isotropization is faced in the same WKB scenario, but starting with two very small quantum anisotropy variables, i.e. assuming that the de-Sitter phase starts when the point-Universe is in the center of the potential, already near to an isotropic configuration.

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