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Dynamical Systems in Quantum Cosmology

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LIST OF PUBLICATIONS

THE CONTENT OF THIS THESIS IS BASED ON THE FOLLOWING RESEARCH PAPERS

- R. Moriconi and G. Montani, *Behavior of the Universe anisotropy in a Big-Bounce cosmology*, Phys. Rev. D - Forthcoming Paper Under Journal Revision(2017)

- R. Moriconi, G. Montani and S. Capozziello, *Big-bounce cosmology from quantum gravity: The case of a cyclical Bianchi I universe*, Phys. Rev. D **94**, 023519 , arXiv:1607.04481 [gr-qc] (2016)

- R. Moriconi, G. Montani and S. Capozziello, *Chaos removal in* $R + qR^2$ *gravity: The Mixmaster model*, Phys. Rev. D **90**, 101503(R), arXiv:1411.0441 [gr-qc] (2014)

- O. M. Lecian, G. Montani and R.Moriconi *Semiclassical and quantum behavior of the Mixmaster model in the polymer approach*, Phys. Rev. D **88**, 103511, arXiv:1311.6004 [gr-qc] (2013)

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List of Abbreviations

ADM	**A**rnowitt-**D**eser-**M**isner
BKL	**B**elinski-**K**halatnikov-**L**ifshitz
CCR	**C**anonical **C**ommutation **R**ules
CMBR	**C**osmic **M**icrowave **B**ackground **R**adiation
FRW	**F**riedmann-**R**oberston-**W**alker
LQC	**L**oop **Q**uantum **C**osmology
LQG	**L**oop **Q**uantum **G**ravity
QFT	**Q**uantum **F**ield **T**heory
RW	**R**oberston-**W**alker
SCM	**S**tandard **C**osmological **M**odel
WDW	**W**heeler-**D**e**W**itt
WKB	**W**entzel-**K**ramers-**B**rillouin
WCR	**W**eyl **C**ommutation **R**ules

Preface

Understanding the initial cosmological singularity is one of the major objectives that a complete theory of Quantum Gravity aims to solve. The works realized by Hawking and Penrose [54] about the theorem on the existence of the singularity and by Belinsky-Khalatnikov-Lifshitz [14],[15],[13],[12],[68] on the chaotic behavior of the early Universe are two of the main contributions that have shed light on the subject. Nevertheless, our knowledge about the dynamics of the Universe near the initial singularity (and more generally about the singularities and open issues in general relativity) remains, at today, very limited.

However, the problems related to General Relativity does not concern only the understanding of the initial singularity. In fact, although it is diametrically opposed energy regimes, the improvements over the last few decades about the astrophysical observations have shown that there are two aspects that general relativity cannot handle: the presence of a dark sector in the energy budget of the observable universe (dark matter and dark energy) and the dominance of the dark energy over matter (ordinary and dark) at present times. As a consequence the expansion of the universe seems to be an accelerated one. A promising way to solve such defects is represented by the extended theories of gravity and they are one of the main topic of this Ph.D. thesis. Corrections to the Einstein-Hilbert action involving higher powers of the Ricci scalar and/or the presence of the Gauss-Bonnet invariant, that bring to the so-called $f(R)$ and $F(R, \mathcal{G})$ theories, are actually two of the most elegant modification that can easily match cosmological and astrophysical observation and that reach the General Relativity as a low curvature limit.

Keeping this issues all in mind, a very common approach believes that the presence itself of such pathologies is the symptom of the fact that we are trying to apply general relativity outside of its validity region, and that it is necessary to introduce corrective measures, not only on the classical point of view. In this sense, the presence of the initial singularity is of great attention for any kind of attempt to quantize the gravitational field and one can expect that a deeper understanding of nature it is necessary to solve it. The role played by the Quantum Cosmology is exactly to study the very early stage of the Universe providing a correct description of the initial singularity (typically through a removal or a regularization).

Another key aspect to consider is to characterize, as fully as possible, how the Universe approaches the singularity, or in other words which class of cosmological models best describes its evolution.

Without any doubt, from this point of view, the Standard Cosmological Model is a milestone in modern physics. The homogeneity and isotropy hypotheses on the Universe large scale structure are sustained from observational evidences and theoretical predictions, as confirmed by the almost absolute homogeneity and isotropy of the Cosmic Microwave Background Radiation and by the agreement between predictions of the primordial nucleosynthesis and the actual abundance of light elements in the Universe. This is why we can argue that the Standard Cosmological Model is able to properly describe all the history of the Universe from now backwards until 10^{-32} seconds after the Big Bang, typically the temporal scale associated to the end of the inflationary stage. Anyway, a series of internal problems that afflict the Standard Cosmological Model (presence of paradoxes as example) suggests the possibility to consider more complex and more general cosmological models to characterize the early stage of the Universe. In this sense, the inflation play the role of the perfect bridge between a generic pre-inflation cosmological scenario (where in principle any kind of cosmological model is allowable) and the actual observable homogeneous and isotropic Universe.

For this and other reasons, instead of taking into account the highly symmetric homogeneous and isotropic spacetimes, described by the Friedmann-Roberston-Walker models, one should expects that the early Universe approaches the singularity with an higher level of generality, in principle without any symmetry imposition as expected by the Generic Cosmological Solution. The perfect intermediate step between the homogeneous and isotropic spacetimes and the Generic Cosmological Solution is represented by the Homogeneous Models (collected in the so-called Bianchi Classification), which are deeply studied in this thesis. The importance of such a cosmological class of models is historically due to the studies of Belinski-Khalatnikov-Lifshitz, which showed the possibility to construct a generic cosmological solution next to the singularity that has all its degrees of freedom available and whose evolution resembling a collection of dynamically independent homogeneous space of the type VIII or IX of the Bianchi Classification, one for each independent horizon.

But the choice of the proper class of cosmological models to describe the early Universe is not the only aspect to consider when the problem of the initial singularity is faced. A crucial point is the quantization procedure. Proceeding with a canonical quantization of the gravitational field in the Hamiltonian formulation, one arrives to formulate the *Wheeler-DeWitt equation*, which determines the evolution of the wave function of the Universe that stands for the description of quantum state of the system. The work space of the Wheeler-DeWitt equation is the infinite-dimensional space of all the possible three-geometries, also known as the Wheeler superspace. Such an equation is in some sense comparable with a Klein-Gordon equation with a variable mass and conceptually represents for the Quantum Gravity what the Schrodinger equation represents for the Quantum Mechanics. As it is well known from its origins, it carries a lot of pathologies, above all two. First of all it brings to the so called *frozen formalism*, which suggests that there is no kind of evolution in Quantum Gravity and makes losing completely the concept of time, and furthermore, as shown in [43], it does not give a clear indication about the behaviour of the initial singularity at the quantum level.

Although the situation is simplified in Quantum Cosmology, where the imposition of the symmetries (as for example homogeneity and isotropy) freezes all but a finite number of degrees of freedom and reduces the space work to a finite dimensional subspace called *minisuperspace*, all the issues formally remain.

Regarding the problem of time, besides being able to consider some internal variables to describe the evolution of the universe (such as, for example, the volume of the universe or a scalar field), several alternative approaches can be adopted in order to overtake this issue and one of the most promising is the Evolutionary Quantum Approach. It relies on the dualism existing between a dust fluid and a physical clock. For this reason, following the prescription suggested by Kuchar and Torre [64],[21], the implementation of the evolutionary theory consists of assuming that the wave function of the Universe evolves with respect to an external parameter t (associated to the dust), which plays the role of a physical clock.

Moreover, a possible way out from the problem of the initial singularity is represented by the Polymer approach[39],[38]. The latter considers the discrete nature of one or more of the variables of the phase space of the particular cosmological model that is taken into account for the quantization. The use of such a modified quantization scheme is justified by the request that a cut-off in the spatial scale, as expected at the Planckian level, would induce a corresponding discrete morphology in the configuration space. The algebra generated from such a statement is in strong analogy with the typical quantum prescription of the Loop Quantum Gravity, whose applications in cosmology (Loop Quantum Cosmology) have as a common denominator the regularization of the initial singularity. The application of approaches like this has started a lot of studies in cosmology in which the Big-Bang singularity is removed in favor of a turning point in the evolution of the Universe, characterized by a non-zero value of the scale factor and a non-diverging value of the energy density. Such a branch of studies is called *Big Bounce Cosmologies*.

The work presented in this Ph.D. thesis has exactly the purpose to provide new quantization procedures for the minisuperspace cosmological models in order to better understand the nature of the initial singularity. The possibility to perform a quantum analysis of the primordial Universe able to provide information about its first instants of life is of absolute interest for the comprehension of the properties of the initial singularity, and, consequently, of the mechanisms at the ground of the birth of our Universe.

The subject of the thesis can be divided in two parts. The first one, composed by the Chapter 1 and Chapter 2, concerns a review of the Literature topics necessary for the comprehension of the original work of the thesis.

In particular, in the Chapter 1 are treated all the "classical " basic knowledge that regards the General Relativity and Cosmology. Indeed, after a brief introduction on the Hamiltonian Formulation of General Relativity and on the Extended Theories of Gravity, the main part of this Chapter is devoted to the detailed analysis of the two main classes of cosmological models: FRW models and Bianchi Models. After the study of the mathematical proprieties of the Bianchi universes, a particular focus is dedicated to the dynamics of one specific model within the classification: the Bianchi IX type, also called Mixmaster model. For such a model are then reported the main set of variables useful for its description, first of all the Misner variables, which provides a clear physical interpretation of the model, and the Misner-Cithrè variables, useful for the independence that the scalar curvature term assumes from the "time"-variable.

In Chapter 2 is given an overview about the "quantum" part of the basic subjects introduced. The Chapter starts with a presentation of the main issues arising from the canonical quantization of the gravitational field and from the formulation of the Wheeler-DeWitt equation. Through the presentation of the concept of the minisuperspace, will be possible to describe the canonical quantization of the flat FRW model, in which the presence of the initial singularity, also from a quantum point of view, will be a clear symptom of the failure of the canonical approach. With this spirit, as a possible way out, in the central part of this Chapter is illustrated the Polymer Quantum Mechanics, a non-equivalent representation of the Schrodinger one, based on the hypothesis than one or more of the configuration variables are discrete. As example, two polymer application on the flat FRW model and on the Bianchi IX model are then provide. The Chapter is closed by the illustration of the Evolutionary Quantum approach, or in other words the existence of an emerging dust fluid with respect to which the evolution is considered, and from the Vilenkin Interpretation of the wave function of the Universe, in which a clear separation between the semiclassical and pure quantum variables is made explicit *a priori* in the shape of the wave function.

The second part of this thesis, which goes from Chapter 3 to Chapter 6, contains completely original contributions.

In Chapter 3 is examined the $f(R) = R + qR^2$ modified theory of gravity, which in the context of the equivalent scalar-tensor picture behaves as a self-interacting scalar field coupled with the ordinary General Relativity. Once it is considered the Mixmaster

Model for this particular $f(R)$ theory, it emerges the existence of a free Kasner regime (formally a Bianchi I model coupled with a scalar field) towards the singularity, *i.e.* a regime in which the chaos is absent. Furthermore, to close the chapter, is presented a possible quantization method for the model.

The Chapter 4 concerned always the extended theories of gravity, in particular the presence of the Gauss-Bonnet invariant in the modified action that describe the gravitational field. The original work illustrated in this Chapter consists in the Noether Symmetry Approach in the framework of Gauss-Bonnet cosmology (namely starting with a modified Einstein-Hilbert Lagrangian $F(R, \mathcal{G})$) when a simple flat FRW model is taken into account. The individuation of the Noether symmetries allow to individuate conserved quantities, which are fundamental for the purpose of simplify the dynamics. The second part of this work is dedicated to the canonical quantization of the system. Following the prescriptions of the Hartle criterion, will be possible to select, from all the possible solutions of the wave function of the Universe, just the ones that exhibits an oscillatory behavior around a central action term. After the selection of such an action will be possible to extract the emerging classical cosmological trajectories from the solutions of the WDW equation.

Then, in Chapter 5 is given the classical and quantum dynamics of a Bianchi I model in the presence of a small negative cosmological constant when a Gaussian Reference Dust Fluid is taken into account. In the framework of the canonical metric approach it is showed that the initial cosmological singularity is removed and it is replaced by a bounce in correspondence to a positive defined value of the dust energy density. A physical interpretation of the Bounce will be provide in term of a correlation between the Cosmological Constant and a characteristic polymer scale related to polymer discretization of the Universe volume.

Finally, Chapter 6 is focused on the analysis of a homogeneous Bianchi I model in presence of a stiff matter contribution, applying the Vilenkin interpretation of the Wave Function of the Universe when a Polymer quantization procedure is performed to the isotropic component of the spatial metric. The goal of this work is to understand if and how the singularity is avoided, how it changes the behaviour of the anisotropies and if it is possible to extend the results of the above mentioned application to the Bianchi IX model.

Chapter 1

Hamiltonian Formulation of General Relativity and Classical Cosmology

This Chapter is devoted to the basic aspects of General Relativity with a particular focus on the Hamiltonian formulation of the dynamics of the gravitational field and the extended theories of gravity. In the context of the Hamiltonian formulation, the classical cosmology will be treat through the study of the Friedmann-Roberston-Walker models and the Bianchi Models. The high generality offered by the homogeneous models will be deeply analyzed and a particular light will be done on Bianchi IX model, also called Mixmaster model. The final part of this Chapter is dedicated to the investigation of the main sets of variables useful to describe the Mixmaster model, first of all the Misner variables.

1.1 Einstein Equations

The main issue of the Einstein theory of gravity is the dynamical character of the space-time metric, described within a fully covariant scheme[63],[79],[76]. The space-time is defined as a four-dimensional manifold $\mathcal{M}$, characterized with a coordinate x^γ, on which a metric tensor $g_{\mu\nu}(x^\gamma)$ is assigned. The definition of distance is express introducing the line element

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu. \tag{1.1}$$

A proper concept of distance allow to define the motion of a free free particle on the manifold $\mathcal{M}$ through the geodesic equation

$$\frac{du^\mu}{ds} + \Gamma^\mu_{\nu\gamma}u^\nu u^\gamma = 0, \tag{1.2}$$

where $u^\mu = \frac{dx^\mu}{ds}$ is the four-velocity of the particle, equivalent to the tangent vector of the trajectory $x^\mu(\lambda)$, and $\Gamma^{mu}_{\nu\gamma}$ are the Christoffel symbols

$$\Gamma^\mu_{\nu\gamma} = \frac{1}{2}g^{\mu\delta}\left(\partial_\gamma g_{\delta\nu} + \partial_\nu g_{\delta\gamma} - \partial_\delta g_{\nu\gamma}\right) \tag{1.3}$$

The field equations that describes their evolution are the *Einstein equations*. This equations can be obtained through a variation of an action that contains a gravitational contribution and a matter contribution. Such an action, that preserves the covariant nature of the space-time, is the Einstein-Hilbert Action[1]:

$$S = -\frac{1}{2k}\int_{\mathcal{M}}\sqrt{-g}(R - 2k\mathcal{L}_m)d^4x \tag{1.4}$$

[1]We use the $(-,+,+,+)$ signature of the metric and the natural unit system $(c = \hbar = 1)$.

where $k = 8\pi G$ is the Einstein constant, g is the determinant of the metric tensor $g_{\mu\nu}$ and R is the Scalar Curvature. The variation of the Action (1.4) with respect to the metric tensor $g_{\mu\nu}$ brings to the Einstein Equations:

$$R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = k T_{\mu\nu}, \tag{1.5}$$

where the matter contribution is represented by the stress-energy tensorT_{ik} and its explicit form is

$$T_{\mu\nu} = \frac{2}{\sqrt{-g}} \left(\frac{\delta(\sqrt{-g}\mathcal{L}_m)}{\delta g^{\mu\nu}} - \frac{\partial}{\partial x^l} \frac{\delta(\sqrt{-g}\mathcal{L}_m)}{\delta(\partial_l g^{\mu\nu})} \right). \tag{1.6}$$

Looking at the equations (1.5) it is evident that the expression on the left side represents the curvature of space-time as determined by the metric and the expression on the right side represents the matter contribution. The Einstein equations show in a clear way the interconnection between the curvature of a given space-time and the presence of a particular form of matter.

1.2 Hamiltonian Formulation of the General Relativity

In order to analyse the canonical quantization of the gravitational field in the next section, it is necessary to introduce the Hamiltonian formulation of General Relativity[79],[76]. Looking at the Einstein-Hilbert Action (1.4), the Lagrangian formulation of general relativity is manifestly covariant under diffeomorphism and the fundamental field is the metric tensor $g_{\mu\nu}$.

In opposition, from the Hamiltonian formulation point of view, there is not a manifestly diffeomorphism covariance. Indeed, this formulation is essentially based on a $3+1$ split of the metric, and the dynamical degrees of freedom are the spatial components of the metric. Formally speaking, this is equivalent to require that the four-dimensional manifold $\mathcal{M}$ can be decomposed in $\mathcal{M} \to \mathbb{R} \times \Sigma$, where Σ is a three-dimensional hypersurface. The usual $3+1$ split is accomplished through the Arnowitt, Deser, Misner (ADM)[2] decomposition of the space-time metric in terms of a lapse function N, a shift vector N_i and an induced spatial metric h_{ij}. To this aim, one begins by constructing the hypersurfaces Σ_t, parameterized by some global time-like variable t. This way, $\mathcal{M}$ can be foliated by a one-parameter family of embedding three-dimensional hypersurfaces. As it is represented in Fig.1.1, such a foliation requires the introduction of a time-like vector n^μ normal to the hypersurfaces Σ_t and moreover an interpretation of the lapse function N and the shift vector N_i can be done from a geometric point of view. The lapse function specify the proper time separation between two successive hypersurfaces Σ_t, Σ_{t+dt} measured in the direction n^μ normal to the first hypersurface. Instead, the shift vector N measures the displacement between the intersection of n^μ on Σ_{t+dt} and the position of x^i on Σ_{t+dt}. The Fig.1.1 also illustrate the notion of distance in terms of N, N_i, h_{ij} as:

$$ds^2 = N^2 dt^2 - h_{ij}(N_i dt + dx_i)(N_j dt + dx_j) \tag{1.7}$$

In addition, a comparison between the (1.7) and the generic proper length in Eq.(1.1) allow to establish the components of the space-time metric respect to N, N_i, h_{ij}. As we will show below, the equivalence between the arbitrary choice of the foliation and the invariance under diffeomorphism guaranteed the general covariance. After the definition of the geometric structure of the space-time let us now consider the gravitational Lagrangian density

$$\mathcal{L}_g = -\frac{1}{2k}\sqrt{-g}R. \tag{1.8}$$

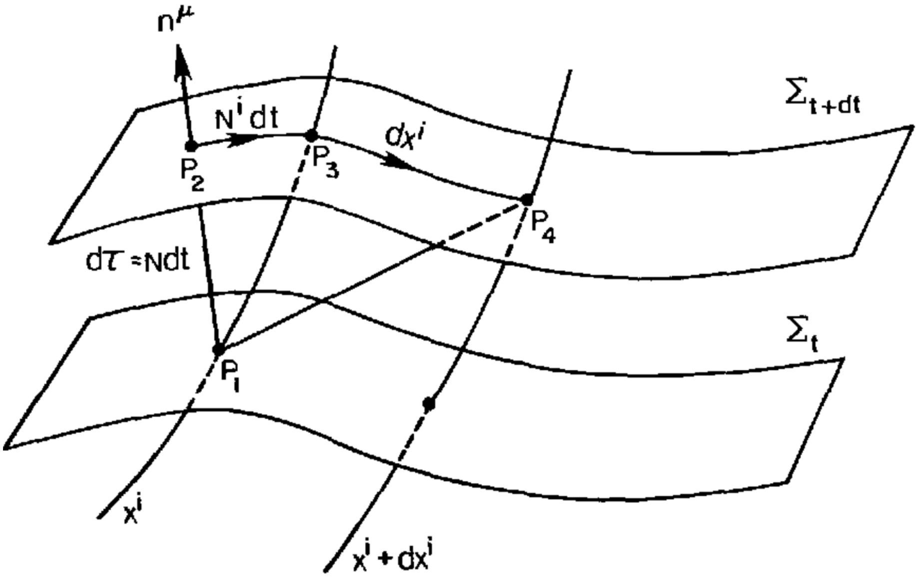

FIGURE 1.1: Geometrical interpretation of two successive hypersurfaces in the space time foliation

In order to define the 4-dimensional invariant scalar curvature R as a function of N, N_i, h_{ij} it is useful to define the *extrinsic curvature* of a generic hypersurfaces Σ_t:

$$K_{ij} = -\frac{1}{2N}\left(\frac{\partial h_{ij}}{\partial t} - \nabla_i N_j - \nabla_j N_i\right), \tag{1.9}$$

which provides the curvature of Σ_t from a 4-dimensional prospective. The extrinsic curvature appears in the so-called *Gauss-Codazzi relation*, which relates the four-dimensional Ricci scalar R to three-dimensional one $\overline{R}$[2]; it explicitly reads as

$$\sqrt{-g}\,{}^4R = N\sqrt{h}(K^2 - \overline{R} - K_{ij}K^{ij}) + 2\frac{d}{dt}(\sqrt{h}K_i^i) + \partial_j(K_l^l N^j - h^{ij}\partial_i N) \tag{1.10}$$

where $\sqrt{-g} = N\sqrt{h}$ and $h = \det(h_{ij})$.

The last two terms in the Eq.(1.10) do not contribute to the dynamics. Indeed, applying the principle of stationary action with a Lagrangian density (1.10), they represent a total differentiation on the edge and then they can be dropped.

Therefore, the gravitational part of the Einstein-Hilbert action (1.4) can be recast in a $3+1$ formalism as

$$S_g(h_{ij}, N, N^i) = \int_{\mathcal{M}} \mathcal{L}_{ADM}\, dt d^3x = -\frac{1}{2k}\int_{\mathcal{M}} N\sqrt{h}(K^2 - K^{ij}K_{ij} - \overline{R})\, dt d^3x \tag{1.11}$$

Using the relation (1.9) and the fact that $\overline{R}$ do not contain time-derivative, we can write the conjugate momenta to the variables (h_{ij}, N, N^i) directly from the Lagrangian density $\mathcal{L}_{ADM}$ in this way:

$$\Pi^{ij} = \frac{\delta \mathcal{L}_{ADM}}{\delta \dot{h}_{ij}} = \frac{\sqrt{h}}{2k}(h^{ij}K_i^i - K^{ij}) \tag{1.12}$$

$$\Pi = \frac{\delta \mathcal{L}_{ADM}}{\delta \dot{N}} = 0 \tag{1.13}$$

[2]The quantity $\overline{R}$ is the analogous of the Ricci scalar but it refers to the three-dimensional hypersurfaces Σ_t. In other words it is built withe the metric h_{ij} instead of the space-time metric$g_{\mu\nu}$

$$\Pi_i = \frac{\delta \mathcal{L}_{ADM}}{\delta \dot{N}^i} = 0 \tag{1.14}$$

The Eqs. (1.13),(1.14), due to the independence of the Lagrangian density from the derivative of (N, N^i), are called *primary constraints*. The term "primary" indicates that the constraint has been obtained without the use of the equation of motion.

To proceed, let us perform a typical technique of the constrained Hamiltonian systems. Let us introduce in the Hamiltonian the Lagrangian multipliers $\lambda(x,t)$ e $\lambda^i(x,t)$ associated to the primary constraints (1.13),(1.14). After this, making use of the *Legendre transformation*, the action (1.11) can be expressed as

$$S_g = \int_{\mathbb{R}} dt \int_{\Sigma} d^3x \left[\dot{h}_{ij}\Pi^{ij} + \dot{N}\Pi + \dot{N}^i\Pi_i - (\lambda\Pi + \lambda^i\Pi_i + N^i\mathcal{H}_i + N\mathcal{H}) \right], \tag{1.15}$$

where

$$\mathcal{H} = \mathcal{G}_{ijkl}\Pi^{ij}\Pi^{kl} - \frac{\sqrt{h}}{2k}\overline{R}, \tag{1.16}$$

$$\mathcal{H}_i = -2h_{ik}\nabla_j\Pi^{kj}, \tag{1.17}$$

$$\mathcal{G}_{ijkl} = \frac{k}{\sqrt{h}}(h_{ik}h_{jl} + h_{jk}h_{il} - h_{ij}h_{kl}), \tag{1.18}$$

are respectively the *superHamiltonian*, the *supermomentum* and the *supermetric*. A proof of the initial freedom in the choose of the $3+1$ slicing of the space-time is given by the Hamiltonian equation for the lapse function and the shift vector, or equivalently considering the variation of the action (1.15) with respect to the conjugate momenta Π and Pi_i. In any case, we obtain

$$\dot{N} = \lambda \qquad \dot{N}^i = \lambda^i \tag{1.19}$$

The previous relations ensure us that the trajectories of N and N^i are completely arbitrary, due to the fact that λ and λ^i are Lagrangian multipliers. The result to have an arbitrary choice for N and N^i is a direct consequence of the principle of general covariance.

If now we take into account the Hamiltonian equations associated to the conjugate momenta Π and Π_i and considering the Eqs.(1.13),(1.14), we obtain the so-called *secondary constraints*:

$$\dot{\Pi} = \frac{\partial(N\mathcal{H})}{\partial N} = \mathcal{H} = 0 \tag{1.20}$$

$$\dot{\Pi}_i = \frac{\partial(N^i\mathcal{H}_i)}{\partial N^i} = \mathcal{H}_i = 0 \tag{1.21}$$

Those relations tell us that the Hamiltonian density, and therefore the Hamiltonian too, is identically zero. Let us attempt to give a physical interpretation of the secondary constraints just obtained. The supermomentum constraint (1.21) represents the freedom in the choice of the reference system, in other words the choice of the metric, to describe the geometry of the spatial metric h_{ij}. In fact, given an infinitesimal spatial variation as $x'^{\mu} = x^{\mu} + \xi^{\mu}$, the transformation for the metric h_{ij} is

$$h'_{ij} = h_{ij} + \delta_{tot}h_{ij} = h_{ij} + 2\nabla_i\xi_j \tag{1.22}$$

while the variation of the action due to the same displacement is

$$\delta S = \int \Pi^{ij}\delta(\partial_t h_{ij}) = \int \Pi^{ij}\partial_t\delta h_{ij} = -2\int \nabla_i\Pi^{ij}\xi_j d^3x = \int \mathcal{H}^i\xi_i d^3x = 0 \tag{1.23}$$

The supermomentum constraint brings to an action invariant under spatial diffeomorphism. The conclusion is that, inside the configuration space within the theory lives, the dynamics of the systems does not depend from the particular representation provides by the metric choice but only from the spatial three-dimensional geometry that characterize the manifold, here indicated as $\{h_{ij}\}$. This brings to conclude that all the information about the dynamics of the gravitational field are collected in the scalar superHamiltonian constraint

$$\mathcal{H} = \mathcal{G}_{ijkl}\Pi^{ij}\Pi^{kl} - \frac{\sqrt{h}}{2k}\overline{R} = 0. \tag{1.24}$$

This analysis shows how the real dynamical variable is the metric h_{ij} and its evolution is ruled by the constraint (1.24).

1.2.1 The ADM Reduction of the Dynamics

The ADM reduction of the dynamics is a procedure that allow to individuate a temporal parameter within the geometrical variables introduced in the Hamiltonian formulation.

In order to emphasize the importance of such a procedure, it is useful to achieve a count of the total degree of freedom of the gravitational field. Considering the Hamiltonian formalism introduced in the previous section, there are initially 20 phase-space functions identified by the sets $\big((N,\Pi),(N^i,\Pi_i),(h_{ij},\Pi^{ij})\big)$. The freedom in the choice of (N, N_i) and the presence of the primary and secondary constraints reduce the total number of functions in the configuration space from 20 to 8. The way to arrive at the final result of 4 phase space functions (corresponding to the two physical degrees of freedom of the gravitational field, i.e. to the two independent polarizations of a gravitational wave in the weak field limit) is the imposition of a particular gauge for the lapse function and the shift vector. To be more schematic let us consider for the 12 variables (h_{ij}, Π^{ij}) a canonical transformation as

$$(h_{ij}, \Pi^{ij}) \to (Q^a, P_a; \phi^r, \pi^r) \tag{1.25}$$

where $a = 1, 2, 3, 4$ e $r = 1, 2$. The eight functions Q^a, P_a are a possible choice of internal variables (and the respectively conjugate momenta) and differ from the two modes ϕ^r(and the conjugate momenta π^r) which represent the physical degrees of freedom of the gravitational field.

Therefore, we can express the superHamiltonian and the supermomentum constraints with respect to the change of variables (1.25), and write the new version of the Lagrangian density

$$\begin{aligned}\mathcal{L}'(N, N^i, Q^a, P_a, \phi^r, \pi^r) &= \\ &= P^a\partial_t Q_a + \pi^r\partial_t\phi^r - N\mathcal{H}(Q^a, P_a, \phi^r, \pi^r) - N^i\mathcal{H}_i(Q^a, P_a, \phi^r, \pi^r).\end{aligned} \tag{1.26}$$

We can now remove 4 non-dynamical variables by using the secondary constraints $\mathcal{H} = 0$ and $\mathcal{H}_i = 0$, where the superHamiltonian after the change of variables explicitly reads as

$$P_a + h_a^{red}(Q, \phi, \pi) = 0 \tag{1.27}$$

Solving the latter constraint respect to P_a and inserting it inside the Lagrangian density (1.26), we remove the other 4 non-dynamical variables and we obtain the so-called *reduced Lagrangian density*

$$\mathcal{L}_{red} = \pi^r\partial_t\phi^r - h_a^{red}(Q, \phi, \pi)\partial_t Q^a = \pi^r\partial_t\phi^r - \mathcal{H}_{red} \tag{1.28}$$

where $\mathcal{H}_{red}$ is the *reduced Hamiltonian density* and the expected number of degrees of freedom has been obtained. It is clear how all the information about the choice of the lapse function and the shift vector have been moved to the term $\partial_t Q^a$. To conclude this section let us underline that in this scheme the equations of motion of the new fields (ϕ^r, π^r) will be obtained from reduced Hamiltonian density as

$$\partial_t \phi^r = \{\phi^r, \mathcal{H}_{red}\} \qquad \partial_t \pi^r = \{\pi^r, \mathcal{H}_{red}\}. \tag{1.29}$$

1.3 The Extended Theories of Gravity

Immediately after the introduction of the General Relativity and the Einstein equations, many attempts to understand if it was the only theory to describe gravitation has been done. Being the General Relativity at the very beginning, the early attempts started essentially by scientific curiosity and they concern the possibility to consider the inclusion of higher order invariants in the Einstein-Hilbert action.

During the XX century, a lot of new theoretical considerations brought more and more interest in higher-order theories of gravity, or in other words to consider modifications of the Einstein–Hilbert action in order to include higher-order curvature invariants with respect to the Ricci scalar[30],[85].

Furthermore, in the last years a new astrophysics and cosmology interest emerges from those kind of theory. The increasingly accurate analysis of the Cosmic Microwave Background Radiation (CMBR) have shown that the principle contributions to the radiation is due, within the total energy contained in the Universe, to the dark matter and in particular to the dark energy. The dominance of the dark energy (it seems to resemble a cosmological constant contribution) over the dark and ordinary matter brings to have an accelerated Universe, in contrast with respect to the ordinary matter domination, where a decelerated behavior takes place.

Starting from this theoretical and observational considerations the question if the General Relativity if sufficient to describe naturally arises. In this view, the extended theories of gravity appear as a possible solution for the explanation of the dark components of the energy density of the Universe and for the interpretation of the gravitational interaction at the relevant scales.

1.3.1 $f(R)$ Theories

We devote this subsection to introduce the simpler modification to deviate from General Relativity, the $f(R)$ theories.

The $f(R)$ theories of gravity are a direct generalization of the Einstein-Hilbert Lagrangian consisting in a replacement of the Ricci Scalar R by a general function $f(R)$[26],[84]:

$$S = -\frac{1}{2k}\int d^4x\sqrt{-g}f(R) \tag{1.30}$$

where g is the determinant of the metric. Performing a variation of the action (1.30) with respect to the metric tensor $g_{\mu\nu}$ leads to the modified Einstein equations

$$f' R_{\mu\nu} - \frac{1}{2} f g_{\mu\nu} - \nabla_\mu \nabla \nu f' + g_{\mu\nu}\nabla_\gamma \nabla \gamma f' = kT_{\mu\nu}, \tag{1.31}$$

where $f' = \frac{df}{dR}$. Through the introduction of the quantity $F(R) = f(R) - R$, it is possible to rewrite the Einstein equations (1.31) in a more treatable way in the form:

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = k(T_{\mu\nu} + T^f_{\mu\nu}) \tag{1.32}$$

The additional term is $T^f_{\mu\nu}$ equal to

$$T^f_{\mu\nu} = \left(\frac{1}{2}F(R) - \nabla_\gamma \nabla \gamma f'\right) g_{\mu\nu} + \nabla_\mu \nabla \nu f', \tag{1.33}$$

and looking at the Eq.(1.32) is evident how the obtained modified theory is an Einstein-like theory with a curvature term as a source. As it is possible to show when the cosmological framework is considered, the presence of those additional terms affect only the late time history of the Universe with an accelerated behavior, typical of dark energy contribution, leaving unchanged the behavior at early times.

The introduction of the additional degree of freedom, related to the presence of the $f(R)$ term, can be translated into a dynamics of a self-interacting scalar field coupled with the Einstein-Hilbert Action, the so-called *Scalar-Tensor framework*[6],[8],[7]. In this approach, a new auxiliary field χ is introduced to get the following equivalent version of the action (1.30):

$$S = -\frac{1}{2k}\int d^4x\sqrt{-g}[f(\chi) - f'(\chi)(R-\chi)]. \tag{1.34}$$

The variation of the action (1.34) with respect to χ provides $f''(\chi)(R-\chi) = 0$, implying $\chi = R$ if $f''(\chi) \neq 0$. By a redefinition of the auxiliary field χ in the form $\varphi = f'(\chi)$ the action becomes

$$S = -\frac{1}{2k}\int d^4x\sqrt{-g}[\varphi R - \chi(\varphi)\varphi + f(\chi(\varphi))]. \tag{1.35}$$

It is now possible to perform a conformal transformation on the metric $g_{\mu\nu} \to \tilde{g_{\mu\nu}} = \varphi g_{\mu\nu}$ and a scalar field redefinition $\varphi \equiv f'(R) \to \phi = \sqrt{\frac{3}{2k}}\ln f'(R)$ in order to obtain

$$S = -\frac{1}{2k}\int d^4x\sqrt{-\tilde{g}}\tilde{R} + \int d^4x\left[\frac{1}{2}\partial^\alpha\phi\partial_\alpha\phi - U(\phi)\right], \tag{1.36}$$

where the potential term $U(\phi)$ has the form:

$$U(\phi) = \frac{-Rf'(R) + f(R)}{2k(f'(R))^2}. \tag{1.37}$$

For small values of the Ricci scalar, the first order correction to the Einstein-Hilbert Lagrangian, is represented by a quadratic correction, i.e.

$$f(R) = R + qR^2. \tag{1.38}$$

By this choice, the potential term (1.37) takes the form

$$U(\phi) = \frac{1}{8kq}\left(1 - 2\exp^{-\sqrt{\frac{2k}{3}}\phi} + \exp^{-2\sqrt{\frac{2k}{3}}\phi}\right). \tag{1.39}$$

This is the effective potential that emerges in the so called Starobinsky-inflation model[87]. Such a model ensures a "slow-rolling" period and it is an inflationary model passing the latest inflation constraint[1].

1.3.2 $F(R, \mathcal{G})$ Theories

The idea of consider other higher-order curvature corrections in Einstein-Hilbert Lagrangian than simply a function $f(R)$ has led to consider several combinations of curvature invariants as for example $R_{\mu\nu}R^{\mu\nu}$ or $R_{\mu\nu\rho\delta}R^{\mu\nu\rho\delta}$. The aim of this approach is to explain the entire cosmological evolution (*i.e.* the early and late time evolution) without using exotic form of matter. In this sense, the Gauss-Bonnet topological invariant $\mathcal{G}$ plays a central role[48],[28]. First of all, it naturally arises in the renormalization procedure in curved space-time. Then, it is constructed in such a way that within its definition are present the Ricci Tensor $R_{\mu\nu}$ and the Riemann Tensor $R_{\mu\nu\rho\delta}$, and so, considering a theory in which R and $\mathcal{G}$ are present, complete the necessary number of curvature degree of freedom needed to extend the General Relativity. Furthemore, the extension of such an extended theory to the cosmological point of view, and in particular to the inflationary stage, shows the existence of a double inflationary phase respectively drives from R and $\mathcal{G}$[41].

Just to introduce the modified Gauss-Bonnet Gravity, that we will consider in the next Chapters in cosmological point-like Lagrangian picture, let us write the most general action, in the vacuum case, that concerns the fields R and $\mathcal{G}$ in this way

$$S = -\frac{1}{2k}\int d^4x\sqrt{-g}F(R, \mathcal{G}), \tag{1.40}$$

where $F(R, \mathcal{G})$ is a function of the Ricci Scalar and the Gauss-Bonnet invariant which is defined as

$$\mathcal{G} = R^2 - 4R_{\mu\nu}R^{\mu\nu} + R_{\mu\nu\rho\delta}R^{\mu\nu\rho\delta}. \tag{1.41}$$

As done in the previous Section, a variation of the action (1.40) with respect to the metric leads to these modified gravitational equations

$$\begin{aligned} R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = \frac{1}{F_R}\Big[&\nabla_\mu\nabla_\nu F_R - g_{\mu\nu}\Box F_R + 2R\nabla_\mu\nabla_\nu F_G - 2g_{\mu\nu}R\Box F_G - \\ &- 4R^\lambda_\mu\nabla_\lambda\nabla_\nu F_G - 4R^\lambda_\nu\nabla_\lambda\nabla_\mu F_G + 4R_{\mu\nu}\Box F_G + 4g_{\mu\nu}R^{\alpha\beta}\nabla_\alpha\nabla_\beta F_G + \\ &+4R_{\mu\alpha\beta\nu}\nabla^\alpha\nabla^\beta F_G - \frac{1}{2}g_{\mu\nu}(RF_R + \mathcal{G}F_G - F(R, \mathcal{G})\Big], \end{aligned} \tag{1.42}$$

where we define the partial derivatives with respect to R and $\mathcal{G}$ of the modified term as

$$F_R = \frac{\partial F(R, \mathcal{G}}{\partial R} \quad , \quad F_G = \frac{\partial F(R, \mathcal{G}}{\partial G} \tag{1.43}$$

and $\Box$ is the d'Alembert operator in curved space-time.

In conclusion of this brief introduction about the Gauss-Bonnet gravity it is worth noting that the modified equations (1.42) reduce to the standard Einstein equations (1.5) when it is restored the condition $F(R, \mathcal{G}) = R$.

1.4 The FRW Cosmological models

We devote this Section to the description of the Standard Cosmological Model (SCM)[63]. It is essentially based on the distribution that the matter and radiation assumed in the actual observed Universe. Indeed, looking at the large observational scales (greater than 100Mpc) we note an incredible regularity in the distribution in any possible direction. This observation brings to the formulation of the *Cosmological Principle*, by which the observable Universe is *homogeneous* and *isotropic* everywhere at large scales. Qualitatively speaking, a universe is homogeneous and isotropic if respectively there are no preferred observers and no preferred directions. It is worth noting that an isotropic space-time is necessary homogeneous while the contrary it is not true, as we will see in the next Section. The most spectacular confirmation of the Cosmological Principle is the (almost perfect) black body spectrum of the CMBR, which is at the temperature $T = 2.726K$ and it is uniform everywhere in the sky.

1.4.1 Field equations for the homogeneous and isotropic Universe

Starting from the Cosmological Principle, the metric that describes such a space-time is the Roberston-Walker (RW) metric

$$ds^2 = dt^2 - a^2(t)\left(\frac{dr^2}{1-Kr^2} + r^2 d\theta^2 + r^2 \sin^2\theta d\phi\right), \tag{1.44}$$

where the coordinates (t, r, θ, ϕ) are comoving coordinates, $a(t)$ is the cosmic scale factor and K, after a proper redefinition of the scale factor, can take only the values $\{+1, -1, 0\}$ if the space is respectively at constant positive, negative, or zero spatial curvature. In the Eq. (1.44) the spatial part of the metric is expressed respect to the spherical coordinates (r, θ, ϕ) and the only dynamical degree of freedom is the scale factor $a(t)$. The geometrical interpretation of the three scalar curvature cases are respectively the 3-sphere ($k = +1$), the hyper-saddle ($k = -1$) and the hyper-plane ($k = 0$).

In order to analyze the dynamics of the homogeneous and isotropic Universe, it is necessary to consider the Einstein equations (1.5) where the RW geometry (1.44) it is taken into account. Such dynamical cosmological models are known as Friedmann-Roberston-Walker (FRW) models. Furthermore, it is also necessary to characterize the matter contribution that appears in the right hand side of the Einstein equations. The requirement for the stress-energy tensor $T_{\mu\nu}$ is to be consistent with the symmetries of the metric (homogeneity and isotropy). For this reason, it would necessary be diagonal and with equal spatial components. The simplest fulfillment of this requirements is the perfect fluid case, with energy density $\rho(t)$ and pressure $p(t)$:

$$T_{\mu\nu} = diag(\rho, -p, -p, -p). \tag{1.45}$$

The left hand side of the Einstein equations can be evaluated in the RW geometry case evaluating the non-zero component of the Ricci Tensor $R_{\mu\nu}$:

$$R_{00} = -3\frac{\ddot{a}}{a} \tag{1.46}$$

$$R_{ij} = -\left[\frac{\ddot{a}}{a} + 2\frac{\dot{a}^2}{a^2} + 2\frac{K}{a^2}\right] g_{ij} \tag{1.47}$$

and the Ricci Scalar R:

$$R = -6\left[\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2} + \frac{K}{a^2}\right], \tag{1.48}$$

where the tensor g_{ij} accounts for the spatial component of the RW geometry.

Inserting the Eqs. (1.45),(1.46),(1.47),(1.48) in the Einstein equations (1.5) we obtain, for the $0-0$ component the so called *Friedmann equation*

$$\frac{\dot{a}^2}{a^2} + \frac{K}{a^2} = \frac{k}{3}\rho, \tag{1.49}$$

while the $i-i$ component leads to the equation

$$2\frac{\ddot{a}}{a}+\frac{\dot{a}^2}{a^2}+\frac{K}{a^2}=-kp. \tag{1.50}$$

Performing a difference between the Eqs. (1.49),(1.50), we obtain an equation that characterize the acceleration $\ddot{a}$ alone:

$$\frac{\ddot{a}}{a}=-\frac{k}{6}(\rho+3p). \tag{1.51}$$

The Eq.(1.51) provides the simplest and easy proof about the existence of the initial singularity, namely the *Big Bang singularity*. Indeed, being the Universe in expansion today we have that $\dot{a}>0$. Furthermore, for the standard matter domination cases (matter, radiation or vacuum) the quantity $(\rho+3p)$ is always positive. This implies that $\ddot{a}<0$ and then at some finite time in the past (usually referred as $t=0$) the scale factor has been equal to zero. This moment is referred as the initial singularity.

1.4.2 Hamiltonian dynamics of the FRW models

The results obtained for the FRW Universe can be replaced in the Hamiltonian formulation framework too. This approach will be useful for the quantization procedure that we will implement in the next chapters. Following the prescriptions in the Section 1.2, we start by considering the ADM line element in the case of homogeneous and isotropic model[79]:

$$ds^2=N^2dt^2-a^2(t)dl^2_{RW}, \tag{1.52}$$

where we consider a generic lapse function $N(t)$ and a shift vector N_i equal to zero due to the homogeneity symmetry. Moreover, the quantity dl^2_{RW} is the spatial part of the RW geometry that we described with the spherical coordinates in the Eq.(1.52). Let us consider now the Einstein-Hilbert action (1.11) for the RW geometry in presence of an energy density contribution $\rho(a)$. The action takes the form

$$S=\int dt\left[\frac{6\pi^2}{kN}(\ddot{a}a^2+a\dot{a}^2+KN^2a)-2\pi^2N\rho a^3\right], \tag{1.53}$$

where we used the homogeneous symmetry to calculate the spatial part of the integration as a factor $2\pi^2$. The previous relation can be rearranged making use of the relation $a^2\ddot{a}=(a^2\dot{a})^\cdot-2a\dot{a}^2$ in order to obtain:

$$S=\int dt\mathcal{L}_{RW}=\int dt\left[-\frac{6\pi^2}{kN}a\dot{a}^2+N\left(\frac{6\pi^2}{k}Ka-2\pi^2\rho a^3\right)\right]. \tag{1.54}$$

The conjugate momenta to the scale factor a can be evaluated from the FRW Lagrangian density $\mathcal{L}_{RW}$ as

$$p_a=\frac{\partial\mathcal{L}_{RW}}{\partial a}=-\frac{12\pi^2}{kN}a\dot{a}\rightarrow\dot{a}=-\frac{kN}{12\pi^2}\frac{p_a}{a}. \tag{1.55}$$

Making use of the relation (1.55) and the Legendre transformation $N\mathcal{H}_{RW} = p_a\dot{a} - \mathcal{L}_{RW}$, the action (1.54) can be recast in the following way:

$$S = \int dt(p_a\dot{a} - N\mathcal{H}_{RW}) =$$
$$= \int dt \left[p_a\dot{a} - N\left(-\frac{k}{24\pi^2}\frac{p_a^2}{a} - \frac{6\pi^2 K}{k}a + 2\pi^2\rho a^3\right)\right]. \quad (1.56)$$

The variation of the action in the form (1.56) with respect to N leads to the superHamiltonian constraint

$$\frac{p_a^2}{a^4} + \frac{144\pi^4}{k^2a^2}K = \frac{48\pi^4}{k}\rho. \quad (1.57)$$

From the superHamiltonian $\mathcal{H}_{RW}$, it is possible to evaluate the Hamiltonian equations for the configuration variables (a, p_a):

$$\dot{a} = N\frac{\partial\mathcal{H}_{RW}}{\partial p_a} = -\frac{kN}{12\pi^2}\frac{p_a}{a} \quad (1.58)$$

$$\dot{p}_a = -N\frac{\partial\mathcal{H}_{RW}}{\partial a} = -\frac{kN}{24\pi^2}\frac{p_a^2}{a^2} + \frac{6\pi^2 KN}{k} - 2\pi^2\frac{d(\rho a^3)}{da}. \quad (1.59)$$

The equivalence between the superHamiltonian constraint (1.57) and the Friedmann equation (1.49) is established choosing the lapse function $N = 1$. Indeed, inserting in the constraint (1.57) the dependence of p_a with respect to $\dot{a}$ given in the Eq.(1.55), for this particular choice of the lapse function we obtain exactly the Friedmann equation (1.49).

Furthermore, substituting the Eq.(1.58) in the Eq.(1.59) and considering the continuity equation for the perfect fluid in the form $\frac{d(\rho a^3)}{da} = -3a^2 p$, we arrive precisely to the spatial component of the Einstein equations (1.50).

In conclusion, we have shown how the variation of the superHamiltonian respect to N, a, p_a leads to a complete description of the dynamics of the FRW models, providing the same information obtained in the previous section with the field equations approach.

The dynamics of the FRW models in the Hamiltonian framework resembles the behavior of a one-dimensional particle, with position and momenta variables respectively (a, p_a), whose evolution is ruled by the model-dependent potential term that appears in the superHamiltonian constraint.

1.5 The Homogeneous Cosmological Models

As said in the previous sections, the SCM represents an exceptional success for the description of the Universe. The accomplishment in considering the symmetries of homogeneity and isotropy to describe the observed Universe has been supported from the observational and theoretical point of view.

Nevertheless, there are some problems. Indeed, even though the paradoxes that emerges in the SCM can be overtaken considering an inflationary phase during the evolution of the Universe, some reasons exists to consider more general models respect to the FRW ones. For example, if we consider the classical early stage of the Universe (before the inflationary stage) as emerged from an initial quantum phase, it is very peculiar to imagine it with an high degree of symmetry as the actual observed Universe. Instead, what it is natural to expect is that the classical phase of the Universe began in conditions of maximal generality and without any symmetry. The possibility to construct a generic cosmological solution for the Einstein Equation has been shown for the first time by V.A.

Belinski, I.M. Khalatnikov and E.M. Lifshitz, who found a solution with all its degrees of freedom available.

The homogeneous and anisotropic models that we present in this Section stand as a natural bridge between the high degree symmetry FRW models and the generic cosmological solution. The starting point to classify all the possible models of this kind is to formally define the concept of homogeneity in cosmology.

A generic homogeneous model with space-time metric $g_{\mu\nu}$ has to preserve the invariance of the spatial line element under suitable group of transformations[65]. It means that the spatial line element

$$dl^2 = h_{\alpha\beta}(t,x)dx^\alpha dx^\beta, \tag{1.60}$$

under the isometry $T : x \to x'$, has to left invariant the 3-dimensional metric $h_{\alpha\beta}(t,x)$ so that in the transformed line element

$$dl^2 = h_{\alpha\beta}(t,x')dx'^\alpha dx'^\beta, \tag{1.61}$$

with the spatial metric $h_{\alpha\beta}(t,x') = h_{\alpha\beta}(t,x)$. In the previous spatial line element the shift vector $N^i = 0$ due to the homogeneity symmetry. In the general case of a non-Euclidean homogeneous three-dimensional space, there are three independent differential forms[3] which are invariant under the transformations T. It is possible to write them as $\omega^a = e^a_\alpha dx^\alpha$, where e^a_α are a set of four linearly independent vectors which respect the condition $e^i_a e_{ib} = \eta_{ab}$ and η_{ab} is a symmetric matrix depending on time only. Hence, the spatial line element (1.60) can be expressed as $dl^2 = \eta_{ab}(e^a_\alpha dx^\alpha)(e^b_\beta dx^\beta)$ with the metric tensor $h_{\alpha\beta} = \eta_{ab}e^a_\alpha e^b_\beta$. The entire element line in the ADM framework takes the form

$$ds^2 = N(t)^2 dt^2 - \eta_{ab}\omega^a\omega^b. \tag{1.62}$$

Respect to the vectors e^a_α (called the tetradic picture) the homogeneity condition can be expressed with the relation

$$C^c_{ab} = \left(\frac{\partial e^c_\alpha}{\partial x^\beta} - \frac{\partial e^c_\beta}{\partial x^\alpha}\right) e^\alpha_a e^\beta_b, \tag{1.63}$$

where C^c_{ab} are constants object anti-symmetric in the lower indexes and they are called *structure constants*. The classification of all the possible homogeneous models that respect the constraint can be done introducing the dual of the constant of structure through the complete anti-symmetric Levi-Civita tensor $\epsilon_{abc} = \epsilon^{abc}$ with respect to which the structure constants takes the form $C^{ab} = \epsilon^{cda}C^b_{cd}$ and the condition (1.63) assumes the form:

$$\epsilon_{bcd}C^{cd}C^{ba} = 0. \tag{1.64}$$

Furthermore, the tensor C^{ab} can be decomposed in symmetric and anti-symmetric part this way:

$$C^{ab} = n^{ab} + \epsilon^{abc}a_c, \tag{1.65}$$

where n_{ab} and $\epsilon^{abc}a_c$ are respectively the symmetric and the anti-symmetric part. This decomposition allows to recast the condition (1.64) as

$$n^{ab}a_b = 0 \tag{1.66}$$

Without loss of generality we can redefine $a_c = (a, 0, 0)$ and the symmetric tensor as a diagonal matrix $n_{ab} = diag(n_1, n_2, n_3)$. This way the latter condition reduces to $an_1 = 0$.

[3] In the Euclidean case the three invariant objects are simply the differential components (dx, dy, dz).

Type	a	n_1	n_2	n_3
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 1.2: Classification of the all possible homogeneous models-

Finally, if we choose to rescale the parameters such that $a \geq 0$ and n_1, n_2, n_3 assume the values $0, \pm 1$, we can collect all the possible combinations of different spaces that respect the condition of homogeneity. This classification, called *Bianchi Classification* and reported in the Fig.1.2, is moreover divided in A-type ($a = 0$) spaces and B-type ($a \neq 0$) spaces. To conclude this section it is worth to underline that three of this spaces represent the non-isotropic generalization of the RW geometry, that are the flat, the open and the closed space. Such spaces (Bianchi I, Bianchi V, Bianchi IX) possess the feature to became, when the isotropy symmetry is restored, respectively the homogeneous and isotropic model with the curvature parameter $K = 0, -1, +1$.

Let us now see what form the Einstein equations assume in the tetradic framework. For convenience let us consider the field equations in the mixed components version

$$R^{\mu}_{\nu} - \frac{1}{2}\delta^{\mu}_{\nu} R = \frac{k}{c} T^{\mu}_{\nu}. \tag{1.67}$$

When the ADM line element (1.62) is taken into account, they acquire the form

$$R^0_0 = -\frac{\partial}{\partial t} K^{\alpha}_{\alpha} - K^{\alpha}_{\beta} K^{\beta}_{\alpha} = \frac{k}{c}\left(T^0_0 - \frac{1}{2}T\right), \tag{1.68}$$

$$R^0_{\alpha} = \left(\frac{\partial K^{\beta}_{\alpha}}{\partial x^{\beta}} - \frac{\partial K^{\beta}_{\beta}}{\partial x^{\alpha}}\right) = \frac{k}{c} T^0_{\alpha}, \tag{1.69}$$

$$R^{\beta}_{\alpha} = -\overline{R}^{\beta}_{\alpha} - \frac{1}{\sqrt{h}} \frac{\partial(\sqrt{h} K_{\alpha\beta})}{\partial t} = \frac{k}{c}\left(T^{\beta}_{\alpha} - \frac{1}{2}\delta^{\beta}_{\alpha} T\right). \tag{1.70}$$

where the extrinsic curvature is, being $N^i = 0$, equals to $K_{\alpha\beta} = -\frac{1}{2N}\frac{\partial h_{\alpha\beta}}{\partial t}$ and the three-dimensional Ricci tensor $\overline{R}_{\alpha\beta}$ is expressed in terms of spatial Christoffel symbols $\overline{\Gamma}^{\gamma}_{\alpha\beta}$ as

$$\overline{R}_{\alpha\beta} = \partial_{\gamma}\overline{\Gamma}^{\gamma}_{\alpha\beta} - \partial_{\alpha}\overline{\Gamma}^{\delta}_{\beta\delta} + \overline{\Gamma}^{\sigma}_{\alpha\beta}\overline{\Gamma}^{\lambda}_{\sigma\lambda} - \overline{\Gamma}^{\nu}_{\alpha\epsilon}\overline{\Gamma}^{\epsilon}_{\beta\nu}, \tag{1.71}$$

$$\overline{\Gamma}^{\gamma}\alpha\beta = \frac{1}{2}h^{\gamma\delta}(\partial_\alpha h_{\delta\beta} + \partial_\beta h_{\alpha\delta} - \partial_\delta h_{\alpha\beta}). \tag{1.72}$$

1.5.1 Bianchi I

The simplest homogeneous solution in the Bianchi classification is the vacuum Bianchi I model, also called *Kasner solution*[65]. In this model all the parameters (a, n_1, n_2, n_3) are null. As a consequence $C_{ab} = 0$ and it is possible to show that also the three-dimensional Ricci scalar (1.71) vanishes.

Then, the Einstein equations (1.68),(1.69),(1.70) leads to

$$\dot{K'}^a_a + K'^b_a K'^a_b = 0 \qquad \frac{1}{\sqrt{\eta}}\frac{\partial(\sqrt{\eta}K'^b_a)}{\partial t} = 0, \tag{1.73}$$

where $\eta = det\eta_{ab}$. From the second equation it is possible to identify a constant of motion, indeed

$$\sqrt{\eta}K'^b_a = \xi^b_a = cost, \tag{1.74}$$

and contracting it with respect to the indexes a and b heads to

$$K'^a_a = \frac{\dot{\eta}}{2\eta} = \frac{\xi^a_a}{\sqrt{\eta}} \longrightarrow \eta = (\xi^a_a)^2 t^2 \tag{1.75}$$

Without loss of generality we can rescale the coordinates in such a way that $\xi^a_a = 1$, ans then, substituting the constant of motion (1.74) in the first equation of the (1.73) the condition $\xi^a_b\xi^b_a = 1$ is achieved. Such a condition, once substituted in the Eq.(1.74), leads to a differential equation for η_{ab}:

$$\dot{\eta}_{ab} = \frac{2}{t}\xi^c_a\eta_{cb} \tag{1.76}$$

The set of coefficients ξ^c_a can be seen as the matrix associated to a given linear transformation. In this sense, if we choose to define its eigenvalues and eigenvectors as $(p_1, p_2, p_3) \in \mathbb{R}$ and $\mathbf{n}^1, \mathbf{n}^2, \mathbf{n}^3$, the previous differential equation admits as solution

$$\eta_{ab} = t^{2p_1}\mathbf{n}^1_a\mathbf{n}^1_b + t^{2p_2}\mathbf{n}^2_a\mathbf{n}^2_b + t^{2p_3}\mathbf{n}^3_a\mathbf{n}^3_b \tag{1.77}$$

Finally, choosing the directions of the vectors $\mathbf{n}^1, \mathbf{n}^2, \mathbf{n}^3$ as the frame directions and rename it as x^1, x^2, x^3, the spatial element line $dl^2 = \eta_{ab}(e^a_\alpha dx^\alpha)(e^b_\beta dx^\beta)$ reduces to

$$dl^2 = t^{2p_1}(dx^1)^2 + t^{2p_2}(dx^2)^2 + t^{2p_3}(dx^3)^2 \tag{1.78}$$

The three arbitrary parameters (p_1, p_2, p_3) are called *Kasner indexes* ans from the relation $\xi^a_a = 1$ and $\xi^a_b\xi^b_a = 1$ they obey the conditions

$$p_1 + p_2 + p_3 = 1 \tag{1.79}$$

$$p_1^2 + p_2^2 + p_3^2 = 1 \tag{1.80}$$

As a consequence, in the Kasner solution we have only one independent parameter, due to the fact that we deal with three indexes and two conditions. Except for the cases when (p_1, p_2, p_3) are $(0, 0, 1)$ and $(-\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$, the three indexes are always different from each other and anyhow two are always positive and one is always negative. Choosing the order $p_1 \leq p_2 \leq p_3$ their values are included in the ranges

$$-\frac{1}{3} \leq p_1 \leq 0 \qquad 0 \leq p_2 \leq \frac{2}{3} \qquad \frac{2}{3} \leq p_3 \leq 1 \tag{1.81}$$

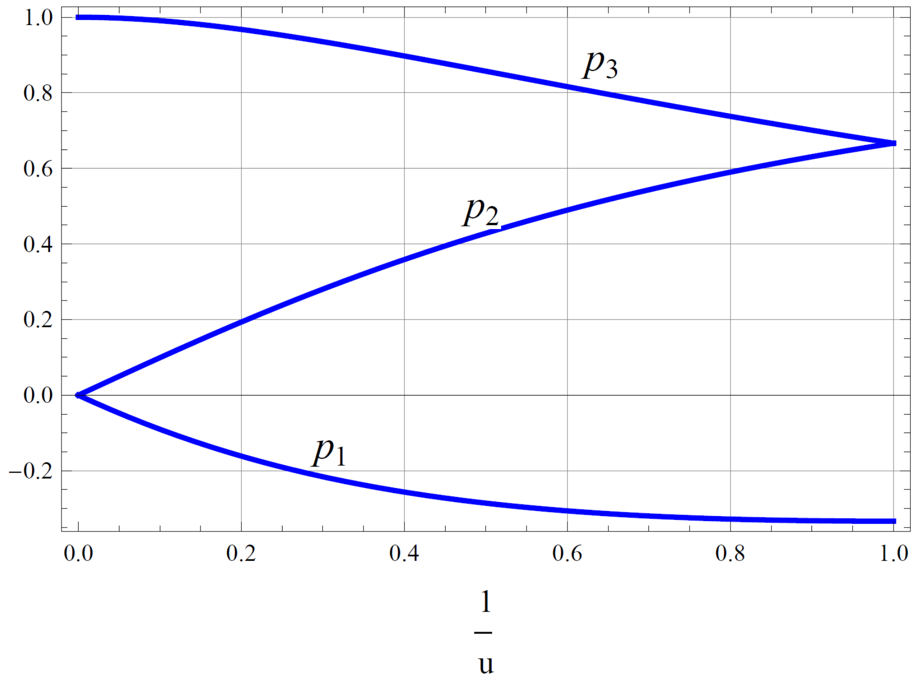

FIGURE 1.3: Evolution of the Kasner indexes p_1, p_2, p_3 as a function of $\frac{1}{u}$

Moreover, the Kasner indexes admit the following parametrization

$$p_1(u) = -\frac{u}{1+u+u^2} \quad p_2(u) = \frac{1+u}{1+u+u^2} \quad p_3(u) = \frac{u(1+u)}{1+u+u^2}, \tag{1.82}$$

where the parameter u takes values in the interval $1 \leq u \leq \infty$. Given the particular form of the parametrization (1.82), all the values of p_i are achieve mapping u in $u' = \frac{1}{u}$ in the interval $0 \leq u \leq 1$ and using the inversion propriety

$$p_1(u' = \frac{1}{u}) = p_1(u) \quad p_2(u' = \frac{1}{u}) = p_3(u) \quad p_3(u' = \frac{1}{u}) = p_2(u) \tag{1.83}$$

In Fig.1.3 is sketched the trend of the Kasner indexes with respect to $\frac{1}{u}$.
In conclusion, we identify the spatial metric (1.78) as the metric of a flat and anisotropic space, which volumes increase proportional to the cosmic time t and where the linear distances along two axes expand and along the third axes contracts. Except to the $(0, 0, 1)$ case[4], this model present a non-eliminable physical singularity in $t = 0$, being the invariants associated to the curvature tensor infinite.

1.5.2 Bianchi II

In order to analyse more complex homogeneous models then the Bianchi I, let us consider a more treatable shape for the Einstein equations[79]. To do this, let us choose three spatial vectors $\{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$ with respect to which the matrix η_{ab} takes a diagonal form. Furthermore, we choose the elements of the diagonal matrix equals to (a^2, b^2, c^2). This way the space metric $h_{\alpha\beta}$ assumes the form

$$h_{\alpha\beta} = a^2 l_\alpha l_\beta + b^2 m_\alpha m_\beta + c^2 n_\alpha n_\beta, \tag{1.84}$$

[4] in which the singularity is eliminated through a change of variable

where the quantities (a^2, b^2, c^2) are three different scale factors. Substituting the metric (1.84) in the Einstein equations (1.68),(1.69),(1.70), they reduce to

$$-R^l_l = \frac{(\dot{a}bc)^\cdot}{abc} + \frac{1}{2(abc)^2}\left[\lambda_l^2 a^4 - (\lambda_m b^2 - \lambda_n c^2)^2\right] = 0 \tag{1.85}$$

$$-R^m_m = \frac{(a\dot{b}c)^\cdot}{abc} + \frac{1}{2(abc)^2}\left[\lambda_m^2 b^4 - (\lambda_l a^2 - \lambda_n c^2)^2\right] = 0 \tag{1.86}$$

$$-R^n_n = \frac{(ab\dot{c})^\cdot}{abc} + \frac{1}{2(abc)^2}\left[\lambda_n^2 c^4 - (\lambda_l a^2 - \lambda_m b^2)^2\right] = 0 \tag{1.87}$$

$$-R^0_0 = \frac{\ddot{a}}{a} + \frac{\ddot{b}}{b} + \frac{\ddot{c}}{c} = 0 \tag{1.88}$$

Being η_{ab} a diagonal matrix, all the non-diagonal components of the equations vanish. The constants $(\lambda_l, \lambda_m, \lambda_n)$=$(C_{11}, C_{22}, C_{33})$ are the only non-vanishing structure constants and their combination select the particular model within the Bianchi Classification. It is worth noting that this framework allow to select only a part of the totality of the Bianchi model. In particular, we can take into account only the model I, II, VI, VII, VIII, IX of the classification. In order to simplify the temporal derivatives that appear in the Einstein equations, it is useful to consider the logarithmic variables

$$\alpha = \ln a \qquad \beta = \ln b \qquad \gamma = \ln c, \tag{1.89}$$

and the new temporal variable τ such that

$$dt = abc d\tau. \tag{1.90}$$

Then, the Eqs. (1.85)-(1.88) with respect to the latter variables show as

$$2\alpha_{\tau\tau} = (\lambda_m b^2 - \lambda_n c^2)^2 - \lambda_l^2 a^4 \tag{1.91}$$

$$2\beta_{\tau\tau} = (\lambda_l a^2 - \lambda_n c^2)^2 - \lambda_m^2 b^4 \tag{1.92}$$

$$2\gamma_{\tau\tau} = (\lambda_l a^2 - \lambda_m c^2)^2 - \lambda_n^2 a^4 \tag{1.93}$$

$$\frac{1}{2}(\alpha + \beta + \gamma)_{\tau\tau} = \alpha_\tau \beta_\tau + \alpha_\tau \gamma_\tau + \beta_\tau \gamma_\tau \tag{1.94}$$

where the indexes τ mean derivatives with respect to τ.

The Bianchi II model is identifies by a set of structure constants $(\lambda_l, \lambda_m, \lambda_n) = (1, 0, 0)$ which reduce the Eqs. (1.85)-(1.88) to

$$\frac{(\dot{a}bc)^\cdot}{abc} = -\frac{a^2}{2(bc)^2} \tag{1.95}$$

$$\frac{(a\dot{b}c)^\cdot}{abc} = \frac{a^2}{2(bc)^2} \tag{1.96}$$

$$\frac{(ab\dot{c})^\cdot}{abc} = \frac{a^2}{2(bc)^2} \tag{1.97}$$

$$\frac{\ddot{a}}{a} + \frac{\ddot{b}}{b} + \frac{\ddot{c}}{c} = 0 \tag{1.98}$$

Looking at the right hand side of the Eqs. (1.95)-(1.97), it can be noted that they plat the role of a perturbation of the free regime, or in other words a perturbation of the Kasner regime. Indeed, if at a certain instant of time t we know that it is possible to neglect such terms, what remain is exactly the Kasner solution analyzed in Section 1.5.1.

The stability of the Bianchi II solution critically depends about the initial conditions. In fact, if the perturbation, that we for example can choose to grow as $a^4 \sim t^{4p_i}$ towards the singularity , is associated to one of the two positive Kasner indexes, so for $t \to 0$ this goes ahead to decrease and finally can be neglected.

On the other hand, if the perturbation is associated to the negative Kasner index, for $t \to 0$ this grows indefinitely and cannot be neglected. This is the case when it is necessary to analyze the full system. For such a perturbation, the Eqs. (1.95)-(1.98) in the logarithmic variables version, reduce to

$$\alpha_{\tau\tau} = -\frac{1}{2}e^{4\alpha} \tag{1.99}$$

$$\beta_{\tau\tau} = \gamma_{\tau\tau} = \frac{1}{2}e^{4\alpha} \tag{1.100}$$

The Eq.(1.99) resembles the equation of motion of a one-dimensional particle that interacts with a infinite potential well; the particle reaches the wall with a certain velocity determined from the previous free Kasner period, bounces against the wall and approaches a new free Kasner regime with a different velocity without any successive interaction with the wall. From this consideration it is clear that the role of the perturbation is to connect one Kasner regime to another one, where each of which is called *Kasner epoch*. The old and the new Kasner indexes in the two Kasner epochs are connected through the so-called *Belinski,Khalatnikov,Lifshitz (BKL) Map*[14]

$$p'_l = \frac{|p_l|}{1-2|p_l|} \quad , \quad p'_m = -\frac{2|p_l| - p_m}{1-2|p_l|} \quad , \quad p'_n = \frac{-2|p_l| + p_n}{1-2|p_l|} \tag{1.101}$$

The main feature that emerges looking at this map is that the transition on the wall moves the negative Kasner indexes from one direction to another one. In particular, after the bounce, the negative power law in t is not any more associated to the l direction but to the m direction:

$$p_l < 0, p_m > 0 \Longrightarrow p'_m < 0, p'_l > 0 \tag{1.102}$$

1.5.3 Bianchi IX

We dedicate this Section to the study of the more general model[5] of the Bianchi classification; the Bianchi IX model[79],[76]. The set of the structure constants for this model is $(\lambda_l, \lambda_m, \lambda_n) = (1, 1, 1)$ and the Einstein equations (1.91)-(1.93) become

$$2\alpha_{\tau\tau} = (b^2 - c^2)^2 - a^4 \tag{1.103}$$

$$2\beta_{\tau\tau} = (a^2 - c^2)^2 - b^4 \tag{1.104}$$

$$2\gamma_{\tau\tau} = (a^2 - b^2)^2 - c^4 \tag{1.105}$$

Let us consider again the negative indexes associated to the direction l. Differently from the Bianchi II case, here the perturbations are present in any directions. In particular, along the l-direction the perturbation grows for $t \to 0$ proportional to a^4 while the perturbations decrease along the other two. In this way, if we consider only the growing terms in the Einstein equations, we obtain precisely the system of equations (1.99),(1.100), whose solution describe the evolution of the metric from the initial Kasner state (1.78) to

[5] The Bianchi VIII too possess the same degree of generality

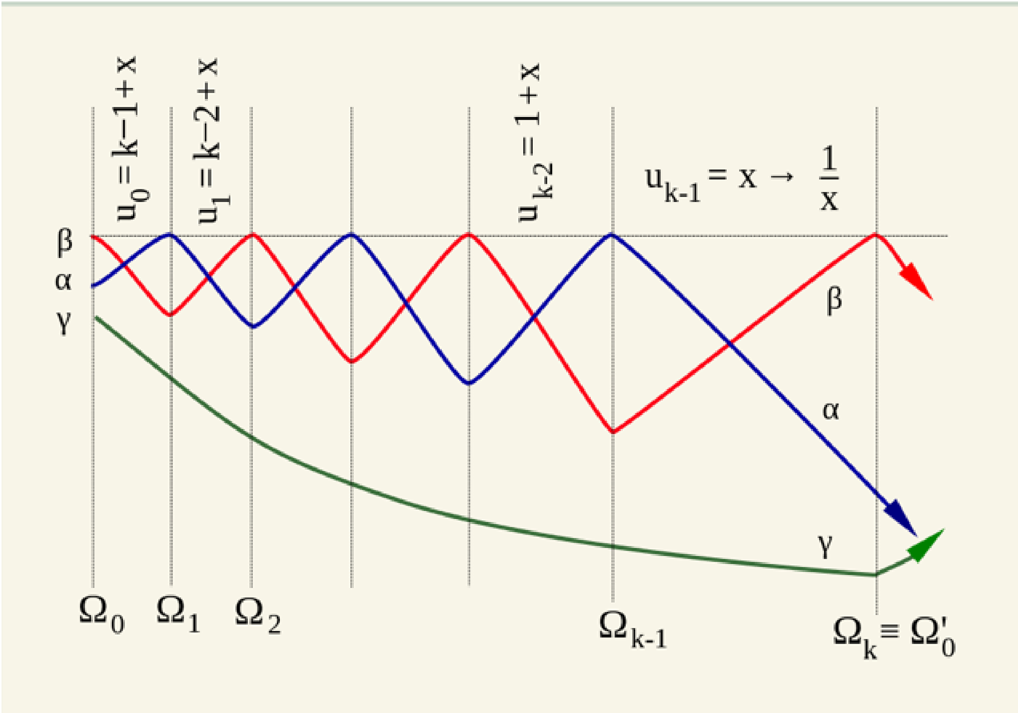

FIGURE 1.4: Oscillatory Behaviour of the Bianchi IX model

another one. Once the transition of the negative index between the l direction and the m direction occurred, following the BKL map (1.101), the dominant term in the right hand sides of the equations is the b^4 term, with the other two perturbation negligible. So, after the successive bounce, we have an exchange in the direction of the negative index from the m direction back to the l direction. This exchange in the l and m direction go ahead until the perturbation along the n direction remains negligible. The collection of successive Kasner epochs until the explosion of the perturbation in the n direction is called *Kasner era*. During the Kasner era the scale factor c, associated to the n direction, decreases monotonically towards the singularity. At the end of the first Kasner era the perturbation c^4 is not negligible anymore and from that moment the negative power exponent is exchanged between the n or l directions or the n or m directions. It is possible to show that this behavior go ahead indefinitely with a continuous interchanges among directions until the singularity. The situation is sketched in the Fig.1.4.

To resume, the evolution of the model towards the singularity consists of successive eras, in which distances along two axes oscillate and along the third axis monotonically decrease while the volume always decreases linearly with respect to the time t.

1.6 Hamiltonian dynamics of the Mixmaster Model

In this Chapter we provide the Hamiltonian formulation of the Mixmaster dynamics, describing in detail how the infinite sequence of Kasner epochs, that characterize the type VIII and IX of the Bianchi classification, takes the suggestive form of an interacting two-dimensional point particle within a potential well. Let us start by considering, in a generic homogeneous space-time, the ADM element line:

$$ds^2 = N(t)^2 dt^2 - h_{\alpha\beta} dx^\alpha dx^\beta, \tag{1.106}$$

where $N(t)$ is the lapse function and where we redefined the three scale factors $\{a(t), b(t), c(t)\}$ in such a way to have a spatial line element of the form:

$$dl^2 = h_{\alpha\beta}dx^\alpha dx^\beta = (e^{q_l}l_\alpha l_\beta + e^{q_m}m_\alpha m_\beta + e^{q_n}n_\alpha n_\beta)dx^\alpha dx^\beta = \eta_{ab}\omega^a\omega^b, \tag{1.107}$$

where we introduced the matrix $\eta_{ab} = diag\{e^{q_l}, e^{q_m}, e^{q_n}\}$ and a set of three invariance form $\omega^a = \omega^a_\alpha dx^\alpha$ with $\omega^a_\alpha = \{l_\alpha, m_\alpha, n_\alpha\}$. In the definition of the spatial line element (1.107), the generalized coordinates $\{q_l, q_m, q_n\}$ are functions of time only. Being the Bianchi IX space-time the selected one to illustrate the Mixmaster model[6], the set of structure constants is $(\lambda_l, \lambda_m, \lambda_n) = (1,1,1)$. In order to introduce the dynamical character of the gravitational field let us consider the Einstein-Hilbert Action in the vacuum case in the Hamiltonian formulation framework, as written in the Eq.(1.11). The first consideration regards the spatial integration of the action. As in the FRW case, due to the homogeneity symmetry, it is possible to isolate the spatial integration with respect to the time integration and this factorization provides a term $(4\pi)^2$. This way, substituting the metric as appears in the line element (1.107), the action for the Bianchi IX model takes the form

$$S_g = \int \mathcal{L}_{IX}(q_a, \dot{q}_a)dt = \int dt \left(-\frac{8\pi^2\sqrt{\eta}}{k}\right)\left[\frac{1}{2N}(\dot{q}_l\dot{q}_m + \dot{q}_l\dot{q}_n + \dot{q}_m\dot{q}_n) - N\overline{R}\right] \tag{1.108}$$

The spatial curvature term can be explicitly evaluated in terms of the generalized coordinates. In particular, we obtain

$$\eta\overline{R} = -\frac{1}{2}\left[\sum_a \lambda_a^2 e^{2q_a} - \sum_{a\neq b}\lambda_a\lambda_b e^{q_a+q_b}\right] \tag{1.109}$$

with $\eta = \det(\eta_{ab}) = e^{\sum_a q_a}$ and $a, b = l, m, n$. Passing from the Lagrangian to the Hamiltonian formulation consists in performing a Legendre transformation and, as an intermediate step, to evaluate the conjugate momenta to the generalized coordinates q_a:

$$p_l = \frac{\partial\mathcal{L}_{IX}}{\partial\dot{q}_l} = -\frac{4\pi^2\sqrt{\eta}}{kN}(\dot{q}_m + \dot{q}_n), \tag{1.110}$$

$$p_m = \frac{\partial\mathcal{L}_{IX}}{\partial\dot{q}_m} = -\frac{4\pi^2\sqrt{\eta}}{kN}(\dot{q}_n + \dot{q}_n), \tag{1.111}$$

$$p_n = \frac{\partial\mathcal{L}_{IX}}{\partial\dot{q}_n} = -\frac{4\pi^2\sqrt{\eta}}{kN}(\dot{q}_l + \dot{q}_m). \tag{1.112}$$

The relations (1.110)-(1.111) allow to write the Legendre transformation

$$N\mathcal{H}_{IX} = \sum_{a=l,m,n} p_a\dot{q}_a - \mathcal{L}_{IX} \tag{1.113}$$

ans to substitute it in the action (1.108) in order to obtain

$$S_g = \int dt(p_a\dot{q}_a - N\mathcal{H}_{IX}) \tag{1.114}$$

[6]Considering the Bianchi VIII with respect to the Bianchi IX leads to the same dynamical proprieties

where the superhamiltonian explicitly reads as

$$\mathcal{H}_{IX} = \frac{k}{8\pi^2\sqrt{\eta}}\left[\sum_a (p_a)^2 - \frac{1}{2}\left(\sum_b p_b\right)^2 - \frac{64\pi^4}{k^2}\eta\overline{R}\right] \tag{1.115}$$

and the scalar constraint is $\mathcal{H}_{IX} = 0$. It is useful to introduce the *anisotropy parameters*, defined as

$$Q_a = \frac{q_a}{\sum_b q_b} \quad , \quad \sum_a Q_a = 1, \tag{1.116}$$

to provides a potential role for the dynamics to the last term in the Eq.(1.115). Indeed, considering the relations (1.116), the scalar curvature term (1.109) becomes

$$\eta\overline{R} = -\frac{1}{2}\left[\sum_a \lambda_a^2 \eta^{2Q_a} - \sum_{b\neq c}\lambda_b\lambda_c\eta^{Q_b+Q_c}\right] = -\frac{1}{2}\left[\sum_a \lambda_a^2 \eta^{2Q_a} - \sum_{b\neq c}\lambda_b\lambda_c\eta^{1-Q_a}\right] \tag{1.117}$$

To analyze the behavior of this term towards the singularity means to consider this object in the limit $\eta \to 0$. The second term, in this limit, is always negligible, while the second one depends critically on the sign of the parameter Q_a; in particular it is negligible if $Q_a > 0$, while is ∞ if $Q_a < 0$. For this reason we can modelized the potential term $\eta\overline{R}$ as an infinitely steep well whose behavior is resumed in

$$-\eta\overline{R} = \sum_a \Theta(Q_a) \quad , \quad \Theta(Q_a) = \begin{cases} \infty, & Q_a < 0 \\ 0, & Q_a > 0 \end{cases} \tag{1.118}$$

From the writing (1.118) is clear hoe the dynamics of the Universe resembles that of a particle moving in a domain D_Q, defined as the space in which the condition $Q_a > 0$ is valid.

1.6.1 The Mixmaster Model in the Misner Variables

The main feature of the generalized coordinates is the connection with the Kasner indexes. In fact, comparing the relations (1.77),(1.107) is possible to establish that

$$q_a(t) = 2p_a \ln t. \tag{1.119}$$

In order to resemble a full point-particle dynamics it is necessary to treat with a diagonal kinetic term in the superHamiltonian constaint. In this optic the generalized coordinates admits a particular transformation variables, that brings to the so-called *Misner variables*[74], which transforms the kinetic term

$$KT = \sum_a p_a^2 - \frac{1}{2}\left(\sum_b p_b)\right)^2, \tag{1.120}$$

in a diagonalized kinetic term:

$$KT = -\frac{1}{24}(-c_1^2 p_\alpha^2 + c_2^2 p_+^2 + c_3^2 p_-^2), \tag{1.121}$$

The generalized coordinates and the Misner variables are linked in the following way:

$$\begin{cases} q_1 = 2p_1 \ln t = 2(\alpha + \beta_+ + \sqrt{3}\beta_-) \\ q_2 = 2p_2 \ln t = 2(\alpha + \beta_+ - \sqrt{3}\beta_-) \\ q_3 = 2p_3 \ln t = 2(\alpha - 2\beta_+) \end{cases} \tag{1.122}$$

With respect to the new variables, the matrix $\eta_{ab} = diag\{e^{q_l}, e^{q_m}, e^{q_n}\}$ exhibits the peculiarity of this frame:

$$\eta_{ab} = e^{2\alpha}(e^{2\beta})_{ab} \longrightarrow (\ln \eta)_{ab} = 2\alpha\delta_{ab} + 2\beta_{ab}. \tag{1.123}$$

Looking at the Eq.(1.123), where the matrix β_{ab} is a three dimensional symmetric matrix with null trace which elements are

$$\beta_{11} = \beta_+ + \sqrt{3}\beta_- \quad , \quad \beta_{22} = \beta_+ - \sqrt{3}\beta_- \quad , \quad \beta_{33} = -2\beta_+, \tag{1.124}$$

is clear the factorization of the α component, which is the variable related to Universe volume, with respect to the $\{\beta_+, \beta_-\}$ one, related to the anisotropies. This is evident inverting the relations (1.122), indeed

$$\alpha = \frac{1}{3} \ln t \tag{1.125}$$

$$\beta_+ = \frac{1 - p_3}{6} \ln t = \frac{1 - p_3}{2} \alpha \tag{1.126}$$

$$\beta_- = \frac{p_1 - p_2}{2\sqrt{3}} \ln t = \sqrt{3}(p_1 - p_2)\alpha \tag{1.127}$$

The proportionality of α with respect to the logarithm of the volume of the Universe clarify its identification with the isotropic component, while $\beta_\pm$ are linked to the anisotropies of the Universe, due to the dependence on the Kasner indexes. With this variables choice, the determinant of the metric η assumes the simple form

$$\eta = \det(\eta_{ab}) = \det(e^{6\alpha} \det((e^{2\beta})_{ab}) = e^{6\alpha} e^{2tr\beta} = e^{6\alpha} \tag{1.128}$$

The action (1.108) for the Bianchi IX model in the Misner variables is rewrite as[75]

$$S_g = \int dt \left(p_\alpha \dot{\alpha} + p_+ \dot{\beta}_+ + p_- \dot{\beta}_- - N\mathcal{H}_{IX} \right) \tag{1.129}$$

where the superHamiltonian takes the form

$$\mathcal{H}_{IX} = \frac{k}{3(8\pi)^2} e^{-3\alpha}(-p_\alpha^2 + p_+^2 + p_-^2 + \mathcal{V}) \tag{1.130}$$

and the term $\mathcal{V}$ is

$$\mathcal{V} = -\frac{6(4\pi)^4}{k^2} \eta \overline{R} = \frac{3(4\pi)^4}{k^2} e^{4\alpha} V(\beta_\pm) \tag{1.131}$$

The potential term $V(\beta_\pm)$ depends on the anisotropies only and its form is

$$V(\beta_\pm) = e^{-8\beta_+} - 4e^{-2\beta_+} \cosh(2\sqrt{3}\beta_-) + 2e^{4\beta_+} \left[\cosh(4\sqrt{3}\beta_-) - 1) \right] \tag{1.132}$$

By the variation of the action (1.129) with respect to the conjugate momenta, a relation

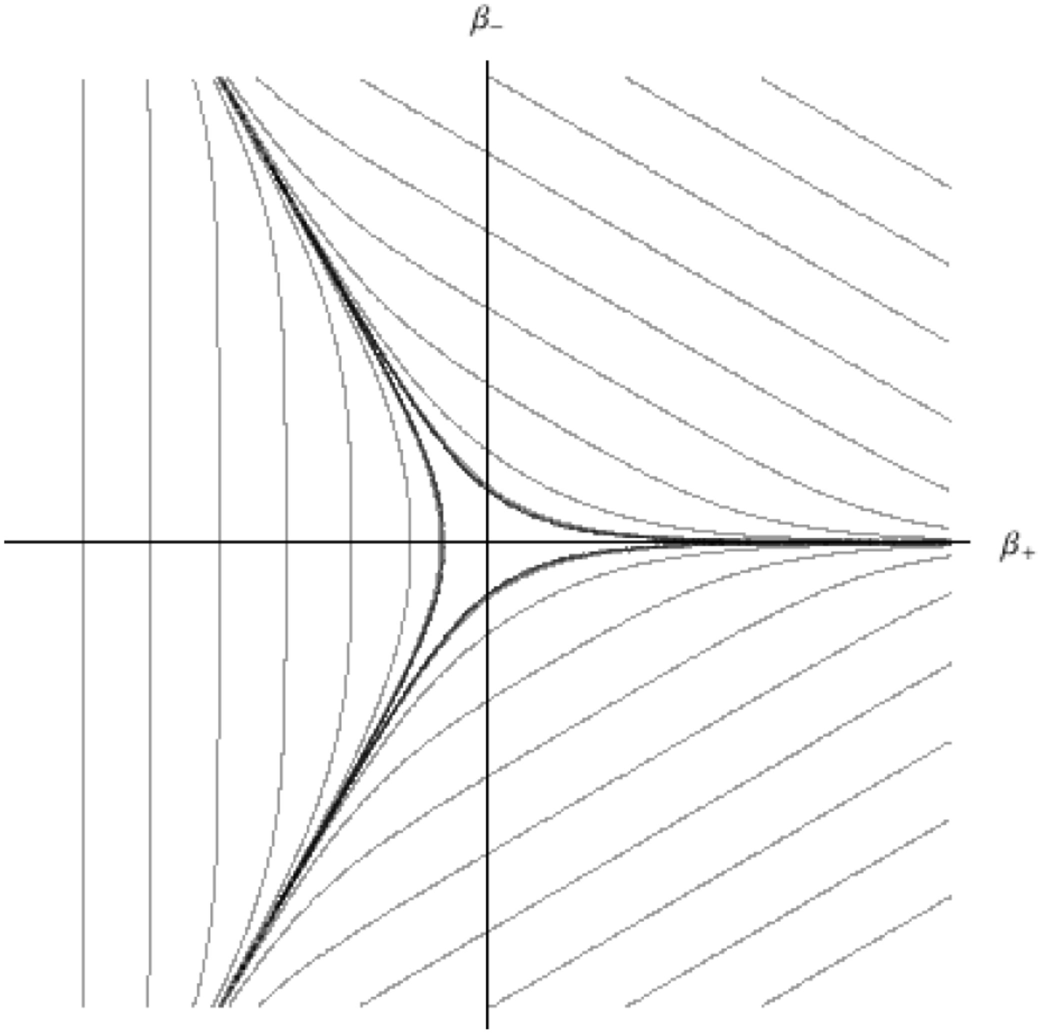

FIGURE 1.5: Equipotential lines of the Bianchi IX model in the (β_+, β_-)

with the Misner variables is obtained:

$$\dot{\alpha} + \frac{2Nk}{3(8\pi)^2} e^{-3\alpha} p_\alpha = 0 \rightarrow p_\alpha = -\frac{6(4\pi)^2}{Nk} e^{3\alpha} \dot{\alpha} \tag{1.133}$$

$$\dot{\beta}_\pm - \frac{2Nk}{3(8\pi)^2} e^{-3\alpha} p_\pm = 0 \rightarrow p_\pm = \frac{6(4\pi)^2}{Nk} e^{3\alpha} \dot{\beta}_\pm \tag{1.134}$$

Naturally, the variation of the action with respect to the lapse function heads to the superHamiltonian constraint

$$\mathcal{H}^s_{BIX} = -p_\alpha^2 + p_+^2 + p_-^2 + \frac{3(4\pi)^4}{k^2} e^{4\alpha} V(\beta_\pm) = 0 \tag{1.135}$$

As soon as we perform an ADM reduction of the dynamics, as prescribed in the Section 1.2.1, with respect to the conjugate momenta p_α, the Bianchi IX reduced Hamiltonian is obtained:

$$-p_\alpha = \mathcal{H}_{ADM} \equiv \sqrt{p_+^2 + p_-^2 + \frac{3(4\pi)^4}{k^2} e^{4\alpha} V(\beta_\pm)}. \tag{1.136}$$

The reduction procedure is complete after the imposition of a particular temporal gauge[7] or in other choosing a particular value for the lapse function N. In this case, the choice is for the temporal gauge $\dot{\alpha} = 1$ that, due to the relation (1.133), says that N_{ADM} is

$$N_{ADM} = -\frac{6(4\pi)^2}{kp_\alpha} e^{3\alpha} = \frac{6(4\pi)^2}{k\mathcal{H}_{ADM}} e^{3\alpha} \tag{1.137}$$

Therefore, looking at the reduced Hamiltonian (1.136), we have all the elements to assert that the Bianchi IX evolution resembles the dynamics a two-dimensional particle, that moves in the $\{\beta_+, \beta_-\}$ plane under the effect of a α-time-dependent potential. In Fig.1.5 are shown the equipotential lines for the potential term at different α times. To evaluate the particle velocity in the anisotropies plane, the reduced Hamiltonian equations can be used:

$$\beta'_\pm = \frac{d\beta_\pm}{d\alpha} = \frac{\partial \mathcal{H}_{ADM}}{\partial p_\pm} = \frac{p_\pm}{\mathcal{H}_{ADM}}, \tag{1.138}$$

$$p'_\pm = \frac{dp_\pm}{d\alpha} = -\frac{\partial \mathcal{H}_{ADM}}{\partial \beta_\pm} = \frac{3(4\pi)^4}{2k\mathcal{H}_{ADM}} e^{4\alpha} \frac{\partial V(\beta_\pm)}{\partial \beta_\pm}, \tag{1.139}$$

to evaluate the *anisotropy velocity* β':

$$\beta' = \sqrt{\left(\frac{d\beta_+}{d\alpha}\right)^2 + \left(\frac{d\beta_-}{d\alpha}\right)^2}. \tag{1.140}$$

The system (1.136) just introduced do not admit an analytic integration. Anyway, some peculiar features can be extracted considering the neighbourhood to the singularity $\alpha \to -\infty$. The Hamiltonian equations allow to rewrite the reduced Hamiltonian in a very interesting form

$$1 = \frac{p_+^2}{\mathcal{H}_{ADM}^2} + \frac{p_-^2}{\mathcal{H}_{ADM}^2} + \frac{3(4\pi)^4}{k^2} \mathcal{H}_{ADM}^{-2} e^{4\alpha} V(\beta_\pm) \tag{1.141}$$

Furthermore, the time variation of the quantity $\ln \mathcal{H}_{ADM}^2$ gives us that

$$\frac{d \ln \mathcal{H}_{ADM}^2}{d\alpha} = 4\left(\frac{3(4\pi)^4}{k^2} \mathcal{H}_{ADM}^{-2} e^{4\alpha} V(\beta_\pm)\right) = 4(1 - \beta'^2), \tag{1.142}$$

that implies, as a first approximation in the limit $\alpha \to -\infty$, the unitarity of the anisotropy velocity (1.140) and the conservation law

$$\frac{d \ln \mathcal{H}_{ADM}^2}{d\alpha} = 0 \to \ln \mathcal{H}_{ADM}^2 = cost \to \mathcal{H}_{ADM} = cost, \tag{1.143}$$

being the potential term negligible. The regime just founded correspond to a reduced problem with Hamiltonian

$$\mathcal{H}_{ADM} = \sqrt{p_+^2 + p_-^2} \tag{1.144}$$

and equations of motion

$$\beta'_\pm = \frac{p_\pm}{\mathcal{H}_{ADM}} = \frac{p_\pm}{\sqrt{p_+^2 + p_-^2}} \tag{1.145}$$

$$p'_\pm = 0 \to p_\pm = cost \tag{1.146}$$

[7] With reference to the Section 1.2.1 means to choose the quantity $\partial_t Q^a$

The latter solution is nothing else that the Hamiltonian formulation of the Kasner solution for the Bianchi I model. In this picture the anisotropic Bianchi I model resembles the dynamics of a two-dimensional free particle with fixed anisotropy velocity determined by the condition $\beta'^2 = 1$. However, a closer inspection reveals an important periodical attitude. As shown in the Fig.1.5 the possibility to neglect the potential is guaranteed just when we are far from the wall, namely near the center of the triangle. When the particle approaches one of the three equivalent sides, the well rises steeply and the effects of the potential must be take into account. If we choose the vertical line of the Figure to analyze this effects, the asymptotic form for the potential (1.131) is

$$V \simeq \frac{1}{3} e^{-8\beta_+} \quad , \quad \beta_+ \to -\infty, \tag{1.147}$$

which is valid for $|\beta_-| < -\sqrt{3}\beta_+$.

When $\alpha \to -\infty$ the term $\frac{3(4\pi)^4}{k^2}\mathcal{H}_{ADM}^{-2} e^{4\alpha} V(\beta_\pm)$ is important in the dynamics just if $V >> 1$ and this is reason why the form 1.147 has been chosen. This condition allows to determine the motion of the potential walls, indeed:

$$\mathcal{H}_{ADM}^{-2} e^{4\alpha} V(\beta_\pm) \simeq 1 \to \beta_+ \simeq \beta_{wall} = \frac{1}{2}\alpha - \frac{1}{8}\ln\left(\frac{k^2}{3(4\pi)^4}\mathcal{H}_{ADM}^2\right) \tag{1.148}$$

where β_{wall} is the position of the wall. The relation (1.148) reveals that, going towards the singularity ($\alpha \to -\infty$), the potential wall moves away from the origin with velocity $|\beta'_{wall}| = \frac{1}{2}$. Being the velocity of the particle far from the wall always equal to unity, it is evident that the particle moves in any moment twice as fast than the walls. So, in a finite interval of time reaches the wall, bounces against the wall and starts for a new free particle regime. After each bounce the particle relative velocity between the particle and the wall is always the same and this imply that the sequence of bounces go ahead without interruption towards the singularity. The single bounce regime just described corresponds to the Hamiltonian formulation of the Bianchi II solution described in the Section 1.5.2 with an associated reduced Hamiltonian

$$\mathcal{H}_{ADM} = \sqrt{p_+^2 + p_-^2 + \frac{(4\pi)^4}{k^2} e^{4\alpha - 8\beta_+}}, \tag{1.149}$$

and Hamiltonian equations

$$\begin{aligned} \beta'_\pm &= \frac{p_\pm}{\mathcal{H}_{ADM}^{II}} \\ \mathcal{H}'_{ADM} &= -2\frac{3(4\pi)^4}{k^2 \mathcal{H}_{ADM}} \exp^{4\alpha - 8\beta_+} \\ p'_+ &= 4\frac{3(4\pi)^4}{k^2 \mathcal{H}_{ADM}} \exp^{4\alpha - 8\beta_+} \\ p'_- &= 0 \longrightarrow p_- = C^-. \end{aligned} \tag{1.150}$$

The system (1.150) can be studied in order to identified two constants of motion

$$\begin{aligned} p_- &= cost, \\ K &= \frac{1}{2}p_+ + \mathcal{H}_{ADM} = cost. \end{aligned} \tag{1.151}$$

The previous constants quantity can be redefined in terms of the ingoing and outgoing velocity. Indeed, by the introduction of incidence and reflection angles θ_i and θ_f, the following parametrization is formulated

$$\begin{aligned}(\beta'_-)_i &= \sin\theta_i,\\ (\beta'_+)_i &= -\cos\theta_i,\\ (\beta'_-)_f &= \sin\theta_f,\\ (\beta'_+)_f &= \cos\theta_f.\end{aligned} \tag{1.152}$$

Putting together the relations (1.151) expressed in terms of the latter parametrization allow to write, remembering that $\beta'_\pm = \frac{p_\pm}{\mathcal{H}_{ADM}}$, an equivalent version of the BKL map (1.101) in terms of a reflection law:

$$\sin\theta_f - \sin\theta_i = \frac{1}{2}\sin(\theta_i + \theta_f) \tag{1.153}$$

The single bounce dynamics can be used to individuate a conservation law valid approaching the singularity. In particular, following the convenience choice used by C.W. Misner in [75], and taking advantage of the geometric properties of this scheme, in the limit close to the singularity ($\alpha \to -\infty$) one finds a conservation law of the form

$$< \mathcal{H}_{ADM}\alpha >= cost. \tag{1.154}$$

Therefore, given two successive bounces (the i-th and the $(i+1)$-th of the sequence) in which α^i expresses the time at which the i-th bounce occurs and $\mathcal{H}^i_{ADM}$ the value of reduced Hamiltonian (1.136) just before the i-th bounce, the relation (1.154) states that

$$\mathcal{H}^i_{ADM}\alpha^i = \mathcal{H}^{i+1}_{ADM}\alpha^{i+1}. \tag{1.155}$$

In other words, the quantity $\mathcal{H}_{ADM}\alpha$ acquires the same constant value as just before each bounce towards the singularity. To resume what founded in this Section, we can conclude that the dynamics of the vacuum Bianchi IX model, also called *Mixmaster model*, consists in a series of successive bounces against the wall, each of which correspond to an exchange in the contracting and expanding directions of the Bianchi II model and it is governed by the reflection law (1.153), alternated by a sequence of free particle regimes with anisotropy velocity $\beta' = 1$. The fixed relative velocity between the particle and the walls implies that bounces go ahead until the singularity is reached. To conclude, the oscillatory regime founded in the Section 1.5.3 is mapped in the never ending bounces of the particle-Universe against the potential walls.

1.6.2 The Mixmaster model in the presence of a Scalar Field

In the previous Section we demonstrate, in the context of the Misner variables, that the main feature of the Mixmaster model, the oscillatory behavior, is equivalent to consider the never-ending bouncing of the particle agianst the potential walls until the singularity. In this Section we show how the oscillations can be suppressed considering the presence of a scalar field[11].

The dynamics of the Mixmaster model is modified by the presence of a scalar field taking into account, in the total Lagrangian density, an adding Lagrangian term of this kind[79]

$$\mathcal{L}_\phi = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi + U(\phi) \tag{1.156}$$

where ϕ is the variable that obey the Klein-Gordon $\partial_\mu\partial^\mu\phi = \Box\phi = \frac{\partial U(\phi)}{\partial\phi}$ and $U(\phi)$ is the selfinteracting potential. For the analysis of the chaotic behavior towards the singularity, we can make the hypotheses to neglect the potential of the scalar field respect to the other terms in the Action. Such a requirement is verified if, in the limit $\alpha \to -\infty$, the potential $U(\phi)$ grows not so much with respect to the scalar curvature potential. Furthermore, we demand that the scalar field is a time-function only. Under this hypothesis the part of the Action related to the scalar field becomes

$$S_\phi = \int \mathcal{L}_\phi dt = \int \frac{1}{2}\dot{\phi}^2 dt = \int (p_\phi \dot{\phi} - N\mathcal{H}_\phi)dt, \tag{1.157}$$

where in the last step the Legendre transformation has been used. The conjugate momenta to the scalar field p_ϕ can be easily evaluated as

$$p_\phi = \frac{\partial \mathcal{L}_\phi}{\partial \dot{\phi}} = \dot{\phi} \tag{1.158}$$

and from the (1.157) we obtain

$$N\mathcal{H}_\phi = \frac{1}{2}p_\phi^2 \tag{1.159}$$

We are now able to write the action of the Mixmaster model in the presence of a scalar field. Remembering the Eq.(1.129), the entire action gets

$$S = S_{BIX} + S_\phi = \int \left[p_\alpha \dot{\alpha} + p_+ \dot{\beta}_+ + p_- \dot{\beta}_- + p_\phi \dot{\phi} - N(\mathcal{H}_{BIX} + \mathcal{H}_\phi)\right] dt. \tag{1.160}$$

without loss of generality, we decide to rescale the conjugate momenta p_ϕ in this manner

$$p_\phi^2 \to \frac{2k}{3(8\pi)^2}p_\phi^2, \tag{1.161}$$

and we choose the temporal gauge (1.137). As always, the dynamics is contained in the superHamiltonian constraint, which for this model in the Misner variables takes the form

$$-p_\alpha^2 + p_+^2 + p_-^2 + p_\phi^2 + \frac{3(4\pi)^4}{k^2}e^{4\alpha}V(\beta_\pm) = 0 \tag{1.162}$$

Following the Misner prescriptions, the realization of the ADM reduction of the dynamics pass to the consideration of α as the time variable, and this leads to the reduced Hamiltonian

$$-p_\alpha = \mathcal{H}_{red} = \sqrt{p_+^2 + p_-^2 + p_\phi^2 + \frac{3(4\pi)^4}{k^2}e^{4\alpha}V(\beta_\pm)} \tag{1.163}$$

As we seen in the Section 1.6.1, far from the potential walls the dynamics reduces to the motion of a free particle, whose trajectories can be studied through the Hamiltonian equations in the case of absence of potential term. For the case in presence of a scalar field those are

$$\begin{cases} \beta'_\pm = \frac{\partial \mathcal{H}^0_{red}}{\partial p_\pm} = \frac{p_\pm}{\mathcal{H}^0_{red}} = \pi_\pm \\ \phi' = \frac{\partial \mathcal{H}^0_{red}}{\partial p_\phi} = \frac{p_\phi}{\mathcal{H}^0_{red}} = \pi_\phi \end{cases} \to \begin{cases} \beta_\pm = \pi_\pm|\alpha| + \beta^0_\pm \\ \phi_\pm = \pi_\phi|\alpha| + \phi^0 \end{cases} \tag{1.164}$$

where the quantity π_+, π_-, π_ϕ are constants. The reduced Hamiltonian that appears in the Eq.(1.164) explicitly reads as

$$\mathcal{H}^0_{red} = \sqrt{p_+^2 + p_-^2 + p_\phi^2} \tag{1.165}$$

Squaring both the sides of the scalar constraint (1.163), it can be written as

$$\pi_+^2 + \pi_-^2 + \pi_\phi^2 = 1 \tag{1.166}$$

In order to analyse the modification induced by the scalar field, it is necessary to reconsider the curvature potential term with respect to the new constants π_+, π_-. Let us begin considering the case without the scalar field $\pi_\phi = 0$. The superHamiltonian constraint reduces to $\pi_+^2 + \pi_-^2 = 1$ and this allow the following parametrization[17]

$$\pi_+ = \cos\theta \quad , \quad \pi_- = \sin\theta. \tag{1.167}$$

Therefore, making use of the Eq.s(1.164), the leading terms of the curvature potential (1.132) assume the form

$$e^{4\alpha}V \simeq e^{4\alpha(1+2\cos\theta)} + e^{4\alpha(1-\cos\theta-\sqrt{3}\sin\theta)} + e^{4\alpha(1-\cos\theta+\sqrt{3}\sin\theta)}. \tag{1.168}$$

In terms of the Eq.(1.168), the instability of the Kasner regime and the subsequent bounces against the walls are expressed by the fact that, for any value of θ, at least one of the three terms at the exponent become negative. This means that, for $\alpha \to \infty$, the potential is not negligible anymore and this moment coincides with the bounce. The situation is drastically different where the scalar field is turned on. Being the associated quantity $\pi_\phi^2 > 0$, the Eq.(1.169) says that

$$\pi_+^2 + \pi_-^2 = 1 - \pi_\phi^2 < 1 \tag{1.169}$$

The presence of the scalar field opens the space of the possible configuration of the system. In particular, the free Kasner regime, identified by the regime in which the scalar curvature potential is negligible, is guarantee if the conditions

$$\begin{cases} 1 + 2\pi_+ > 0, \\ 1 - \pi_+ - \sqrt{3}\pi_- > 0, \\ 1 - \pi_+ + \sqrt{3}\pi_- > 0, \end{cases} \tag{1.170}$$

contemporaneously hold. Such a situation is realized for $\pi_+^2 < 1/2$ and $\pi_-^2 < 1/12$, correspondent to $2/3 < \pi_\phi^2 < 1$. The scalar field influences such dynamics so that for values that satisfying the conditions latter conditions there are not further bounces and the solution approaches a final free Kasner regime. In other words, after a finite number of bounces the point-Universe will never reach the potential walls again. In this sense an appropriate configuration of the scalar field removes the chaotic Mixmaster dynamics toward the classical cosmological singularity.

1.6.3 The Misner-Chitrè Variables

The picture of the Misner variables described in the previous Section is a very efficient contest in which analyze the Mixmaster model. The main reasons are the clear factorization of the metric in isotropic and anisotropic components, the simple geometry that characterize the potential walls (*i.e.* the triangular domain) and the fact that the two dimensional $\{\beta_+, \beta_-\}$ space over which the point-Universe evolves is a zero curvature variety, having an associated Ricci scalar $R = 0$.

However, a very unpleasant feature in the Misner variables is that the living domain for the point-Universe depends on the "time" variable. This peculiarity, although it was clear from the wall velocity (1.148), results evident writing the anisotropy parameters

(1.116) with respect to the Misner variables. The living domain for the point-Universe is therefore obtained as the region in which the three conditions

$$\begin{aligned} Q_1 &= \frac{1}{3} + \frac{\beta_+ + \sqrt{3}\beta_-}{3\alpha} > 0, \\ Q_2 &= \frac{1}{3} + \frac{\beta_+ - \sqrt{3}\beta_-}{3\alpha} > 0, \\ Q_3 &= \frac{1}{3} - \frac{2\beta_+}{3\alpha} > 0, \end{aligned} \tag{1.171}$$

are simultaneously verified. The presence of the time variable α in the conditions (1.171) is the reason why the potential walls are not fixed during the evolution towards the singularity. Despite this is not a problem at a classical level, as we will show in the next Chapter, the quantization of a system with a time-dependent domain will be a challenge when the imposition of a boundary condition for the wave function of the Universe is taken into account.

For this reason let us consider the Misner-Cithrè like variables[32],[56] $\{\tau, \xi, \theta\}$, connected with the Misner variables in the following way:

$$\begin{aligned} \alpha &= -e^{\tau}\xi, \\ \beta_+ &= e^{\tau}\sqrt{\xi^2 - 1}\cos\theta, \\ \beta_- &= e^{\tau}\sqrt{\xi^2 - 1}\sin\theta, \end{aligned} \tag{1.172}$$

where $-\infty < \tau < \infty$ is the new "time" variable, $1 < \xi < \infty$, $0 \leq \theta < 2\pi$. The anisotropy parameters in this set of variables are independent of the time variable τ. Indeed,

$$\begin{aligned} Q_1 &= \frac{1}{3} - \frac{\sqrt{\xi^2 - 1}}{3\xi}\left(\cos\theta + \sqrt{3}\sin\theta\right) > 0, \\ Q_2 &= \frac{1}{3} - \frac{\sqrt{\xi^2 - 1}}{3\xi}\left(\cos\theta - \sqrt{3}\sin\theta\right) > 0, \\ Q_3 &= \frac{1}{3} + 2\frac{\sqrt{\xi^2 - 1}}{3\xi}\cos\theta > 0. \end{aligned} \tag{1.173}$$

The Action (1.129) and the superHamiltonian (1.130) in these new variables read as

$$S_g = \int dt\left(p_\tau\dot{\tau} + p_\xi\dot{\xi} + p_\theta\dot{\theta}_- - N\mathcal{H}_{MC}\right), \tag{1.174}$$

$$\begin{aligned} \mathcal{H}_{MC} = \frac{k}{3(8\pi)^2}e^{-2\tau+3\xi e^{\tau}}\Bigg[-p_\tau^2 + p_\xi^2(\xi^2-1) + \frac{p_\theta^2}{(\xi^2-1)} &+ \\ + \frac{3(4\pi)^4}{k^2}e^{2\tau+4e^{\tau}\xi}V_{IX}(\tau,\xi,\theta)\Bigg], \end{aligned} \tag{1.175}$$

where p_τ,p_ξ and p_θ are the conjugate momenta to the Misner-Cithrè variables $\{\tau, \xi, \theta\}$. As always, the variation of the action with respect the lapse function gives the superHamiltonian constraint $\mathcal{H}_{MC} = 0$.

In this case, the reduction of the dynamics is realized solving the scalar constraint with respect to the conjugate momenta p_τ and this brings to

$$-p_\tau = \mathcal{H}_{ADM} = \sqrt{p_\xi^2(\xi^2-1) + \frac{p_\theta^2}{(\xi^2-1)} + \mathcal{V}e^{2\tau}}, \tag{1.176}$$

with

$$\mathcal{V} = \frac{3(4\pi)^4}{k^2} e^{4e^\tau \xi} V_{IX}(\tau, \xi, \theta). \tag{1.177}$$

The analysis of the potential term $\mathcal{V}$ shows the same infinite potential well behavior as

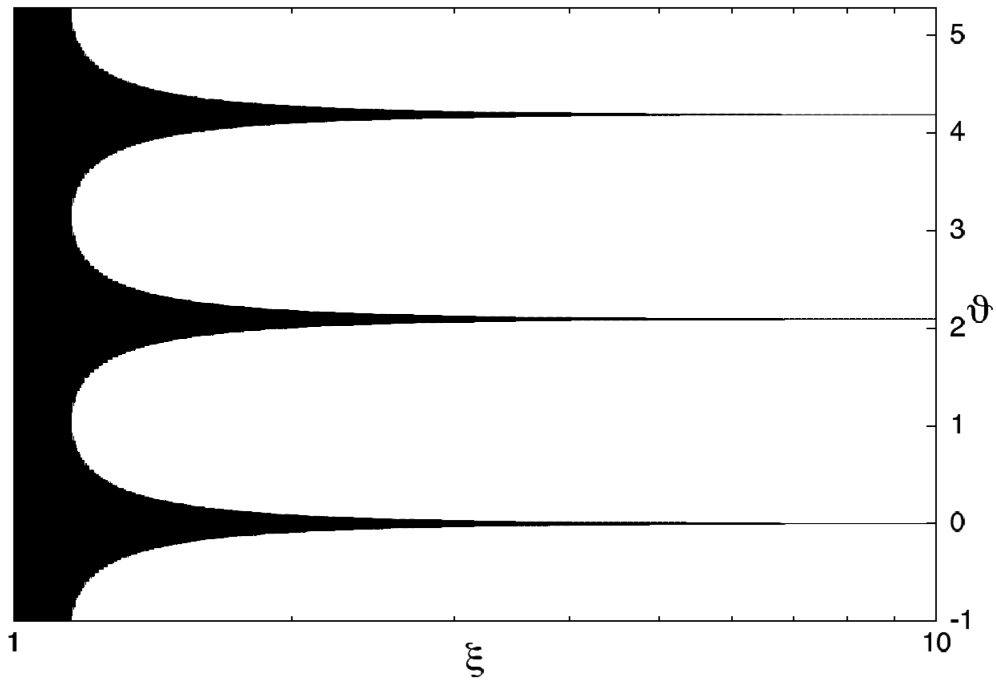

FIGURE 1.6: The region of the configuration space where the conditions (1.173) are fulfilled

in the Misner framework and this allow to assert that the Hamiltonian (1.175) reproduces the dynamics of a two-dimensional particle that moves in the $\{\xi, \theta\}$ plane inside the fixed (respect to the time variable τ) allowed domain defined as the region where the conditions (1.171) are valid at the same time. The portion in the configuration plane within which the potential term is negligible is reported in the Fig. 1.6.
When the particle is far from the wall, the potential term is negligible and the reduced Hamiltonian takes the form

$$-p_\tau = \mathcal{H}_{ADM} = \sqrt{p_\xi^2(\xi^2-1) + \frac{p_\theta^2}{(\xi^2-1)}}. \tag{1.178}$$

In formal analogy with the Eqs. (1.141) and (1.142), it is possible to demonstrate that the reduced Hamiltonian (1.178), that in the zero potential case it is renamed $\mathcal{H}_{ADM} = \epsilon$, becomes asymptotically for $\tau \to \infty$ a constant of motion. Naturally, in the evolution towards the singularity, this condition is valid always with the exception of the instants when the particle bounces against the walls.

The conservation of the quantity ϵ allows to determine the nature of the two dimensional manifold that describes the $\{\xi,\theta\}$-system. By following the standard Jacobi procedure[93] it is achieved a connection between the configuration variables, the conjugate momentas and the elements of the metric associated to the two-dimensional manifold through the relation

$$\dot{q}^a = g^{ab}p^b. \tag{1.179}$$

The time derivatives can be evaluated in terms of the reduced Hamiltonian equations

$$\dot{\xi} = \frac{\partial \mathcal{H}_{ADM}}{\partial p_\xi} = \frac{1}{\epsilon}(\xi^2 - 1)p_\xi \tag{1.180}$$

$$\dot{\theta} = \frac{\partial \mathcal{H}_{ADM}}{\partial p_\theta} = \frac{1}{\epsilon}\frac{p_\theta}{(\xi^2 - 1)} \tag{1.181}$$

Using the Eqs.(1.180) and (1.181) in the Eq.(1.179), the only non-zero elements of the metric are the diagonal elements

$$g^{\xi\xi} = \frac{1}{\epsilon}(\xi^2 - 1) \quad , \quad g^{\theta\theta} = \frac{1}{\epsilon}\frac{1}{(\xi^2 - 1)}. \tag{1.182}$$

that leads to a line element

$$ds^2 = \epsilon^2\left[\frac{d\xi^2}{(\xi^2 - 1)} + (\xi^2 - 1)d\theta^2\right]. \tag{1.183}$$

It is easy to demonstrate that the scalar curvature associated to the latter element line is $R = -\frac{2}{\epsilon^2}$, therefore the metric has negative curvature. Therefore the point-Universe moves over a negatively curved bidimensional space.

1.6.4 The Poincaré Half Plane

An alternative set of variables that holds the propriety to have fixed domain and a simple geometry is represented by the Poincarè variables[61],[88] (u, v), defined with respect to the Misner-Cithrè variables $\{\xi,\theta\}$ as

$$\xi = \frac{1 + u + u^2 + v^2}{\sqrt{3}v}. \tag{1.184}$$

$$\theta = -\arctan\left(\frac{\sqrt{3}(1 + 2u)}{-1 + 2u + 2u^2 + 2v^2}\right), \tag{1.185}$$

with $-\infty < u < \infty$ and $0 < v < \infty$. The $\{u, v\}$ configuration space is called *Poincarè half-plane*. In this picture, the anisotropy parameters conditions (1.173) assume the simple form

$$\begin{aligned} Q_1 &= \frac{-u}{1 + u + u^2 + v^2} > 0, \\ Q_2 &= \frac{1 + u}{1 + u + u^2 + v^2} > 0, \\ Q_3 &= \frac{u(u + 1) + v^2}{1 + u + u^2 + v^2} > 0. \end{aligned} \tag{1.186}$$

As shown in the Fig.(1.7), the conditions (1.186) composed the boundaries of the living domain, precisely two vertical lines in $u = -1$ and $u = 0$ and a semicircle centered in $v =$

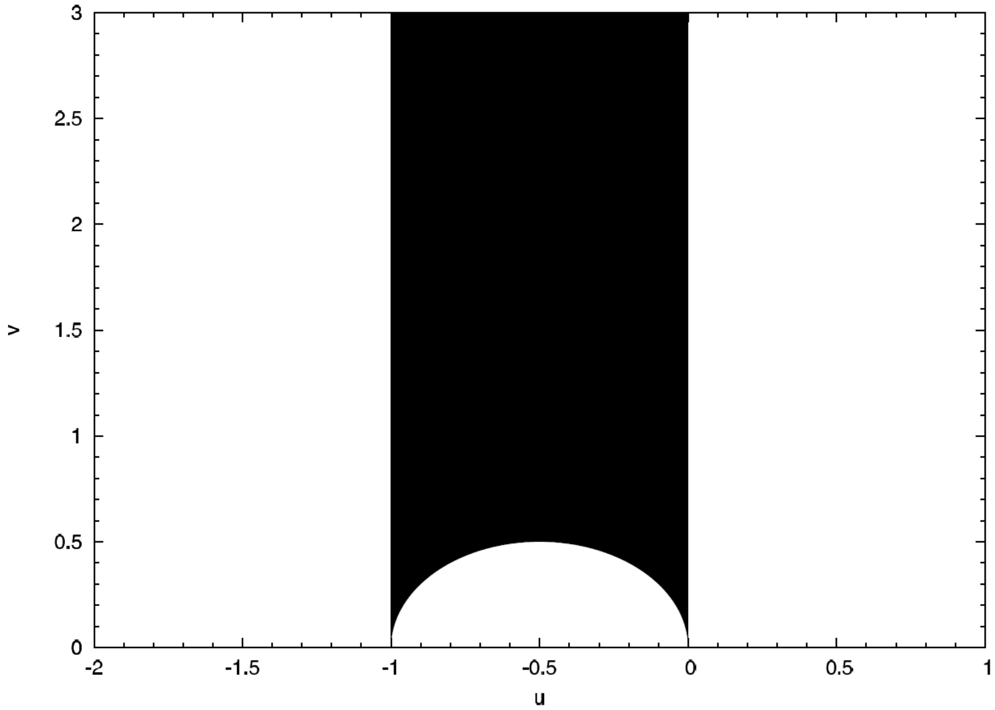

FIGURE 1.7: The region of the configuration space in the Poincare upper half-plane where the conditions (1.186) are fulfilled

0. The time-like variable τ is leaving unchanged in the Poincarè half-plane description. As in the Misner-Cithrè case, the particle Universe moves inside the living domain over a negatively curved space without the effects of the potential term, except for the moments in which the particle bounces against the walls and turn back inside the region.

In this optic, it is interesting to write, for the aims of the next chapters, the very treatable form that the reduced Hamiltonian assume in the case of absence of the potential term. The Hamiltonian (1.178) becomes

$$\mathcal{H}_{ADM} = v\sqrt{p_u^2 + p_v^2}, \tag{1.187}$$

where p_u and p_v are the conjugate momenta to the Poincarè variables$\{u, v\}$.

Chapter 2

Quantum Cosmology

In this Chapter we face the canonical approach to the quantization of the gravitational field. We start deriving the Wheeler-DeWitt equation implementing to an operator the classical superHamiltonian constraint. Such an equation shows the existence of the so called frozen formalism, which suggests the apparent absence of the concept of evolution in quantum gravity. For this reason will be analyzed a couple of mechanism to introduce a notion of time inside the theory. The first one concerns the possibility to individuate a time variable at the classical level before to implement the quantization of a reduced Hamiltonian system. In the second one, instead, we firstly perform the quantization of the whole system and then recognize a physical time at the quantum level. The concept of the minisuperspace allow to simplify the problem transferring the focus from the quantum gravity to the quantum cosmology. In this framework will be illustrated the canonical quantization of the flat FRW model, to the aim to see the presence of the singularity also in the quantum regime. As a possible method to avoid the singularity, will be introduced the basic concepts of the polymer quantum mechanics, an alternative representation of the quantum mechanics whose algebra correspond to the algebra of the Loop Quantum Gravity when a finite number of degree of freedom is considered, *i.e* when the Loop Quantum Cosmology is taken into account. The application of this alternative representation of the quantum mechanics to the cosmological model, which leads to the so called Polymer Quantum Cosmology, will be showed in a couple of interesting case: the Flat FRW model and the Mixmaster model. Finally, the chapter is closed by the illustration a couple of quantization method for cosmological model: the evolutionary quantum approach, correspondent to the category of the "time before quantization" method, that consists in consider an incoherent dust as a physical clock to describe the evolution of the gravitational field and the Vilenkin interpretation of the wave function, belonging to the category "time after quantization" method, which allows to provide a proper definition of probability in quantum cosmology. Finally, will be illustrated

2.1 Wheeler-De Witt Equation

We devote this Section to illustrate the canonical quantization of gravitational field in the metric formalism, also called Quantum Geometrodynamics[33]. As demonstrated in the Hamiltonian formulation Section 1.2, the description of the gravitational field is governed by the dynamics of the system subjected to the constraints (1.20),(1.21). The analysis of this secondary class constraints provides that the evolution of the system is ruled by the superHamiltonian constraint, while the supermomentum constraint established that the configuration space of canonical gravity is the infinite-dimensional space of all the possible three-geometries and it is called *Wheeler Superspace*.

The usually canonical quantization of the gravitational field consists in the quantization of such a constrained system and it is called *Dirac Scheme*. The first step is to implement the classical Poisson brackets for the configuration variables

$$\{h_{\alpha\beta}(x,t), h_{\gamma\delta}(x',t)\} = 0, \tag{2.1}$$

$$\{\Pi^{\alpha\beta}(x,t), \Pi^{\gamma\delta}(x',t)\} = 0, \tag{2.2}$$

$$\{h_{\alpha\beta}(x,t), \Pi^{\gamma\delta}(x',t)\} = \delta^{\gamma}_{(\alpha}\delta^{\delta}_{\beta)}\delta^3(x-x'), \tag{2.3}$$

in the quantum commutation relations

$$[\widehat{h}_{\alpha\beta}(x,t), \widehat{h}_{\gamma\delta}(x',t)\} = 0, \tag{2.4}$$

$$\{\widehat{\Pi}^{\alpha\beta}(x,t), \widehat{\Pi}^{\gamma\delta}(x',t)\} = 0, \tag{2.5}$$

$$\{\widehat{h}_{\alpha\beta}(x,t), \widehat{\Pi}^{\gamma\delta}(x',t)\} = i\delta^{\gamma}_{(\alpha}\delta^{\delta}_{\beta)}\delta^3(x-x'). \tag{2.6}$$

The objects $\{\widehat{h}_{\alpha\beta}, \widehat{\Pi}^{\alpha\beta}\}$ are the correspondent quantum operators to the classical configuration variables. The widely used representation for the quantum operators concerns the association of multiplicative operators for "position" variables and differential operators for "momenta" variables. Given the entire set of space variables, this corresponds to

$$N \to \widehat{N} \quad , \quad N_i \to \widehat{N_i} \quad , \quad h_{ij} \to \widehat{h_{ij}} \tag{2.7}$$

$$\Pi \to \widehat{\Pi} = -i\frac{\delta}{\delta N} \quad , \quad \Pi^i \to -\widehat{\Pi^i} = -i\frac{\delta}{\delta N_i} \quad , \quad \Pi^{ij} \to \widehat{\Pi^{ij}} = -i\frac{\delta}{\delta h_{ij}} \tag{2.8}$$

Then, it is necessary to impose that the quantum physical states are the only ones annihilated by the quantum version of the classical constraints. To be consistent, given a functional of state $\Psi(N, N_i, h_{ij})$, called the *wave function of the Universe*, the quantum counterparts of the primary constraints (1.13),(1.14) select the physical states such that

$$\widehat{\Pi}\Psi = -i\frac{\delta\Psi}{\delta N} = 0 \qquad \widehat{\Pi^i}\Psi = -i\frac{\delta\Psi}{\delta N_i} = 0 \tag{2.9}$$

Such a relations imply the wave function of the Universe does not depend on (N, N_i), or in other words it does not depends on the particular classical foliation realized but becomes a functional of the three-metric only $\Psi(h_{ij})$. Let us now consider the secondary constraints, starting from the supermomentum constraint. Substituting the quantum differential operators (2.8) in the Eq.(1.20), we obtain

$$\widehat{\mathcal{H}^i}\Psi = 2i\nabla_j\frac{\delta\Psi}{\delta h_{ij}} = 0 \tag{2.10}$$

The latter relation implies that the wave function of the Universe does not depend on the particular metric used to represent the geometry; it is therefore defined on the whole class of the three-geometries and, how it is possible to show considering an infinitesimal spatial transformation, it is invariant under spatial diffeomorphisms. This condition is expressed by the dependence

$$\Psi = \Psi(\{h_{ij}\}). \tag{2.11}$$

At the end, the obtained space of configuration over which the canonical quantum gravity exists is exactly the Wheeler superspace mentioned at the beginning of this Section.

The last constraint to consider is the superHamiltonian one, that generate all the dynamical information about the system. Let us promote configuration variables to quantum operators and require that the quantum counterpart of the superHamiltonian annihilates the physical states. This brings to the formulation of the famous *Wheeler-DeWitt* *equation*(WDW), which explicitly reads as

$$\widehat{\mathcal{H}}\Psi = \mathcal{G}_{ijkl}\frac{\delta^2\Psi}{\delta h_{ij}\delta h_{kl}} - \frac{\sqrt{h}}{2k}\overline{R}\Psi = 0. \tag{2.12}$$

The WDW equation is a second order differential equation defined on the configuration space and not on the physical space-time. The disappear of the space-time description at the quantum level can be viewed as the analog of the absence of the classical particle trajectory when the quantum mechanics is implemented. At first sight emerge the factor-order ambiguity that affects the WDW equation and in the Eq.(2.12), although not exists a real prescription order, we choose the simplest possible factor ordering that is the one with all the operators $\widehat{\Pi}^{ij}$ next to the supermetric term $\mathcal{G}_{ijkl}$.

2.2 The Problem of Time

After the selection of the physical state via the imposition of the primary and secondary constraints on the wave function of the Universe, we are able to say something about the dynamics of the system. First of all, from the classical form of the action (1.15), we can define the Hamiltonian of the system as

$$\mathbf{H} \equiv \int_\Sigma d^3x(\lambda\Pi + \lambda^i\Pi_i + N^i\mathcal{H}_i + N\mathcal{H}). \tag{2.13}$$

Considering the action of the primary and secondary constraints operators, the quantum counterpart of the Hamiltonian $\widehat{\mathbf{H}}$ have to annihilates the physical states. This brings to a Schrödinger-like euqation such as

$$i\frac{\partial\Psi}{\partial t} = \widehat{\mathbf{H}}\Psi = 0. \tag{2.14}$$

The functional of state Ψ results independent of time and apparently there is not a quantum evolution. This is the so-called *frozen formalism* ans seems to suggest that the gravitational field does not evolves from a quantum point of view. This is the reason why such an issue is also identified as the *problem of time*[57].

The main motivation that gives rise to this problem is the intrinsic nature of the two theory, quantum mechanics and general relativity. Indeed, in quantum mechanics the evolution is described with respect to a parameter, the time, which is an external fixed one, and the events occur with respect on it.In Quantum Field Theory (QFT) the situation is formally the same, due to the fact the the events take place with respect to a fixed background metric, the Minkowski one. Instead, in General Relativity the key aspect is the fact that the object to study is the metric evolution itself, with no background metric as a reference. Any kind of selection of "time" parameter to describe the evolution involve something that belongs to the metric itself.

The absence of a clear notion of time leads countless inconveniences. In fact, the standard Copenhagen interpretation and the QFT become meaningless without it. Furthermore, concepts like probability and measurement need to be redefined in a physics without a proper time description.

Anyway, some techniques to face with the problem of time and to introduce some kind of evolution exist. Here we illustrate the key steps of two important approaches to introduce a time evolution: the *time before quantization approach* and the *time after quantization approach*.

2.2.1 Time before quantization

This type of approach can be resumed essentially in three schematic steps:

- The identification of a time coordinate Q_A at the classical level.
- The explicit individuation of P_A, the conjugate momenta to the time variable, in the superHamiltonian and then the resolution of the scalar constraint

$$P_A + h_A = 0, \tag{2.15}$$

  where h_A is the physical reduced Hamiltonian which evolution is described with respect to the time variable Q_A.
- Finally, performing a canonical quantization of the expression (2.15), arrive to a Schrödinger-like equation

$$i\frac{d\Psi}{dQ_A} = \widehat{h}_A\Psi. \tag{2.16}$$

The notion of "time" is therefore implemented before the quantization procedure and there are typically two kind of possible formulations.

The first one concerns the selection of a time variable from the gravitational configura-tion space. In this way the constraints are solved classically and the subsequent quantiza-tion leads to the Schrödinger-like equation (2.16). This is called *internal time approach* and essentially it consists in the quantum implementation of the reduced ADM Hamiltonian illustrated in Section 1.2.1.

The second method regards the possibility to consider the presence of an external matter fields and to describe the evolution of the gravitational field using them as *matter clocks*. This procedure was firstly introduce by Kuckar and Torre in this paper[64]. As we will see in details in a next Chapter, this method takes into account an incoherent dust fluid contribution with respect to which the realization of a proper clock for the quantum system is possible.

Despite Both the method provides an evolutionary quantum dynamics for the grav-itational field, they are basically different. In fact, in the internal time approach, only a part of the configuration space is quantizied while the selected time variable is treats as a classical part. The case of the presence of external matter field, instead, is based on the full quantization of the configuration space. In the following chapters we will show how this difference is crucial in the cosmological context.

2.2.2 Time after quantization

This approach replies the logical path that leads to the WDW equation and to the frozen formalism previously introduced. A conceptual time recovering is possible also in this framework.

The first attempt consists to observe the similarity between the WDW equation (2.12) and the Klein-Gordon equation in curved space-time, witch explicitly reads as

$$g^{ij}\nabla_i\nabla_j\phi + m^2\phi = 0 \tag{2.17}$$

A formal analogy can be seen considering the potential term of the WDW equation as a varying mass term of a KG equation. Starting from this analogy, the Hilbert space for a quantum gravity theory can be built from the Klein-Gordon-like inner product, selecting the positive frequency in order to deal with a well-defined probability, as happen in the KG theory. The real difference is due to the fact that the potential term of the WDW equation can assume positive and negative values, differently from the mass term of the KG equation m^2 which is always a positive quantity. This aspect, nevertheless having chosen the positive frequency, brings to the impossibility to declare the positivity of the inner product.

The second chance to recover a time notion after the quantization is based on the *semiclassical interpretation*. The main idea of this approach, mainly introduced in the originally Vilenkin's work [92] and that will be analyze in detail in the following sections, is that time does not exist at fundamental level but emerges as an approximate feature only under some suitable conditions. This concept means in practice that the wave functional is expanded in a Wentzel-Kramers-Brillouin(WKB)-like form from which a time variable is extracted. The main advantages of this method is the definition of a genuine probabilistic interpretation and an automatic appearance of a Schrodinger-like equation without imposing some classical a-priori selection. As a final remark, anyway, the choice of a particular state for the wave function of the Universe with respect to another one and the real description of the system when the pure Planck regime is approached remain as two of the major issues.

2.3 The Concept of Minisuperspace

The Quantum Cosmology aims to apply the laws of the quantum mechanics for the description of the entire Universe. Being the Universe the macroscopical object for excellence, the attempt to describe it in a quantum context seems to be in contrast with the fact that the quantum effects are relevant only at microscopiscal scales. However, the existence of a regime in which the whole Universe is similar to a quantum object cannot be excluded. For example in proximity of the initial singularity the energy and the dimension of the Universe suggest such a behavior as expected.

The real difficult is to establish a connection between Quantum Gravity and Quantum Cosmology even if at first sight there is not. Indeed, the quantum gravity is the quantum description of a just one of the field that characterize the Universe and in this aspect is not different from the other fields (like the electromagnetic one). What suggests that the quantum cosmology should be a derivation of the quantum gravity is the dominant behavior at large scales of the latter one. In this sense, the Quantum Cosmology stands as the natural laboratory to test the validity of the Quantum Gravity.

Let us see, from a practical perspective, what means to apply the quantum framework introduced in the previous sections to the cosmological models. As shown in the Section 2.1, the canonical quantization method brings to consider the work space as the infinite dimensional space of all the possible three-geometries, also known as the Wheeler Superspace. Effectively, the presence of infinite number of degree of freedom make the problem intractable and the only way out is the restriction of the analysis to a finite dimensional subspace through the imposition of particular symmetries. The resulting finite dimensional subspace obtained after the freezing of some degree of freedom is called *minisuperspace*. The symmetries to be imposed to select a particular minisuperspace model are nothing else that the homogeneity (and isotropy) that characterize the cosmological models. This procedure greatly simplifies the quantum evolution of the system; first of all the supermomentum constraint is automatically satisfied (it simply represent the quantum preservation of the diffeomorphism invariance) and then the WDW equation becomes a single equation that lives in the configuration space but that is valid for any spatial point. Despite there is no clear evidence that the reduction at the minisuperspace is a genuine process, the quantum implementation of such a models should put lights to some crucial questions that arise at the classical level, mostly for the description of the Universe towards the initial singularity.

Let us consider now a generic n-dimensional minisuperspace model that contains as a special cases the FRW models and the Bianchi models. Such a homogeneous system is characterizes by a zero shift vector $N^i = 0$, a space independent lapse function $N = N(t)$ and a line element as

$$ds^2 = N^2(t)dt^2 - h_{\alpha\beta}(x,t)dx^\alpha dx^\beta. \tag{2.18}$$

The three-metric $h_{\alpha\beta}$ depends on a finite number of coordinates q^A, differently from the non-minisuperspace case in which the three metric has an infinite dimensional degree of freedom dependence. The vacuum Eisntein-Hilbert action in this minisuperspace system is given by

$$S = \int dt[p_A\dot{q}^A - N(\mathcal{G}^{AB}p_Ap_B + U(q)], \tag{2.19}$$

where p_A is the conjugate momenta to the variable q_A, $\mathcal{G}^{AB}$ is the minisupermetric and $U(q)$ is the potential term. The scheme provides here is nothing else that a generalization that contains the FRW models and Bianchi models cases illustrated in Chapters 1 as particular cases. The variation of the action (2.19) with respect of the lapse function gives the superHamiltonian constraint

$$\mathcal{H} = \mathcal{G}^{AB}p_Ap_B + U(q) = 0. \tag{2.20}$$

In the same way of three-metric $h_{\alpha\beta}$, the minisupermetric is the finite degree of freedom reduced version of the entire super metric $\mathcal{G}^{\alpha\beta\gamma\delta}$.

The reduction to the minisuperspace, at the classical level, leads to a system formally equivalent to the motion of a particle moving in a n-dimensional curved space time, determined by the minisupermetric $\mathcal{G}^{AB}$, under the action of the potential $U(q)$.

The application of the canonical quantization procedure on this models leads to the WDW equation

$$\widehat{\mathcal{H}}\Psi = (-\nabla^2 + U)\Psi = 0, \tag{2.21}$$

where the symbol ∇_A denotes the covariant derivative constructed from the minisupermetric and the laplacian ∇^2 is defined as

$$\nabla^2 = \nabla_A\nabla^A = \frac{1}{\sqrt{\mathcal{G}}}\partial_A(\sqrt{\mathcal{G}}\mathcal{G}^{AB}\partial_B), \tag{2.22}$$

where $\mathcal{G} = |det\mathcal{G}_{AB}|$.

2.4 Quantization of the flat FRW model

In this Section we discuss about the simplest application of the canonical quantization to the cosmological models: the WDW framework of the flat FRW Universe filled with a massless scalar field. The line element of the FRW models is write in the Hamiltonian formulation in the Eq.(1.52) and the variables $\{a, p_a\}$ represent the tw-dimensional phase-space of the model. The superHamiltonian (1.57), referred to a generic form of matter, in the particular case of the scalar field, for which the relation $\rho = \frac{\phi^2}{a^6}$ holds, assumes the form

$$\mathcal{H}_{FRW\phi} = -\frac{k}{24\pi^2}\frac{p_a^2}{a} + 2\pi^2\frac{p_\phi^2}{a^3} = 0, \tag{2.23}$$

where we choose the case $K = 0$ of the FRW classification.

The presence of the classical singularity can be shown simply inserting the Hamiltonian equation $\dot{a} = \frac{\partial \mathcal{H}}{\partial p_a} = -\frac{k}{12\pi^2}\frac{p_a}{a}$ in the scalar constraint. This brings to the following differential equation for the scale factor:

$$\dot{a} = \pm\sqrt{\frac{k}{3}\frac{p_\phi}{a^2}}, \tag{2.24}$$

whose solution is

$$a(t) = \left(\sqrt{3k}p_\phi t\right)^{\frac{1}{3}}. \tag{2.25}$$

The latter relation is sketched in the Fig. 2.1. From the figure is evident the singular

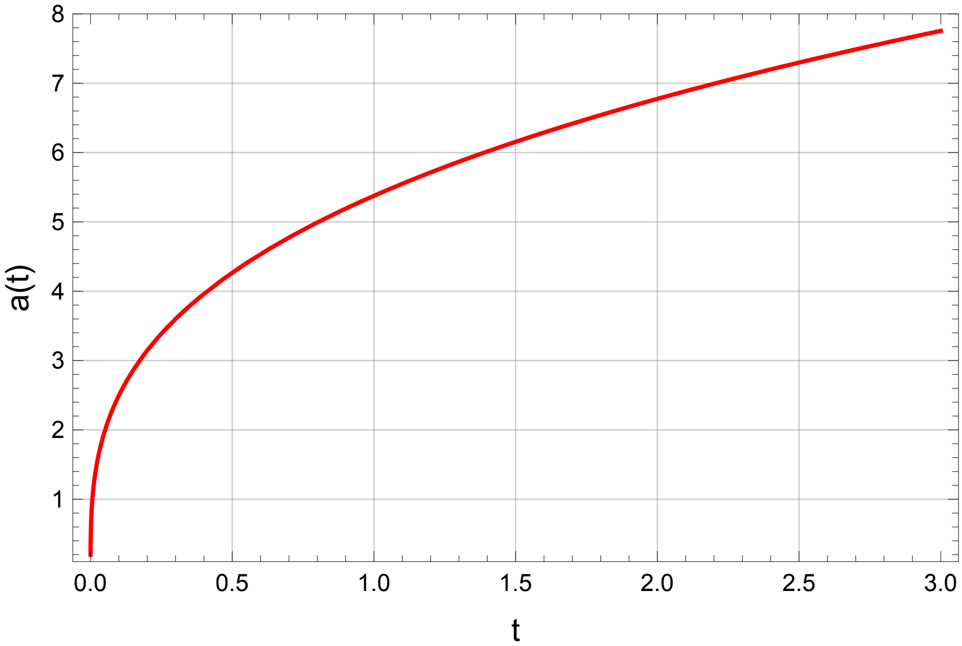

FIGURE 2.1: The singular behavior of the scale factor approaching the limit $t \to 0$, as highlighted from the presence of the value $a = 0$.

behavior for the scale factor in correspondence of the value $t = 0$. In the extraction of the solution we have chosen the plus sign of the solution in order to deal an expanding Universe and impose the integration constant equal to zero to fix the big bang singularity exactly in $t = 0$.

The same singular classical behavior can be highlighted using the scalar field as a relational time. Solving the scalar constraint (2.23) with respect to p_ϕ, the reduced Hamiltonian is obtained

$$-p_\phi = \mathcal{H}_{red} = \frac{k}{3(4\pi^2)^2} a p_a. \tag{2.26}$$

Therefore, the evolution of the scale factor with respect to the scalar field relational time is governed by the Hamiltonian equation

$$a' = \frac{\partial a}{\partial \phi} = \frac{\partial \mathcal{H}_{red}}{\partial p_a} = \frac{k}{3(4\pi^2)^2} a. \tag{2.27}$$

Solving the previous differential equation leads to the following behavior for the scale factor

$$a(\phi) = a_0 e^{\frac{k}{3(4\pi^2)^2}(\phi-\phi_0)}. \tag{2.28}$$

The classical initial singularity is always present and is reached in correspondence of the value $\phi = -\infty$.

Let us now performing a canonical quantization of such a system. This consists in the association of the differential operators to the conjugate momentas in the following manner

$$\widehat{p}_a \to -i\partial_a \quad , \quad \widehat{p}_\phi \to -i\partial_\phi, \tag{2.29}$$

and to the application of the quantum operator associated to superHamiltonian constraint (2.23) to the wave function of the Universe $\psi(a,\phi)$, *i.e.* the WDW equation:

$$\left(\partial_\phi^2 - \frac{k}{48\pi^4}a^2\partial_a^2\right)\psi(a,\phi) = 0. \tag{2.30}$$

The absence of a potential term for the scalar field allow to argue the shape for the wave function as $\psi(a,\phi) = e^{i\omega\phi}\varphi_\omega(a)$ and from this it is possible to reduce the WDW equation to an eigenvalue problem for the scale factor part of the wave function:

$$\left(\omega^2 + \frac{k}{48\pi^4}a^2\partial_a^2\right)\varphi(a) = 0. \tag{2.31}$$

The solution for this equation is

$$\varphi(a) = C_+ a^{\frac{1}{2}+\sqrt{\frac{1}{4}-\frac{48\pi^4\omega 2}{k}}} + C_- a^{-\frac{1}{2}+\sqrt{\frac{1}{4}-\frac{48\pi^4\omega 2}{k}}}. \tag{2.32}$$

The entire wave function $\psi(a,\phi)$, in the limit $a \to 0$ towards the singularity exhibits a diverging behavior.

Furthermore, from the analytic solution of the $\psi(a,\phi)$ it is possible to build the wave packet peaked at late times around particular classical initial values and analyze its dynamics towards the singularity. Choosing $B(\omega)$ as a Gaussian weight packet, a superposition of the just obtained eigenfunctions can be realized as

$$\Psi_\omega(a,\phi) = \int d\omega B(\omega)e^{i\omega\phi}\varphi_\omega(a) \tag{2.33}$$

Accomplishing a numerical integration for the wave packet evolution, a localized wave packet around the classical trajectory is always obtained. In particular, selecting an initial state peaked around the classical late times Universe (roughly speaking the actual observed Universe), the most probable state during the evolution, *i.e.* the position of the maximum of the wave packet, remains always peaked around the classical trajectory until the fall in the initial singularity. This undoubtedly indicates that the classical singularity is not solved by the WDW formalism.

2.5 Polymer Quantum Cosmology

The conclusions about the standard WDW approach of the flat FRW model filled with a scalar field of the previous section clearly demonstrate the main failure of the canonical quantization: the non-avoidance of the initial singularity at the quantum level. Such a pathology addresses us to consider different paths to implement a quantum prescription. A very promising way out is expressed in the application to the cosmological models of the Polymer Quantum Mechanics.

The Polymer representation of quantum mechanics is a non-equivalent representation of the usual Schrödinger quantum mechanics, based on a different kind of Canonical

Commutation Rules (CCR). From a physical point of view this kind of representation allows the description of the quantum system in presence of a cutoff. This scheme is central when dealing the properties of a background-independent canonical quantum theory of gravity as for example the algebra used in Loop Quantum Gravity (LQG). In particular, when a system with a finite number of degrees of freedom is considered, the holonomy-flux algebra of the LQG reduces to a polymer-like algebra, also called Loop Quantum Cosmology (LQC). This theory can be regarded as the implementation of this quantization technique in the minisuperspace dynamics. The last consideration is the quantum-field point of view. In this sense, the polymer representation is substantially equivalent to introducing a lattice structure on the space.

In this Section we briefly summarize the fundamental features of the polymer quantization scheme necessary to apply this kind of cut-off physics to the cosmological model. In other words, we will formulate what is called Polymer Quantum Cosmology in order to provide a proper description of the initial singularity.

To introduce the concept of equivalence among different representations, we start by considering a simple one dimensional system, described with respect to the phase space variables (q, p). In ordinary Quantum Mechanics, the quantization of any system begins considering the implementation from the Poisson brackets of the configuration variables[66]

$$\{q, p\} = 1 \tag{2.34}$$

to the commutators of the correspondent quantum operators

$$[\widehat{q}, \widehat{p}] = i\hbar\widehat{I}, \tag{2.35}$$

and the definition of the space over which the quantum states live, naturally the Hilbert space $\mathcal{H} = L^2(\mathbb{R}, d\mu)$. The relations (2.35) are known as the CCR. The next point is the choice of the base (or polarization) on which the description is given. We have two choices: the position base and the momenta base. Obviously, the choice of a particular polarization imply the structure of the basis vectors. In particular, choosing the q-polarization, the action of the operator $\widehat{q}$ on the basis vectors assumes the eigenvalue equation form

$$\widehat{q}|q\rangle = q|q\rangle \tag{2.36}$$

with the states normalized with the Dirac delta function

$$\langle q|q'\rangle = \delta(q - q') \tag{2.37}$$

In quantum mechanics the generic state is described by the wave function, which in the Dirac scheme is represented by the Ket $|\psi\rangle$. Its projection on the base gives

$$\langle q|\psi\rangle = \psi(q), \tag{2.38}$$

from which follows that

$$\langle q|\widehat{q}|\psi\rangle = q\langle q|\psi\rangle = q\psi(q) \tag{2.39}$$

Taking into account the Eq. (2.35),a possible representation for the operator $\widehat{p}$ in the position base is

$$\widehat{p} = -i\hbar\frac{d}{dq}, \tag{2.40}$$

and then

$$\langle q|\widehat{p}|\psi\rangle = -i\hbar\frac{d}{dq}\psi(q). \tag{2.41}$$

In the same way, it is possible to repeat the previous consideration in the p-polarization. The action of the operator $\widehat{p}$ on the base gives the eigenvalue problem

$$\widehat{p}|p\rangle = p|p\rangle, \tag{2.42}$$

and as before the states are normalized with the Dirac delta function. In this case the projection of the Ket $|\phi\rangle$ on the base vectors $|p>$ leads to

$$\langle p|\phi\rangle = \phi(p), \tag{2.43}$$

where this time the wave function depends on the momenta p. Therefore, in this base we have

$$\langle p|\widehat{p}|\psi\rangle = p\langle p|\psi\rangle = p\psi(p) \tag{2.44}$$

The parallelism with the previous case is completed with the individuation of the operator $\widehat{q}$ in this polarization, which is

$$\widehat{q} = i\hbar\frac{d}{dp} \tag{2.45}$$

This allow to write also the analog of the Eq.(2.41) as

$$\langle p|\widehat{q}|\psi\rangle = i\hbar\frac{d}{dp}\psi(p). \tag{2.46}$$

A schematic resume says that in the q-polarization we have that

$$\widehat{q}\psi(q) \rightarrow q\psi(q) \qquad \widehat{p}\psi(q) \rightarrow -i\hbar\frac{d}{dq}\psi(q). \tag{2.47}$$

while in the p-polarization we have

$$\widehat{q}\phi(p) \rightarrow i\hbar\frac{d}{dp}\phi(p) \qquad \widehat{p}\phi(p) \rightarrow p\phi(p). \tag{2.48}$$

As shown for this simple case, the standard quantization procedure involves the assignment of a differential operator. However, there may be physical reasons for which such assignment is not possible. For example, there are theories for which the configuration of the space has a lattice structure. In these cases, being impossible to define a limit of the difference quotient (or in other words to define a derivative), we cannot associate differential operators to the conjugate momenta of the variables defined on the lattice. However, a physical theory on the lattice can be constructed by associating them the *difference operators*. The way to build the differences operators is through the quotient operators, which are the analog of the difference quotient for the derivatives. In this way, we can basically define two different types of quotient operators acting on appropriate spaces of functions. If we take a function $f[\mathbb{R}]$ defined on the real space we can define two kind of quotient operators:

- **Additive**

$$D^a f(x) = \frac{f(x+a) - f(x-a)}{(x+a) - (x-a)} = \frac{f(x+a) - f(x-a)}{2a} \quad , \quad a \in \mathbb{R} \quad , \quad a \neq 0 \tag{2.49}$$

- **Multiplicative**

$$D^s f(x) = \frac{f(sx) - f(s^{-1}x)}{sx - s^{-1}x} = \frac{1}{x}\frac{f(sx) - f(s^{-1}x)}{s - s^{-1}} \quad , \quad s \in \mathbb{R} \quad , \quad s \neq 1 \tag{2.50}$$

These quotients can be seen as the operators that acts on different lattice theory. In particular, starting from them, we can identify the *Additive lattice*

$$\mathcal{L}_a = \{x_0 + ja | j \in \mathbb{Z}, x_0 \in \mathbb{R}\} \tag{2.51}$$

and the *multiplicative lattice*

$$\mathcal{L}_s = \{x_0 s^j | j \in \mathbb{Z}, x_0 \in \mathbb{R}, x_0 \neq 0\} \tag{2.52}$$

As expected, from the Eq.s(2.49),(2.50), we note respectively that in the limit $a \to 0$ and $s \to 1$ (*i.e.* the removal of the lattice) the equations reduce to the definition of the limit of the difference quotient.

2.5.1 Stone-Von Neumann Theorem

The CCR used in the relation (2.35) are not the only starting points to describe the quantum kinematics. A very important and equivalent alternative form are the *Weyl Commutation Rules*(WCR)[38]. Let us start considering the unitary transformations generate from the operators $(\widehat{q}, \widehat{p})$[51]. These will be very useful to define in the following the difference operators for polymer quantum kinematics. They are:

$$U(\alpha) = e^{\frac{i}{\hbar}\alpha\widehat{q}} \qquad V(\beta) = e^{\frac{i}{\hbar}\beta\widehat{p}} \qquad \alpha, \beta \in \mathbb{R}. \tag{2.53}$$

It is possible to demonstrate that starting from the latter definitions we obtain the WCR:

$$U(\alpha)V(\beta) = e^{\frac{i}{\hbar}\alpha\beta}V(\beta)U(\alpha) \tag{2.54}$$

In other words, any couple of unitary operators $(\{U(\alpha)\}, \{V(\beta)\})$ that act on a given Hilbert space provides provides a representation in the Weyl form if they satisfy the rules (2.54).

With this background we are now able to give some definitions necessary to introduce an important theorem.

An *irreducible* representation is a representation that has no nontrivial invariant subspaces of the Hilbert space.
Furthermore, given two sets of representations $(\{U(\alpha)\}, \{V(\beta)\})$ and $(\{U(\alpha)'\}, \{V(\beta)'\})$ that act on two different Hilbert spaces $\mathcal{H}$ and $\mathcal{H}'$, they are *unitarily equivalent* only if exists a unitary operator $W : \mathcal{H} \to \mathcal{H}'$ such that

$$WU(\alpha)W^* = U(\alpha)'_b \qquad WV(\beta)W^* = V(\beta)' \qquad \forall\alpha, \beta \in \mathbb{R}. \tag{2.55}$$

Finally, a representation is called $(\{U(\alpha)\}, \{V(\beta)\})$ is called *regular* if the transformations

$$\alpha \to U_\alpha \qquad \beta \to V_\beta \tag{2.56}$$

are continuous transformations (given a generic function φ that belongs to the Hilbert space $\forall\varphi \in \mathcal{H}$ the transformation $a \to \langle\varphi|U_a\varphi\rangle$ is continuous). If now we consider a couple of groups of unitary operators $\{U(\alpha), V(\beta)\}$ that satisfy the WCR and make the hypothesis that they are regular and irreducible, we can enunciate the
Stone-Von Neumann Theorem: *Every regular and irreducible representation of the CCR are unitary equivalent to the Schrödinger representation.*

This theorem says that all representations of the quantum mechanics that show the properties listed above are equivalent to the Schrödinger one. Historically this theorem has been used to demonstrate the equaivalence between the Schrödinger and the Heisenberg representation.

We will make use, in the following, of the Stone-Von Neumann theorem to demonstrate how the polymer quantum mechanics is a non-equivalent representation of the usual Schrödinger one.

2.5.2 Kynematical properties

To introduce the basic concepts of the polymer quantum mechanics we start by considering the kynematics of a simple one-dimensional quantum system[39]. Let us take a set of kets $|\mu_i\rangle$, with $\mu_i \in \mathbb{R}$ and discrete index $i = 1, ..., N$. The vectors $|\mu_i\rangle$ belong to the Hilbert space $\mathcal{H}_{poly} = L^2(\mathbb{R}_b, d\mu_H)$[1]. The inner product between two kets is $\langle\nu|\mu\rangle = \delta_{\nu,\mu}$ and the state of the system is described by a generic linear combination of them

$$|\psi\rangle = \sum_{i=1}^{N} a_i |\mu_i\rangle. \tag{2.57}$$

One can identify two fundamental operators in this Hilbert space: a *label operator* $\widehat{\varepsilon}$ and a *shift operator* $\widehat{s}(\lambda)$. They act on the kets as follows

$$\widehat{\varepsilon}|\mu\rangle = \mu|\mu\rangle \quad , \quad \widehat{s}(\lambda)|\mu\rangle = |\mu+\lambda\rangle. \tag{2.58}$$

In order to associate physical operators to the abstract objects (2.58), we consider again the one-dimensional system described by the phase space variables (q, p). With regards of what said before, we make the physical choice to assign a discrete character for the position variable q and we will see the implications for the descriptions of the states of the system in both the polarizations.

p-polarization

Let us begin considering the momenta polarization. The projection of a generic state on the base is

$$\phi(p) = \langle p|\psi\rangle \tag{2.59}$$

However, we have, as in the Schrödinger representation, that the projection on the basis vectors are

$$\phi_\mu(p) = \langle p|\mu\rangle = e^{-\frac{i}{\hbar}\mu p} \tag{2.60}$$

It is now interesting to evaluate the action of the operator $V(\lambda)$, introduced in the Eq.(2.53) on $\phi_\mu(p)$. This application shows that

$$V(\lambda)\phi_\mu(p) = V(\lambda)e^{-\frac{i}{\hbar}\mu p} = e^{\frac{i}{\hbar}\lambda p}e^{-\frac{i}{\hbar}\mu p} = e^{\frac{i}{\hbar}(-\mu+\lambda)p} = \phi_{\mu+\lambda}(p) \tag{2.61}$$

Recalling the definition (2.58), the identification of the operator $V(\lambda)$ with the shift operator $\widehat{s}(\lambda)$ is immediate.

Furthermore, we can identify the position operator $\widehat{q}$ with the label operator. Indeed, the action of the position operator on the projection $\phi_\mu(p)$ gives

$$\widehat{q}\phi_\mu(p) = -i\hbar\frac{d}{dp}e^{-\frac{i}{\hbar}\mu p} = \mu e^{\frac{i}{\hbar}\mu p} = \mu\phi_\mu(p) \tag{2.62}$$

[1]The set of square-integrable functions defined on the Bohr compactification of the real line $\mathbb{R}_b$ with a Haar measure $d\mu_H$

Given the definition of $U(\alpha)$ in the (2.53), the previous equality allow to demonstrate that

$$\lim_{\alpha\to 0}\langle\varphi_\mu|U_\alpha|\varphi_\mu\rangle = \lim_{\alpha\to 0}\langle\varphi_\mu|e^{i\alpha\widehat{q}}|\varphi_\mu\rangle = \lim_{\alpha\to 0}\langle\varphi_\mu|e^{i\alpha\mu}|\varphi_\mu\rangle = \lim_{\alpha\to 0} e^{i\alpha\mu}\langle\varphi_\mu|\varphi_\mu\rangle = 1, \tag{2.63}$$

or in other words the continuity of the relation. Moreover, in this way is possible to see from the application of the position operator on the base vector that

$$\widehat{q}|\mu\rangle = -i\lim_{\alpha\to 0}\alpha^{-1}(U(\alpha)-I)|\mu\rangle = \mu|\mu\rangle \tag{2.64}$$

The last relation demonstrate that the operator $\widehat{q}$ i the generator of the transformation for $U(\alpha)$.

To complete the scheme, we should demonstrate that the operator $\widehat{p}$ is the generator for $V(\lambda)$. Nevertheless, this cannot be achieved because, even if we take an infinitesimal separation parameter λ, two successive vectors $|\mu\rangle$ and $|\mu+\lambda\rangle$ will be always orthogonal, indeed:

$$\langle\varphi_\mu|V_\lambda|\varphi_\mu\rangle = \langle\varphi_\mu|\widehat{s}(\lambda)|\varphi_\mu\rangle = \langle\varphi_\mu|\varphi_{\mu+\lambda}\rangle = \begin{cases}1, & \lambda = 0\\ 0, & \lambda\neq 0\end{cases} \tag{2.65}$$

The Eq.(2.65) says that does not exist a continuous transformation such that $\lambda\to\langle\mu|V_\lambda\mu\rangle$ as in the label operator case. Such a discontinuity drops the assumption of regularity, prevents a genuine definition of the operator $\widehat{p}$ and causes the fall of the Stone-Von Neumann theorem.

In conclusion the polymer representation of the quantum mechanics results non-equivalent to the Schrödinger one.

q-polarization

Let us now formally repeat the same steps above in the q-polarization.

$$\phi(q) = \langle q|\psi\rangle \tag{2.66}$$

This time the projection of the state vectors assume a particular form, making use of a completeness relation:

$$\phi(q)_\mu = \langle q|\mu\rangle = \langle q|\int_{\Re_b} d\mu_H|p\rangle\langle p|\mu\rangle = \int_{\Re_b} d\mu_H\langle q|p\rangle e^{\frac{i}{\hbar}\mu p} = \tag{2.67}$$

$$\int_{\Re_b} d\mu_H e^{-\frac{i}{\hbar}pq}e^{\frac{i}{\hbar}\mu p} = \delta_{q,\mu}$$

How become the shift and label operators in this polarization? It is natural to expect an opposite representation but the preservation of the same features. As in the previous polarization case, the operator $\widehat{p}$ does not exist. This time the reason is the presence of the Kronecker delta function in the definition. Indeed, $\widehat{p}\to -i\hbar\frac{d}{dq}$ in this polarization, we have that the operation

$$\widehat{p}\phi_\mu(q) = -i\hbar\frac{d}{dq}\delta_{q,\mu} \tag{2.68}$$

is inconsistent. Aniway, for the operator V is always valid the identification with the shift operator

$$V(\lambda)\phi(q) = \phi(q+\lambda) \tag{2.69}$$

and $\widehat{q}$ acts as a multiplicative operator:

$$\widehat{q}\phi_\mu(q) = \mu\phi_\mu(q) \tag{2.70}$$

We can conclude the kynematics sections by saying that is impossible, in both the polarization, to define a differential operator as a limit of a difference quotient. This is a direct consequence of the physical choice to assign to the spce variable q a discrete nature. Nothing prevented us, in principle, to choose the momenta variable as a discrete one. In that case the conclusions would have been similar, with the difference that in both the polarization we would find the non-existence of the operator q.

2.5.3 Dynamics

To characterize the dynamical properties of this simple model, it is necessary to investigate the system from the Hamiltonian point of view. A one-dimensional particle of mass m in a potential $V(q)$ is describing by the Hamiltonian

$$H = \frac{p^2}{2m} + V(q). \tag{2.71}$$

Being q a discrete variable, we cannot define, in the p-polarization, the operator $\widehat{p}$ as a differential operator. The standard procedure to go beyond this problem consists in defining a subspace $\mathcal{H}_{\gamma_a}$ of $\mathcal{H}_{poly}$. This subspace contains all vectors that live on the lattice of points identified by the lattice spacing λ

$$\gamma_\lambda = \{q \in \mathbb{R} | q = n\lambda, \forall n \in \mathbb{Z}\}, \tag{2.72}$$

where λ has the dimensions of a *length*.
The basis vector takes the form $|\mu_n\rangle$ (where $\mu_n = \lambda n$) and the states are defined as a linear combination of them:

$$|\psi\rangle = \sum_n b_n |\mu_n\rangle. \tag{2.73}$$

The basic realization of the polymer quantization is to approximate the term corresponding to the non-existent operator (this case $\widehat{p}$), and to find for this approximation an appropriate and well-defined quantum operator. The operator $\widehat{V}$ is exactly the shift operator $\widehat{s}$, in both polarizations. Through this identification, it is possible to exploit the properties of $\widehat{s}$ to write an approximate version of $\widehat{p}$. For $p \ll \frac{\hbar}{\lambda}$, one gets

$$p \simeq \frac{\hbar}{\lambda}\sin\left(\frac{\lambda p}{\hbar}\right) = \frac{\hbar}{2i\lambda}\left(e^{i\frac{\lambda p}{\hbar}} - e^{-i\frac{\lambda p}{\hbar}}\right) \tag{2.74}$$

and then the new version of $\widehat{p}$ is

$$\widehat{p}_\lambda|\mu_n\rangle = \frac{i\hbar}{2\lambda}\left(|\mu_{n-1}\rangle - |\mu_{n+1}\rangle\right). \tag{2.75}$$

One can define an approximate version of $\widehat{p}^2$. For $p \ll \frac{\hbar}{\lambda}$, one gets

$$p^2 \simeq \frac{2\hbar^2}{\lambda^2}\left[1 - \cos\left(\frac{\lambda p}{\hbar}\right)\right] = \frac{2\hbar^2}{\lambda^2}\left[1 - e^{i\frac{\lambda p}{\hbar}} - e^{-i\frac{\lambda p}{\hbar}}\right] \tag{2.76}$$

and then the new version of $\widehat{p}^2$ is

$$\widehat{p}^2_\lambda|\mu_n\rangle = \frac{\hbar^2}{\lambda^2}\left[2|\mu_n\rangle - |\mu_{n+1}\rangle - |\mu_{n-1}\rangle\right]. \tag{2.77}$$

Remembering that $\widehat{q}$ is a well-defined operator as in the canonical way, the approximate version of the starting Hamiltonian (2.71) is

$$\widehat{H}_\lambda = \frac{1}{2m}\widehat{p}^2_\lambda + V(\widehat{q}). \tag{2.78}$$

The Hamiltonian operator $\widehat{H}_\lambda$ is a well-defined and symmetric operator belonging to $\mathcal{H}_{\gamma_\lambda}$.

2.5.4 Free Polymer Particle

The simplest Hamiltonian system for a one-dimensional system is the free particle. Let us analyze the case of the free polymer particle in the p-polarization. The first step is to consider the classical Hamiltonian approximation

$$H_\lambda \simeq \frac{\hbar^2}{m\lambda^2}\left[1 - \cos\left(\frac{\lambda p}{\hbar}\right)\right] \tag{2.79}$$

For what said in Section 2.5.3, for this approximate version of the Hamiltonian is possible to implement a quantization procedure. Therefore, given a wave function $\psi(p)$, they obey the eigenvalue problem:

$$\widehat{H}_\lambda\psi(p) = E_\lambda\psi(p) \longrightarrow \left[\frac{\hbar^2}{m\lambda^2}\left(1 - \cos\left(\frac{\lambda p}{\hbar}\right)\right) - E_\lambda\right]\psi(p) = 0 \tag{2.80}$$

From the previous equation can be explicitly written the energy spectrum

$$E_\lambda = \frac{\hbar^2}{m\lambda^2}\left[1 - \cos\left(\frac{\lambda p}{\hbar}\right)\right] \leq \frac{2\hbar^2}{m\lambda^2} = E^{max}_\lambda, \tag{2.81}$$

from which we argue that, independently from the choice of the polymer scale λ, due to the presence of the trigonometric function, the system assumed a limited spectrum. Of course, in the limit $\lambda \to 0$ the spectrum (2.81) reduces to the typical free particle in the Schrödinger representation:

$$E_\lambda = \frac{\hbar^2}{m\lambda^2}\left[1 - \cos\left(\frac{\lambda p}{\hbar}\right)\right] \xrightarrow[a\to 0]{} \frac{p^2}{2m} \tag{2.82}$$

while the upper limit reduces to

$$E^{max}_\lambda = \frac{2\hbar^2}{m\lambda^2} \xrightarrow[\lambda\to 0]{} \infty \tag{2.83}$$

Let us take a look to the shape of the eigenfunctions. In this representation is easy to verify that the solution for $\psi(p)$ is

$$\psi(p) = A\delta(p - P_\lambda) + B\delta(p + P_\lambda) \tag{2.84}$$

dove

$$P_\lambda = \frac{\hbar}{\lambda} \arccos\left(1 - \frac{m\lambda^2}{\hbar^2} E_\lambda\right) \tag{2.85}$$

Through an inverse Fourier transform the eigenfunctions can be expressed also in the q-polarization. However, considering the lattice structure for the variable q, the eigenfunctions of p that preserve such a structure are all of the form $e^{\frac{i}{\hbar}\lambda np}, n \in \mathbb{Z}$. These functions are periodic, with period $\frac{2\pi\hbar}{\lambda}$. In terms of the inner product this imply that the integral on the momenta is evaluated over the interval$p \in (-\frac{\pi\hbar}{a}, \frac{\pi\hbar}{a})$. Therefore, the eigenfunctions in the position polarization are

$$\psi(q) = \frac{1}{\sqrt{2\pi}} \int_{-\frac{\pi\hbar}{a}}^{\frac{\pi\hbar}{a}} \psi(p) e^{\frac{i}{\hbar}pq} = \frac{1}{\sqrt{2\pi}} \int_{-\frac{\pi\hbar}{a}}^{\frac{\pi\hbar}{a}} \left[A\delta(p - P_a) + B\delta(p + P_a)\right] e^{\frac{i}{\hbar}pq} = \tag{2.86}$$

$$= \frac{\sqrt{2\pi}\hbar}{a} \left(Ae^{\frac{iqP_a}{\hbar}} + Be^{-\frac{iqP_a}{\hbar}}\right)$$

If the configuration of the momenta is comparable with respect to the value $\frac{\pi\hbar}{a}$, then we expect that the approximation will be gross e far from the standard case. On the other side, staying in the region where the approximation is valid guarantees the validity of the substitution.

2.5.5 Polymer Particle in a Box

Another relevant case to study is the polymer particle in a box. The physical system presented here consists in a one-dimensional particle confined along segment of length $L = N\lambda, N \in \mathbb{N}$. In this case the potential $V(q) = V(n\lambda)$ can be modelized as an infinitely height wall such that

$$V(q) = \begin{cases} \infty, & x > L, x < 0 \\ 0, & 0 < x < L \end{cases} \tag{2.87}$$

Essentially, the particle behaves as a free particle inside the box and, due to the infinitely height wall, he cannot pass over. In terms of the associated quantum system, this imply the necessity to impose some boundary condition for the wave function of the free particle case (2.86). In particular we require that

$$\psi(0) = \psi(L) = 0. \tag{2.88}$$

After the imposition of the conditions (2.88) on the wave function (2.86) we obtain

$$\psi(0) = \frac{\sqrt{2\pi}\hbar}{\lambda}(A + B) = 0 \longrightarrow A = -B \tag{2.89}$$

$$\psi(L) = \frac{\sqrt{2\pi}\hbar}{\lambda} A\left(e^{\frac{iLP_\lambda}{\hbar}} - e^{-\frac{iLP_\lambda}{\hbar}}\right) = \frac{\sqrt{2\pi}\hbar}{\lambda} A \sin\left(\frac{LP_\lambda}{\hbar}\right) = 0 \rightarrow LP_\lambda = n\pi\hbar \quad n \in \mathcal{Z}$$

Putting together the previous equations leads to an eigenfunction form

$$\psi(q) = \frac{2\sqrt{2\pi}\hbar}{\lambda} A \sin\left(\frac{n\pi q}{L}\right) \tag{2.90}$$

The energy spectrum can be calculated simply applying the boundary conditions to the Eq.(2.81). In this case the correspondent spectrum is limited and discrete.

$$E_{\lambda,n} = \frac{\hbar^2}{m\lambda^2}\left[1 - \cos\left(\frac{\lambda n\pi}{L}\right)\right] \tag{2.91}$$

Performing the limit $\lambda \to 0$ the Eq.(2.91) reduces to the standard spectrum of a particle in a box :

$$\lim_{\lambda\to 0} E_{\lambda,n} = \lim_{\lambda\to 0}\frac{\hbar^2}{m\lambda^2}\left[1 - \cos\left(\frac{\lambda n\pi}{L}\right)\right] = \frac{\pi^2 n^2\hbar^2}{2mL^2} \tag{2.92}$$

2.5.6 Polymer Quantization of the flat FRW model

We close this Section applying the formalism of the Polymer Quantum Mechanics to the flat FRW model of the Section 2.4. If we choose to use ϕ as the time relational variable, it does not represent a good candidate to implement the quantum prescription. This means that the conjugated momenta to the scalar field can be promoted as a standard differential operator. Therefore, for what said previously, we have the freedom to choose the variable to discretize among the two conjugated ones $\{a, p_a\}$. The physical problem illustrated here concerns the hypotheses to introduce a lattice structure for the scale factor variable a and, as a consequence, for the conjugate momentap_a it is not possible to build a differential operator. The implementation of the whole Polymer Quantum problem starts by considering the effective Hamiltonian that contains the approximation of the non-existing operator. Therefore, the polymer paradigm substitution (2.76) allows the replacement[2]

$$p_a^2 \to \frac{2}{\lambda^2}\left[1 - \cos\left(\lambda p_a\right)\right], \tag{2.93}$$

and the obtained effective superHamiltonian is[91]

$$\mathcal{H}_\lambda = -\frac{k}{24\pi^2}\frac{2}{\lambda^2}\left[1 - \cos\left(\lambda p_a\right)\right]\frac{1}{a} + 2\pi^2\frac{p_\phi^2}{a^3} = 0. \tag{2.94}$$

Before to consider the quantization of such a constraint it is useful to study the semiclassical dynamics of the just obtained system. As in the standard the classical trajectories can be evaluated through the Hamiltonian equations. In particular, as in the standard case, we can estimated the variation of the the scale factor as

$$\dot{a} = \frac{\partial\mathcal{H}_\lambda}{\partial p_a} = -\frac{k}{12\pi^2 a}\frac{\sin(\lambda p_a)}{\lambda} \tag{2.95}$$

The previous relation can be inserted in the scalar constraint making use of the trigonometric relation $\cos(\arcsin(x)) = \sqrt{1-x^2}$. This brings to a differential equation for the scale factor as

$$\dot{a} = \sqrt{\frac{k}{3}}\frac{p_\phi}{a^2}\sqrt{1 - \frac{12\pi^4\lambda^2 p_\phi^2}{k}\frac{1}{a^2}}. \tag{2.96}$$

The crucial presence of the polymer structure is manifest looking at the existence of a particular value

$$a^* = \frac{12\pi^4\lambda^2 p_\phi^2}{k} \tag{2.97}$$

[2] To avoid burdening in the notation has been chosen $\hbar = 1$.

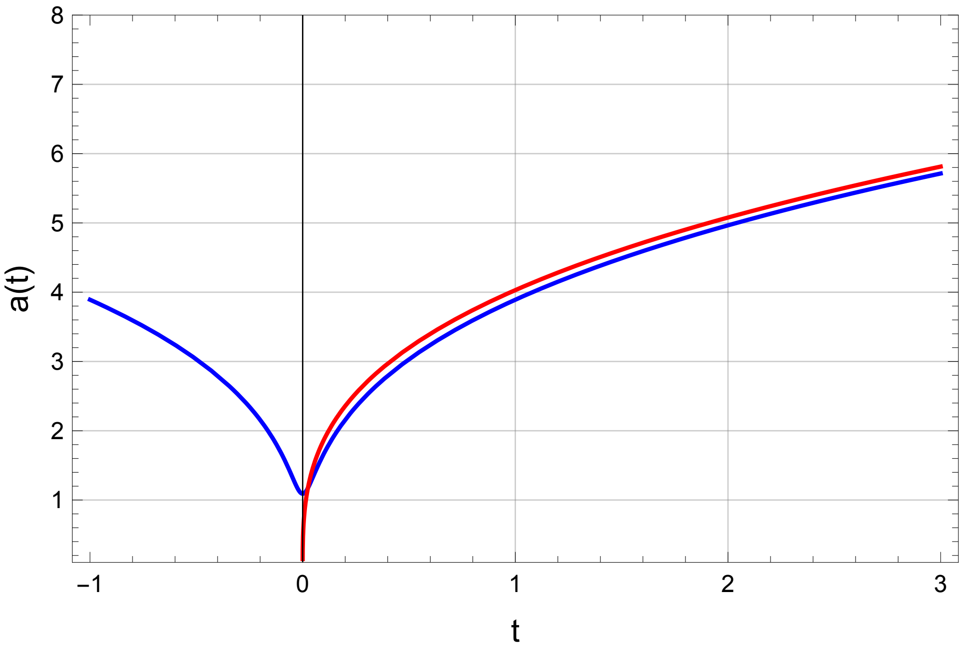

FIGURE 2.2: A comparison between the standard trajectory (red) and the polymer trajectory (blue). In the polymer representation the singularity is avoided and a bounce occurs.

for which the derivative of the scale factor changes its sign. The identification of such a value with a minimum for the scale factor is possible by solving the Eq.(2.96) which gives

$$a(t) = \sqrt{-\frac{12\pi^4\lambda^2 p_\phi^2}{k} + \frac{48(18)^{1/3}\pi^8\lambda^4 p_\phi^4}{k^2 B(t)^{1/3}} + \left(\frac{3}{2}\right)^{1/3} B(t)^{1/3}}. \tag{2.98}$$

The quantity $B(t)$ that appears in latter equation is defined as

$$B(t) = kp^2t^2 + \frac{1152\pi^{12}\lambda^6 p_\phi^6}{k^3} + \sqrt{k^2p^4t^4 + \frac{2304\pi^{12}\lambda^6 p_\phi^8 t^2}{k^2}}. \tag{2.99}$$

The evolution towards the singularity of the scale factor in the polymer case is reported in the Fig. 2.2 in comparison with the standard one. The blue trajectory represents the polymer solution, for which is clear that, in correspondence of the initial singularity the scale factor reach a minimum, namely the value a^* in the Eq.(2.97). Such a value connects a collapsing phase with a successive expanding phase. In this sense, the classical Big-Bang singularity is replaced, in the polymer representation, by a semiclassical *Big-Bounce*.

The extension to the whole polymer quantum problem will consist in the quantum implementation of the superHamiltonian constraint (2.94), namely it leads to the polymer WDW equation. Without loss of generality, we choose to describe the wave function of the universe in the p-polarization for the scale factor part and in the q-polarization for the scalar field part. This choice for the operators formally brings to the quantum problem

$$\left\{\frac{2}{\lambda^2}\left[1-\cos\left(\lambda p_a\right)\right]\partial_{p_a}^2 + \frac{48\pi^4}{k}\partial_\phi^2\right\}\psi(p_a,\phi) = 0 \tag{2.100}$$

As in Section 2.4, the wave function can be factorized as $\psi(p_a, \phi) = e^{i\omega\phi}\varphi_\omega(p_a)$ and the WDW equation (2.100) recasts the form of an eigenvalue problem for the $\varphi_\omega(p_a)$:

$$\left\{ \frac{2}{\lambda^2} \left[1 - \cos(\lambda p_a)\right] \partial^2_{p_a} - \frac{48\pi^4\omega^2}{k} \right\} \varphi(p_a) = 0 \tag{2.101}$$

Unfortunately, the previous differential equation does not admit an immediate analytic solution as in the standard case and for this reason we cannot compare it with the standard case. Anyway, the WDW equation (2.101) can be rearranged in order to highlight the presence of a trigonometric potential term such that:

$$\left\{ \partial^2_{p_a} - \frac{48\pi^4\omega^2}{k} \frac{1}{\sin^2(\lambda p_a)} \right\} \varphi(p_a) = 0 \tag{2.102}$$

The form of the potential term resemble in some sense a simplified version of the trigonometric Poschl-Teller (PT) potential, whose explicit form is

$$V(r) = \frac{V_1}{\sin^2(\alpha r)} + \frac{V_2}{\cos^2(\alpha r)}. \tag{2.103}$$

In [70] and [52], this kind of potential emerges in the context of the Dirac theory, used for example to describe the diatomic molecular vibration or the repulsive action agent on a nucleon. In those works the associated Schrodinger equations admit analytically solution in presence of PT potential. Therefore, a possible solution for the WDW equation (2.102) can be founded taking inspiration from the problems cited above and giving particular values to the parameters in such a way to reduce the general Schrodinger equation in presence of a trigonometric PT potential to the differential equation that appears in Eq.(2.102). Once obtained the wave function in this way, although it is totally to prove, in principle we can expect that the wave packet builds around a certain semiclassical state with the wave function $\psi(p_a, \phi)$, should remains peaked around semiclassical trajectory also in the crossing of the Big-Bounce. This would ensure that the full quantum regime would not differs too much from the corresponding semiclassical polymer dynamics previously founded.

2.6 Quantization of the Mixmaster model: a comparison between standard and polymer approach

In this Section we firstly provide the quantization of the Bianchi IX cosmological model in the Misner picture, in order to show an important feature of the quantum system: the conservation of the quantum numbers associated to the anisotropies when the singularity is approached. Moreover, in the second part of this Section we demonstrate how the implementation of a polymer structure for the anisotropies degrees of freedom induces important modifications both from the semilcassical and the quantum point of view.

2.6.1 Misner picture of the Quantum Mixmaster model

Let us start performing a canonical quantization of the Mixmaster model. As always, it consists in considering the commutation relations

$$[\widehat{q}_a, \widehat{p}_b] = i\delta_{ab}, \tag{2.104}$$

which are satisfied for $\widehat{p_a} = -i\frac{\partial}{\partial q_a} = -i\partial_a$ where $a, b = \alpha, \beta_+, \beta_-$. By replacing the canonical variables with the corresponding operators, the quantum behaviour of the Universe is given by the quantum version of the superhamiltonian constrain (1.135), *i.e.* the WDW equation for the Bianchi IX model

$$\widehat{\mathcal{H}}_{IX}\Psi(\alpha,\beta_\pm) = \left[\partial_\alpha^2 - \partial_+^2 - \partial_+^2 + \frac{3(4\pi)^4}{k^2}e^{4\alpha}V(\beta_\pm)\right]\Psi(\alpha,\beta_\pm), \tag{2.105}$$

where $\Psi(\alpha,\beta_\pm)$ is the wave function of the Universe which provides information about the physical state of the Universe. In the original work of C.W.Misner[75], although it is not clearly claimed, the form of the wave function is done making use of the *adiabatic approximation*. According to this approximation, the shape of the wave function is such that

$$\Psi = \sum_n \chi_n(\alpha)\phi_n(\alpha,\beta), \tag{2.106}$$

and the α-evolution is principally contained in the $\chi_n(\alpha)$ coefficients, while the functions $\phi_n(\alpha,\beta)$ depend on α parametrically only. In terms of the components of the wave functions, the adiabatic approximation is therefore expressed by the condition

$$|\partial_\alpha\chi_n(\alpha)| \gg |\partial_\alpha\phi_n(\alpha,\beta)|. \tag{2.107}$$

By applying the condition (2.107), the WDW Eq.(2.105) reduces to an eigenvalue problem related to the reduced Hamiltonian $\mathcal{H}_{ADM}$ via

$$\widehat{\mathcal{H}}^2_{ADM}\phi_n = E_n^2(\alpha)\phi_n = \left[-\partial_+^2 - \partial_-^2 + \frac{3(4\pi)^4}{k^2}e^{4\alpha}V(\widehat{\beta_\pm})\right]\phi_n. \tag{2.108}$$

However, even without finding the exact expression of the eigenfunctions, one may gain important information about the system from a quantum point of view near the initial singularity. From Fig.(1.5), one can see how the potential (6.101) can be modelized as an infinitely steep potential well with a triangular base. In the Misner original work, the strong hypothesis to replace the triangular box with a squared box having the same area L^2 is proposed. This way, the problem describing a two-dimensional particle in a squared box with infinite walls is recovered. In this case, the eigenvalue problem becomes

$$\widehat{\mathcal{H}}^2_{ADM}\phi_{n,m} = \frac{\pi^2(m^2+n^2)}{L^2(\alpha)}\phi_{n,m}, \tag{2.109}$$

where $m, n \in \mathbb{N}$ are the quantum numbers associated to (β_+, β_-). By a direct calculation, we can derive $L^2(\alpha) = \frac{3\sqrt{3}}{4}\alpha^2$, such that the eigenvalue is

$$E_{n,m} = \frac{2\pi}{3^{3/4}\alpha}\sqrt{m^2+n^2}. \tag{2.110}$$

As demonstrated in [55], substituting the eigenvalue expression (2.110) in the Eq.(2.105), the self-consistence of adiabatic approximation is ensured. Therefore, we can substituted the eigenvalue (2.110) in the conservation law (1.154), in order to estimate the quantum numbers behavior towards the singularity. One can see in Eq.(2.110) that the eigenvalue spectrum is unlimited from above, such that, for sufficiently high occupation numbers, the replacing $\mathcal{H}_{ADM} \simeq E_{n,m}$ is a good approximation. This way, for $\alpha \to -\infty$, Eq.(1.154) becomes

$$< \mathcal{H}_{ADM}\alpha > \xrightarrow[\alpha\to-\infty]{} < \sqrt{m^2+n^2} >= cost. \tag{2.111}$$

Being the current state of the Universe anisotropies characterized by a classical nature, i.e. $\sqrt{m^2+n^2} >> 1$, we can say, by Eq.(2.111), that this quantity is constant approaching the singularity. This way, the quantum state of the Universe related to the anisotropies remains classical for all the backwards history until the singularity.

2.6.2 Semiclassical Polymer approach to the Mixmaster model

We devote this subsection to an interesting cosmological application of the polymer quantum mechanics on the Mixmaster model, illustrated in [67]. As we have seen in Section 2.4, the starting point for the implementation of the Polymer Quantum Mechanics is to individuate the effective semiclassical superHamiltonian for which the non-existing operator is well-defined. It is important to underline that here, "semiclassical" means that we are working with a modified super Hamiltonian constraint obtained as the lowest order term of a WKB expansion for $\hbar \to 0$. At this level, the modified theory is subject to a deterministic dynamics. Following a precise physical interpretation, one can choose to define the anisotropies of the Universe (β_+, β_-) as discrete variables leaving the characterization of the isotropic variable α unchanged, which here plays the role of time. This procedure formally consists in the replacement

$$p_\pm^2 \to \frac{2}{a^2}\left[1-\cos(ap_\pm)\right], \tag{2.112}$$

which modifies the superHamiltonian constraint (1.135) as

$$-p_\alpha^2 + \frac{2}{a^2}\left[2-\cos(ap_+)-\cos(ap_-)\right] + \frac{3(4\pi)^4 e^{4\alpha}}{k^2}V(\beta_\pm) = 0. \tag{2.113}$$

We define $-p_\alpha \equiv H_{poly}$ as the *reduced Hamiltonian*, such that one gets

$$-p_\alpha \equiv H_{poly} = \sqrt{\frac{2}{a^2}\left[2-\cos(ap_+)-\cos(ap_-)\right] + \frac{3(4\pi)^4 e^{4\alpha}}{k^2}V(\beta_\pm)}. \tag{2.114}$$

Starting from the new Hamiltonian formulation (2.114), we can get the following set of the Hamiltonian equations as

$$\begin{aligned} \beta'_\pm &= \frac{d\beta_\pm}{d\alpha} = \frac{\sin(ap_\pm)}{aH_{poly}}, \\ p'_\pm &= \frac{dp_\pm}{d\alpha} = \frac{3(4\pi)^4}{2kH_{poly}}e^{4\alpha}\frac{\partial V(\beta_\pm)}{\partial\beta_\pm}. \end{aligned} \tag{2.115}$$

This modification leaves the potential $V(\beta_\pm)$ and the isotropic variable α unchanged. Therefore, even in the modified theory, the walls move in the 'outer' direction with velocity $|\beta'_w| = \frac{1}{2}$ and the initial singularity is not expected to be removed.
Let us start by analyzing the system far from the wall, i.e. with $V \simeq 0$. As one can see in (2.115) when $V \simeq 0$, the anisotropy velocity is modified if it is compared to the standard case. In particular, the behavior of $\beta_\pm$ is proportional to the time α, as in the standard theory, but with a different coefficient, i.e.

$$\beta_\pm \propto \frac{\sin(ap_\pm)}{\sqrt{4-2[\cos(ap_+)+\cos(ap_-)]}}\alpha. \tag{2.116}$$

In particular, by the definition of the anisotropy velocity (1.140), one obtains

$$\beta' = \sqrt{\frac{\sin(ap_+)^2 + \sin(ap_-)^2}{4 - 2[\cos(ap_+) + \cos(ap_-)]}} = r(a, p_\pm). \tag{2.117}$$

It is worth noting that $r(a, p_\pm)$ is a bounded function ($r \in [0, 1]$) of parameters that remains constant between one bounce and the following one. From Eq.(2.116), we have a Bianchi I model modified by the *polymer* substitution. As a consequence of this feature, also in the modified theory, the anisotropies behave respect to α in a proportional way. The first important semiclassical result is the relative motion between wall and particle. From (2.117), one can observe the existence of allowed values of (ap_+, ap_-), such that the particle velocity is smaller than the wall velocity β'_w. Therefore, the condition for a bounce is

$$\beta' = \sqrt{\frac{\sin(ap_+)^2 + \sin(ap_-)^2}{4 - 2[\cos(ap_+) + \cos(ap_-)]}} > \frac{1}{2} = \beta'_w. \tag{2.118}$$

It means that the infinite sequence of bounces against the walls, typical of the Mixmaster Model, takes place until condition (2.118) is valid. When $r < \frac{1}{2}$, the particle becomes slower than the potential wall and reaches the singularity without no other bounces. The introduction of the *polymer* structure for the anisotropies acts in a very similar way with respect to a massless scalar field for the Bianchi IX model, as analyzed in Section 1.6.2. This brings us to claim that in the semiclassical polymer scheme of the Mixmaster model the chaotic behavior is removed in favor of a final free particle regime preserved until the singularity.

A second important observation is that the relation (1.155) remains valid until $r < \frac{1}{2}$ or in other words when the particle become slower than the potential wall. When it happens, approaching the singularity we have that $\alpha \to -\infty$ while H_{poly} remains constant without changes. In this sense, when the outgoing momenta configuration of the j-th bounce is such that $r < \frac{1}{2}$, the quantity $H^j_{poly}\alpha^j$ is no longer a constant of motion.

The last semiclassical result is the modified reflection law for the single bounce. As in the standard case, one can introduce a parametrization for the particle velocity components, before and after a single bounce, which takes into account also the different ingoing and outgoing particle velocity. A way to realize such a parametrization is

$$\begin{aligned}
(\beta'_-)_i &= r_i \sin\theta_i, \\
(\beta'_+)_i &= -r_i \cos\theta_i, \\
(\beta'_-)_f &= r_f \sin\theta_f, \\
(\beta'_+)_f &= r_f \cos\theta_f.
\end{aligned} \tag{2.119}$$

where (θ_i, θ_f) are the incidence and the reflection angles and (r_i, r_f) are the anisotropy velocities before and after the bounce. This parametrization can be used to re-express the same couple of constants of motion (with respect to the standard case) obtained from the analysis of the dynamics of the bounce against the wall

$$\begin{aligned}
p_- &= cost, \\
K &= \frac{1}{2}p_+ + H_{poly} = cost.
\end{aligned} \tag{2.120}$$

The expression of p_+ as function of β' can be obtained from (2.115):

$$p_+ = \frac{1}{a}\arcsin(a\beta'_+ H_{poly}). \tag{2.121}$$

This way, by a substitution of Eq.(2.121) in Eq.(2.120), remembering $\arcsin(-x) = -\arcsin(x)$ and using the parametrization (2.119), one obtains

$$\frac{1}{2a}\arcsin(-ar_i H^i_{poly}\cos\theta_i) + H^i_{poly} = \frac{1}{2a}\arcsin(ar_f H^f_{poly}\cos\theta_f) + H^f_{poly}. \tag{2.122}$$

Now we express r and H_{poly} as functions of a, p_+, p_-:

$$\frac{1}{2}[\arcsin(\sqrt{\sin(ap^i_+)^2 + \sin(ap^i_-)^2}\cos\theta_i) + \arcsin(\sqrt{\sin(ap^i_+)^2 + \sin(ap^i_-)^2}\frac{\cos\theta_f\sin\theta_i}{\sin\theta_f})] =$$
$$= \sqrt{4 - 2(\cos(ap^i_+) + \cos(ap^i_-)} - \frac{\sin\theta_i}{\sin\theta_f}\sqrt{\frac{\sin(ap^i_+)^2 + \sin(ap^i_-)^2}{\sin(ap^f_+)^2 + \sin(ap^f_-)^2}[4 - 2(\cos(ap^f_+ + \cos(ap^f_-)]}. \tag{2.123}$$

To perform a direct comparison with the standard case, a Taylor expansion up to second order for $ap_\pm << 1$ for Eq.(2.123) is needed. This way, after standard manipulation, the reflection law rewrites

$$\frac{1}{2}\sin(\theta_i + \theta_f) = \sin\theta_f\sqrt{1 + \frac{a^2}{4}\frac{(p^i_+)^4 + (p^i_-)^4}{(p^i_+)^2 + (p^i_-)^2}} - \sin\theta_i\sqrt{1 + \frac{a^2}{4}\frac{(p^f_+)^4 + (p^f_-)^4}{(p^f_+)^2 + (p^f_-)^2}}. \tag{2.124}$$

Defining $R = \frac{a^2}{4}\frac{p_+^4 + p_-^4}{p_+^2 + p_-^2}$, one has

$$\frac{1}{2}\sin(\theta_i + \theta_f) = \sin\theta_f\sqrt{1 + R_i} - \sin\theta_i\sqrt{1 + R_f}. \tag{2.125}$$

We obtain for $ap_\pm << 1$ a modified reflection law that, differently from the standard case, depends on two parameters (R, θ). Obviously, in the limit $ap_\pm \to 0$, i.e. switching off the *polymer* modification, the standard reflection law (1.153) is recovered.

2.6.3 Polymer Mixmaster model

We now analyse the quantum properties of the Mixmaster model when the full polymer quantization is implemented[67]. Starting from the semiclassical effective superHamiltonian (2.113), we recall the physical choice to discretized the anisotropies (β_+, β_-) leaving unchanged the characterization of the isotropic variable α.

As in the Misner picture, we require that the form of the wave function takes into account the adiabatic approximation, then one searches a solution as

$$\Psi(p_\pm, \alpha) = \chi(\alpha)\psi(\alpha, p_\pm). \tag{2.126}$$

With no changes in the effective dynamics, one can choose to describe the $\chi(\alpha)$ component of the wave function in the q-polarization and the $\psi(\alpha, p_\pm)$ component of the wave function in the p-polarization.

Therefore, as illustrated in the Section 5.4, one applies the formal substitution $\widehat{p}^2_\pm \to \frac{2}{a^2}[1 - \cos(ap_\pm)]$ which act on the wave function of the Universe in a multiplicative way. Of course, the conjugated momenta p_α have a well-defined operator of the form $\widehat{p}_\alpha = -i\partial_\alpha$. This way, we can obtain the WDW equation for the *polymer* Mixmaster model writing the quantum version of superHamiltonian in (2.113), that is

$$[-\partial^2_\alpha + \frac{2}{a^2}(1 - \cos(ap_+)) + \frac{2}{a^2}(1 - \cos(ap_-)) + \frac{3(4\pi)^4}{k^2}e^{4\alpha}V(\beta_\pm)]\Psi(p_\pm, \alpha) = 0. \tag{2.127}$$

Before continuing with the analysis of the above polymer WDW equation in order to extract the quantum properties of this system, is important to underline a key point. The conservation of quantum numbers associated to the anisotropies, as obtained by C.W.Misner in the standard quantum theory (see Eq.(2.111)), is essentially based on a fundamental propriety of the Mixmaster Model: the presence of chaos. Nevertheless, as shown in the study of the relative motion between the particle and the wall in the semi-classical regime (2.118), the chaos is removed for discretized anisotropies of the Universe. This way, one cannot obtain for the modified theory a conservation law towards the singularity as in the standard case. For a quantum description, the *polymer* wavepackets for the theory are needed. By a semiclassical analysis of the relational motion between the wall and the particle, as in Sec.2.6.2, the polymer modification implies for the particle different condition for the reach of the potential wall. This way, it behaves as a free particle (no potential case $V = 0$) or as a particle in a box (infinitely steep potential well case).

In the free particle case, the potential term $V(\beta_\pm)$ is negligible in the WDW equation. The application of the condition due to the adiabatic approximation (2.107) reduces the Eq.(2.127) to a free-particle eigenvalue problem

$$\widehat{H}^2_{poly}\psi(p_\pm) = k^2\psi(p_\pm) = \left[\frac{2}{a^2}(2-\cos(ap_+)-\cos(ap_-))\right]\psi(p_\pm). \tag{2.128}$$

From the structure of the eigenvalue problem (2.128), one can write $\widehat{H^2}_{poly} = \widehat{H^2}_+ + \widehat{H^2}_-$. As a consequence, it is possible to describe the anisotropic wave function as $\psi(p_\pm) = \psi_+(p_+)\psi_-(p_-)$. This way, one obtains the two independent eigenvalue problems

$$\begin{aligned}(\widehat{H^2_+} - k_+^2)\psi_+(p) &= \left[\frac{2}{a^2}[1-\cos(ap_+)] - k_+^2\right]\psi_+(p) = 0,\\ (\widehat{H^2_-} - k_-^2)\psi_-(p) &= \left[\frac{2}{a^2}[1-\cos(ap_-)] - k_-^2\right]\psi_-(p) = 0.\end{aligned} \tag{2.129}$$

where $k^2 = k_+^2 + k_-^2$. These eigenvalue problems can be treated as in Sec.2.5.4 and, by a similar procedure, one can easily verify that the momentum wave functions $\psi_+(p)$ and $\psi_-(p)$ have the form

$$\begin{aligned}\psi_+(p_+) &= A\delta(p_+ - p_a^+) + B\delta(p_+ + p_a^+),\\ \psi_-(p_-) &= C\delta(p_- - p_a^-) + D\delta(p_- + p_a^-),\end{aligned} \tag{2.130}$$

where A, B, C, D are integration constants and p_a^+,p_a^- are defined as

$$\begin{aligned}p_a^+ &= \frac{1}{a}\arccos\left(1 - \frac{k_+^2a^2}{2}\right),\\ p_a^- &= \frac{1}{a}\arccos\left(1 - \frac{k_-^2a^2}{2}\right).\end{aligned} \tag{2.131}$$

From Eq.'s (2.129), the eigenvalue k^2 is given by

$$k^2 = k_+^2 + k_-^2 = \frac{2}{a^2}\left[2-\cos(ap_+)-\cos(ap_-)\right] \leq k^2_{max} = \frac{8}{a^2}, \tag{2.132}$$

i.e. a bounded and continuous eigenvalue is found.

Now one can obtain $\psi(\beta_\pm)$ by performing a Fourier transform for $\psi(p_\pm) = \psi_+(p_+)\psi_-(p_-)$, such that

$$\psi_k(\beta_\pm) = \int\int dp_+ dp_- \psi(p_\pm) e^{ip_+\beta_+} e^{ip_-\beta_-} = \\ = C_1 e^{ip_a^+\beta_+} e^{ip_a^-\beta_-} + C_2 e^{ip_a^+\beta_+} e^{-ip_a^-\beta_-} + C_3 e^{-ip_a^+\beta_+} e^{ip_a^-\beta_-} + C_4 e^{-ip_a^+\beta_+} e^{-ip_a^-\beta_-}, \quad (2.133)$$

where $C_1 = AC$, $C_2 = AD$, $C_3 = BC$, $C_4 = BD$. We are now able to build up the *polymer* wave packet for the wave function of the Universe. We choose to integrate the packet on the energies k_+, k_-. As a consequence of the modified dispersion relations (2.131), the energies eigenvalues k_+, k_- can only take values within the interval $[-\frac{2}{a}, +\frac{2}{a}]$. Therefore, we have

$$\Psi(\beta_\pm, \alpha) = \iint_{-\frac{2}{a}}^{\frac{2}{a}} dk_\pm A(k_\pm) \psi_{k_\pm}(\beta_\pm) \chi(\alpha), \quad (2.134)$$

where $A(k_+, k_-) = e^{-\frac{(k_+-k_+^0)^2}{2\sigma_+^2}} e^{-\frac{(k_--k_-^0)^2}{2\sigma_-^2}}$ is a Gaussian weighting function, $\sigma_\pm^2$ are the variances along the two directions (β_+,β_-) and $k_\pm^0$ are the energies eigenvalues around which we build up the wave packet. Let us note from Eq.(2.134) that the polymer structure modifies the standard wave packet related to the plane wave in terms of the anisotropies component as a consequence of Eqs.(2.131), *i.e.* the modified dispersion relations.
The shape for the isotropic component of the wave function in the free particle case is $\chi(\alpha) = e^{-i\int_0^\alpha k dt} = e^{-i\sqrt{k_+^2+k_-^2}\alpha}$. This shape is a solution of the WDW equation $\partial^2\chi(\alpha) + k^2\chi(\alpha) = 0$ obtained by the application of the adiabatic approximation (2.107). Furthermore, the self-consistence of this approximation is ensured.

We analyze the problem of a polymer particle in a box according to the Misner hypothesis about the substitution of the triangular box by a square domain having the same area L^2, as in Section2.6.1. Furthermore, following the semiclassical results in Sec.2.6.2, one takes into account the outside wall velocity defining the side of square box L as

$$L(\alpha) = L_0 + |\alpha|, \quad (2.135)$$

where L_0 is the side of the square box when $\alpha = 0$. With the squared box substitution, the potential can be modelized as

$$V(\beta_\pm) = \begin{cases} \infty, & \beta_\pm > \frac{L(\alpha)}{2} \quad , \quad \beta_\pm < -\frac{L(\alpha)}{2} \\ 0, & -\frac{L(\alpha)}{2} < \beta_\pm < \frac{L(\alpha)}{2} \end{cases}. \quad (2.136)$$

We can obtain a solution for $\psi(\beta_\pm)$ in the same way of Sec.2.6.2, recalling that the potential form (2.136) implies this kind of boundary conditions for $\psi(\beta_\pm)$ along the two directions

$$\psi_\pm\left(-\frac{L_0}{2} - \frac{\alpha}{2}\right) = \psi_\pm\left(+\frac{L_0}{2} + \frac{\alpha}{2}\right) = 0. \quad (2.137)$$

When one applies the conditions (2.137) separately along the two directions (β_+, β_-), one obtains

$$\psi_+(\beta_+) = A\left[e^{\frac{in\pi\beta_+}{L_0+\alpha}} - e^{\frac{-in\pi\beta_+}{L_0+\alpha}} e^{-in\pi}\right], \\ \psi_-(\beta_-) = B\left[e^{\frac{im\pi\beta_-}{L_0+\alpha}} - e^{\frac{-im\pi\beta_-}{L_0+\alpha}} e^{-im\pi}\right]. \quad (2.138)$$

This way, $\psi(\beta_\pm)$ is the product of the two separate wave functions $\psi_+(\beta_+)$ and $\psi_-(\beta_-)$. Thus, one gets[3]

$$\psi_{n,m}(\beta_\pm,\alpha) = \psi_+(\beta_+)\psi_-(\beta_-) = \\ = \frac{1}{2(L_0+\alpha)}\left[e^{\frac{in\pi\beta_+}{L_0+\alpha}} - e^{\frac{-in\pi\beta_+}{L_0+\alpha}}e^{-in\pi}\right]\left[e^{\frac{im\pi\beta_-}{L_0+\alpha}} - e^{\frac{-im\pi\beta_-}{L_0+\alpha}}e^{-im\pi}\right], \tag{2.139}$$

where A, B are integration constants and $(n,m) \in \mathbb{Z}$ are quantum numbers associated to the anisotropies degrees of freedom. Due to the presence of the integers quantum numbers (n,m), a bounded and discrete eigenvalue spectrum is obtained.

$$k^2 = k_+^2 + k_-^2 = \frac{2}{a^2}\left[2 - \cos\left(\frac{an\pi}{L_0+\alpha}\right) - \cos\left(\frac{am\pi}{L_0+\alpha}\right)\right] \tag{2.140}$$

As in the free polymer particle case, one builds the wave packet. However, in this case, one cannot integrate on a limited domain of energies $k_\pm$, and a sum over all quantum numbers n, m between $-\infty$ and ∞ is necessary. This way,

$$\Psi(\beta_\pm,\alpha) = \sum_{n,m=-\infty}^{+\infty} B(n,m)\psi_{n,m}(\beta_\pm,\alpha)e^{-i\int_0^\alpha \sqrt{\frac{2}{a^2}\left[2-\cos\left(\frac{an\pi}{L_0+t}\right)-\cos\left(\frac{am\pi}{L_0+t}\right)\right]}dt}, \tag{2.141}$$

where $B(n,m) = e^{-\frac{(n-n^*)^2}{2\sigma_+^2}}e^{-\frac{(m-m^*)^2}{2\sigma_-^2}}$ is a Gaussian weighting function and n^*, m^* are the quantum numbers around which we build up the wave packet.

Let us note that, differently from the free particle case, the presence of the polymer structure modifies the standard wave packet related to a particle in a box in terms of the isotropic components. It happens because, in the wave packet (2.141), the energies $k_\pm$ are expressed through (n,m), namely the quantum numbers associated to the anisotropies.

As from Eq.(2.141), one chooses a shape for the isotropic component

$$\chi(\alpha) = e^{-i\int_0^\alpha k(t)dt} = e^{-i\int_0^\alpha \sqrt{\frac{2}{a^2}\left[2-\cos\left(\frac{an\pi}{L_0+t}\right)-\cos\left(\frac{am\pi}{L_0+t}\right)\right]}dt}. \tag{2.142}$$

In this case, Eq.(2.142) is a solution of the WDW equation $\partial^2\chi(\alpha) + k(\alpha)^2\chi(\alpha) = 0$ obtained by means of the adiabatic approximation (2.107) in the asymptotic limit $\alpha \to -\infty$. In this limit, the self-consistence of the adiabatic approximation is ensured. The form of the isotropic component of the wave function (2.142) is also an exact solution for the Schrödinger equation associated to the ADM reduction. Both in the case of a free particle (2.134) and in the one of a particle in a box (2.141), it is not possible to perform an analytic integration for the wave packets. This way, in order to obtain the quantum behaviour of the wave packets near the cosmological singularity, we evaluate them via numerical integrations.

Behaviour of the free particle

In the case of a free particle, we perform the numerical integration choosing the parameters which select semiclassical initial conditions concerning a particle with velocity smaller than the wall one ($r < \frac{1}{2}$). One appreciates, in Fig. 2.3, the behavior towards the singularity (formally for $|\alpha| \to \infty$) of the absolute value of the wave packet $|\Psi(\alpha,\beta_\pm)|$ in

[3] It is possible to evaluate the constant AB by requesting that $|\psi_{n,m}(\beta_\pm)|^2 = 1$ over all the square box. This way, $AB = \frac{1}{2(L_0+\alpha)}$ is obtained.

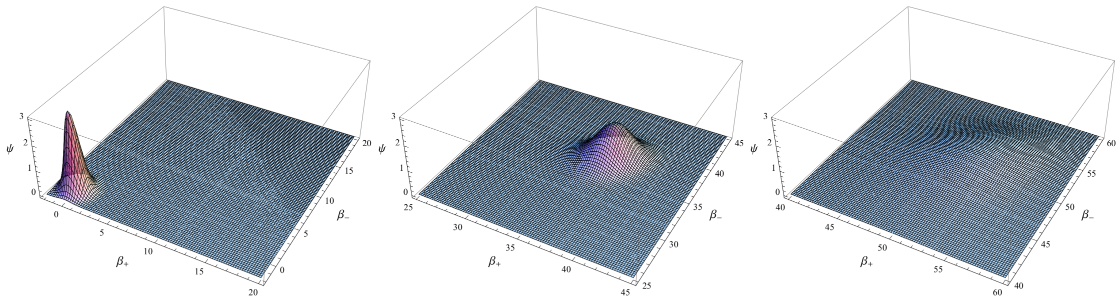

FIGURE 2.3: The evolution of the *polymer* wave packet $|\Psi(\alpha,\beta_\pm)|$ for the free particle case respectively for the values of $|\alpha| = 0, 50, 150$. The numerical integration is done for this choice of parameters: $a = 0.07, k_+ = k_- = 25, \sigma_+ = \sigma_- = 0.7$. They select an initial semiclassical condition of a particle with a velocity smaller than the wall velocity. It is worth noting that the particular choice of the parameters couple $(a, \sigma_\pm)$ is done because this way the condition $a << \frac{1}{\sigma_\pm}$ is valid. It is referred to the condition that the typical *polymer* scale a be much smaller than the characteristic width of the wave packet $\frac{1}{\sigma_\pm}$.

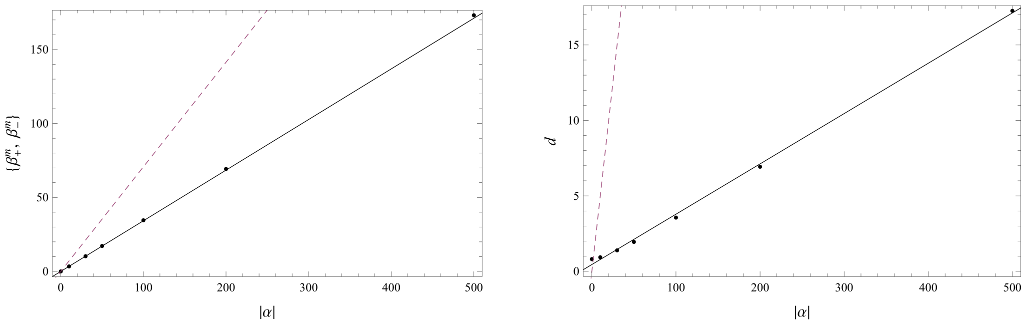

FIGURE 2.4: The solid line in the first graph represents the *polymer* semiclassical trajectory identified by the choice of the initial conditions. The dashed line represents the classical trajectory followed by a wave packet built with the wave function of the standard case, namely starting from the classical superHamiltonian constrain (1.135). The points in the second graph represent the evolution of the spread d as a function of $|\alpha|$. The solid line represents the best fit for the points while the dashed line represents the evolution of the wall position $|\beta_w| = \frac{1}{2}|\alpha|$.

Eq.(2.134). It is interesting to study the evolution of $\beta^m_\pm$, i.e. the wave packet maximum position. This way, we can see which trajectory the wave packet follows towards the singularity. As we can see in the first graph in Fig. 2.4, the behavior of the maximum position is completely overlapping with the semiclassical trajectory selected by our choice of the initial conditions. In this sense, the *polymer* wave packet follows the semiclassical trajectory until the singularity. This feature is not undermined by the spread d of the wave packet, i.e. the delocalization of the wave packet, as expressed by the distance between the maximum position of the wave packet and the edge of the region identified by the full width at half maximum. Obviously, one expects that the spread velocity is really smaller than the wall velocity. Otherwise, it would be possible for that the wave packet to reach the potential wall. In that case, the description of the quantum system with the wave packets for the free particle would not be correct. The second graph in Fig. 2.4 represents the spread evolution, and we can see it follows a linear behavior (solid line) with a slope much smaller than $|\beta'_w| = \frac{1}{2}$, i.e. the one related to the behavior of the wall position (dashed line). This assures that the quantum representation of the system near the singularity for the free particle case is well described by the wave packet representation.

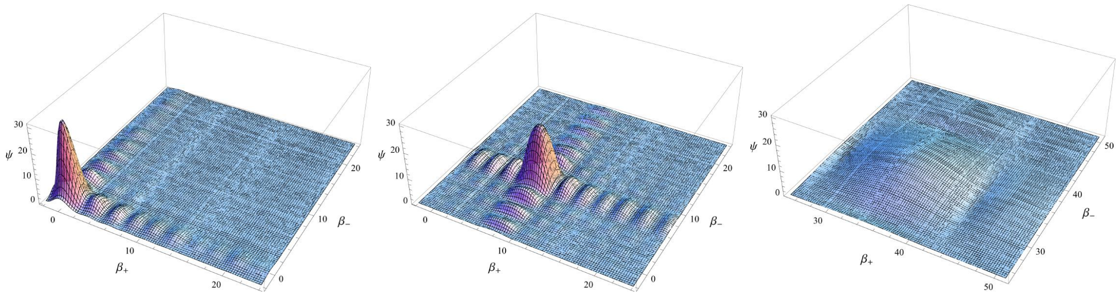

FIGURE 2.5: The evolution of the *polymer* wave packet $|\Psi(\alpha,\beta_\pm)|$ respectively for $|\alpha| = 0, 20, 200$. The numerical integration is done for this choice of parameters: $a = 0.014, n^* = m^* = 3000, \sigma_+ = \sigma_- = 50, L_0 = 52$. They select an initial condition of a particle inside a squared box with velocity smaller than the wall velocity. This time, the particular choice of the parameters $(a, \sigma_\pm, L_0)$ it is done because this way the condition $a << \frac{L(\alpha)}{\sigma_\pm}$ is valid. It concerns the condition that the typical *polymer* scale a is very smaller than $\frac{L(\alpha)}{\sigma_\pm}$, i.e. the correct dimensional quantity related with the width of the wave packet.

Behaviour of the Particle in a box

The numerical integration related to the *polymer* wave packet (2.141) has to face a significant technical difficulty. As a consequence of Eq.(2.140), the conjugated momenta $p_\pm$ turn into a discretized variables. Therefore, we select for the particle in a box the initial semiclassical condition considering the substitution

$$ap_+ \to \frac{an\pi}{L_0+\alpha} \quad , \quad ap_- \to \frac{am\pi}{L_0+\alpha}. \tag{2.143}$$

It is worth noting that the initial condition of the particle depends on α, such that one deals with a *time*-dependent condition. In this subsection, the influence of quantum numbers n, m on the dynamics is investigated. For this reason, one introduces six data sets with different values of quantum numbers (n^*, m^*) and box side L_0

$$\begin{cases} a = 0.014 \\ n_0 = 1000 \\ m_0 = 1000 \\ L_0 = 17 \\ \sigma_+ = 50 \\ \sigma_- = 50 \end{cases} \begin{cases} a = 0.014 \\ n_1 = 2000 \\ m_1 = 2000 \\ L_1 = 34 \\ \sigma_+ = 50 \\ \sigma_- = 50 \end{cases} \begin{cases} a = 0.014 \\ n_3 = 3000 \\ m_3 = 3000 \\ L_3 = 52 \\ \sigma_+ = 50 \\ \sigma_- = 50 \end{cases}$$
$$\begin{cases} a = 0.014 \\ n_4 = 6000 \\ m_4 = 6000 \\ L_4 = 103 \\ \sigma_+ = 50 \\ \sigma_- = 50 \end{cases} \begin{cases} a = 0.014 \\ n_4 = 8000 \\ m_4 = 8000 \\ L_4 = 137 \\ \sigma_+ = 50 \\ \sigma_- = 50 \end{cases} \begin{cases} a = 0.014 \\ n_5 = 10000 \\ m_5 = 10000 \\ L_5 = 172 \\ \sigma_+ = 50 \\ \sigma_- = 50 \end{cases}. \tag{2.144}$$

They select the same initial condition of a particle slower than potential wall ($r < \frac{1}{2}$) and we show in Fig. 2.5 the evolution of $|\Psi(\alpha,\beta_\pm)|$ for the first data set. As in the free particle case, the wave packet spreads with α, *i.e.* it delocalizes until it disappears in a finite α time. The real difference between the free particle case and the particle in a box case is

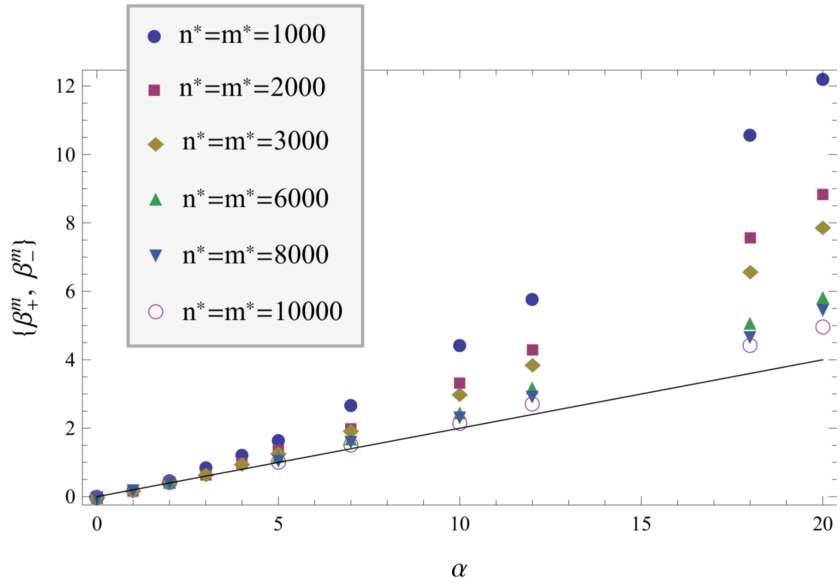

FIGURE 2.6: The points in the graph represent the evolution of the wave packet maximum position $\beta_\pm^m$ as a function of $|\alpha|$ for all data sets. The solid line represents the *polymer* semiclassical trajectory identified by the choice of the initial conditions.

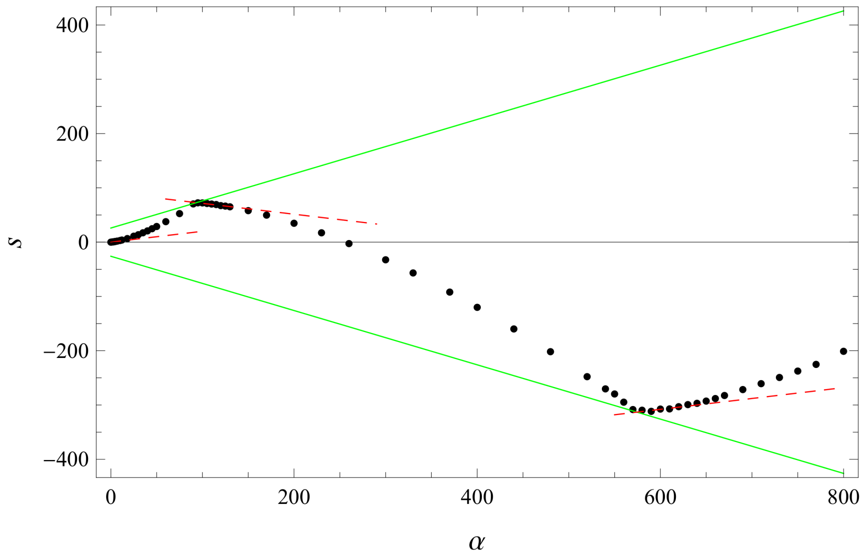

FIGURE 2.7: The points represent the evolution of the wave packet maximum position $\beta_\pm^m$ as a function of $|\alpha|$ for $a = 00.14, n^* = m^* = 3000, \sigma_+ = \sigma_- = 50, L_0 = 32$. The two solid lines represent the α-evolution of the position of two opposite wall of the square box. At last, the dashed lines represent the *polymer* semiclassical trajectory identified by the choice of the initial conditions that the wave packet follow after each bounce for a finite α-time.

the trajectory followed by the wave packet. If we study the evolution of the wave packet maximum position $\beta_\pm^m$ for the all data sets, we observe that the trajectory followed by the wave packet moves away from the *polymer* semiclassical trajectory identified by the initial condition, as we can see in Fig. 2.6. The separation from the *polymer* semiclassical trajectory depends on the quantum numbers n^*, m^*. In particular, the larger n^*, m^*, the longer the semiclassical trajectory is followed. Anyway, no matter how large they are, in a finite time α, the wave packet stops following the semiclassical trajectory, is directed to the potential wall and reaches it. As in Fig. 2.7, this behavior is repeated for every

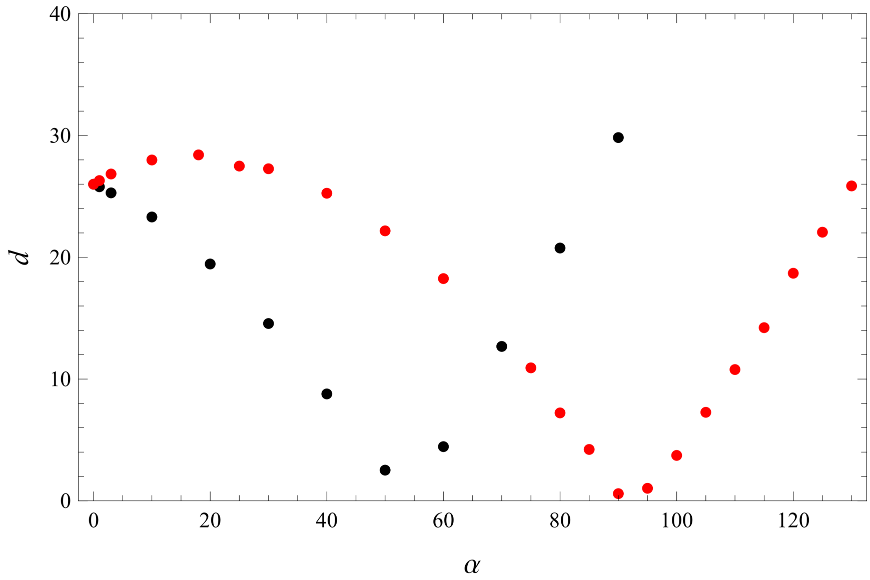

FIGURE 2.8: The red points represent the evolution of the distance d between the wave packet maximum position and the potential wall for $r < \frac{1}{2}$. The black points represent the evolution of the distance d between the wave packet maximum position and the potential wall for $r > \frac{1}{2}$.

unexpected bounce against the wall. This way, it is not possible to choose an initial semi-classical state (*i.e.* large n^*, m^*) conserved until the singularity. This result is opposite with respect to the one in Eq.(1.154), where in the standard theory the state remains classical until the singularity. It happens because we have a *time*-dependent initial condition (as in Eq.(2.143), it depends on α) that changes the particle velocity. This behavior is explained considering the two different data sets

$$\begin{cases} a_1 = 0.014 \\ n_1^* = m_1^* = 3000 \\ L_1 = 26 \\ \sigma_+ = \sigma_- = 50 \end{cases} \qquad \begin{cases} a_2 = 0.014 \\ n_2^* = m_2^* = 400 \\ L_2 = 26 \\ \sigma_+ = \sigma_- = 50 \end{cases} . \tag{2.145}$$

They respectively select a particle with initial velocity $r < \frac{1}{2}$ and with $r > \frac{1}{2}$. The first one is related to a particle in a box which semiclassically cannot reach the potential wall, while the second one is related to a particle in a box which semiclassically reaches the potential wall. For our purposes, we take two data sets with same values of $a, \sigma_\pm, L_0$ but with different n^* and m^*.

In Fig. 2.8, the evolution of the distance d between the wave packet maximum position and the potential wall in the two cases towards the singularity is described.

When the first one is still traveling, the second one has already bounced on the wall and it is traveling again. The red (light grey) points indicate the (expected) velocity change due to the dynamical initial condition (2.143). Thus, we can conclude that, when the potential is taken into account as an infinite well, any kind of a free semiclassical information is lost.

2.7 Evolutionary Quantum Approach

Here we take into account the evolutionary quantum theory, as it is analysed in [64],[21]. In these works it is considered a system of normal Gaussian coordinates $X^\mu = (T, X^i)$, or in other words a synchronous reference system, for which the line element of the metric takes the form:

$$ds^2 = -dT^2 + h_{ij} dX^i dX^j, \tag{2.146}$$

where the indices $\{i, j\}$ are summed over the spatial directions and h_{ij} is the spatial metric. In this way four components of the space-time metric $g_{\mu\nu}$ are fixed by the *Gaussian conditions*:

$$g_{00} + 1 = 0 \quad , \quad g_{0i} = 0. \tag{2.147}$$

The physical meaning of the previous conditions is more clear in the context of the ADM formalism where the space-time metric $g_{\mu\nu}$ is replaced by N,N^i,h_{ij} and the line element is

$$ds^2 = N^2 dt^2 - h_{ij}(N^i + dx^i)(N^j + dx^j). \tag{2.148}$$

If we make a comparison between the line elements (2.146) and (2.148) it is clear that the conditions (2.147) are equivalent to

$$N = 1 \quad , \quad N^i = 0, \tag{2.149}$$

where the foliation of the space-time is such that $t = T$ and $x^i = X^i$. The relations (2.149) tell us that everywhere the proper time between two neighbouring leaves is the same and that there is no displacement, with respect to the normal projection, between one leaves and another. If now we want to implement the Gaussian conditions in the action principles of general relativity, for example in the vacuum case, we can follow two ways: in the first one we impose the conditions after the variation of the Einstein-Hilbert action, while in the other case we adjoin them to the action, making use of Lagrangian multipliers technique, before the variation.

When we proceed in the first manner, we deal with the Einstein-Hilbert Action in vacuum

$$S^G = -\frac{1}{2\kappa} \int d^4x \sqrt{-g} R, \tag{2.150}$$

and a variation of this action with respect to the space-time metric $g_{\mu\nu}$ leads to the Einstein equations in vacuum:

$$G_{\mu\nu} = R_{\mu\nu} - \frac{1}{2} g_{\mu\nu} R = 0. \tag{2.151}$$

As shown in Section 1.2, an equivalent form of the action (2.150) is obtained in the ADM formalism and it is written as

$$S^G[h_{ij}, N, N^i] = \int_{\mathbb{R}} dt \int_{\Sigma} d^3x \left[\dot{h}_{ij} P^{ij} - (N^i \mathcal{H}_i^G + N \mathcal{H}^G)\right] \tag{2.152}$$

where the superscript G for the superHamiltonian and superMomentum specifies the gravitational origin of the terms. As always, the variation with respect to N and N^i gives the secondary constraints:

$$\mathcal{H}^G = \mathcal{H}_i^G = 0. \tag{2.153}$$

The Hamilton equations for h_{ij} and P_{ij}, once fixed $N = 1$ and $N^i = 0$, provide, together with the constraints (2.153), the Einstein equations in the synchronous reference frame.

The second way to proceed consists of adding the coordinate conditions (2.147) in the Einstein-Hilbert action by the multipliers M and M_i in such a way that an extra term S^F

appears in the action:

$$S[g_{\mu\nu}, M, M_k] = S^G + S^F, \tag{2.154}$$

with

$$S^F[g_{\mu\nu}, M, M_k] = -\frac{1}{2\kappa}\int d^4x \left[-\frac{1}{2}M\sqrt{-g}(g^{00}+1) + M_i\sqrt{-g}g^{0i}\right] \tag{2.155}$$

and where we defined the quantity:

$$\begin{cases} M := -\frac{\mathcal{H}^G}{\sqrt{h}}, \\ M_i := \frac{\mathcal{H}^G_i}{\sqrt{h}}. \end{cases} \tag{2.156}$$

Clearly the variation of the action (2.154) introduces a source term in the Einstein equations. The role of Lagrangian multipliers M, M_k is clear if we write the action (2.154) in the ADM formalism, in order to obtain:

$$S[h_{ab}, N, N^i, M, M_k] = \int_{\mathbb{R}} dt \int_{\Sigma} d^3x[\dot{h}_{ij}P^{ij} - (N^i\mathcal{H}^G_i + N\mathcal{H}^G) + \\ -\frac{1}{2}M\sqrt{h}(N - N^{-1}) + M_i\sqrt{h}NN^i]. \tag{2.157}$$

If we perform a variation by M and M_i we obtain the Gaussian conditions (2.149), while a variation with respect to N and N^i gives the Eqs. (2.156) and fix the multipliers M and M_i as functions of the canonical variables h_{ij}, P^{ij}. If we use the Eqs. (2.149) and (2.156) to eliminate the presence of the mutipliers N, N^i and M, M_i, the action (2.157) clearly reduces to the canonical action (2.154), so the two way to implement the Gaussian Conditions are equivalent.

Looking at the action (2.154), it is not invariant under arbitrary transformations of space-time coordinates and this is due to the fact that we have introduced a privileged coordinate system, *i.e* the normal Gaussian coordinates. However, it is always possible to restore the diffeomorphism invariance making a parametrization of the coordinates. It means that if we take the Gaussian coordinates as a functions of a arbitrary coordinates x^α in such a way that $X^\mu = (T(x^\alpha), X^i(x^\alpha))$ the action (2.154) can be expressed as:

$$S[g_{\alpha\beta}, M, M_k, X^\mu] = S^G + S^F = \\ = -\frac{1}{2\kappa}\int d^4x\sqrt{-g}R - \frac{1}{2\kappa}\int d^4x\sqrt{-g}\left[-\frac{1}{2}M(g^{\alpha\beta}T_{,\alpha}T_{,\beta}+1) + M_i g^{\alpha\beta}T_{,\alpha}X^i_{,\beta}\right], \tag{2.158}$$

that is manifestly invariant under arbitrary transformations of x^α.

The form of the action (2.158) allows us to understand the nature of the source of the gravitational field, described by that part of the action appearing in the second row. In [64] this source term is defined as *Gaussian Reference Fluid*.

The variation of the action (2.158) by the metric $g_{\alpha\beta}$ gives the Einstein equations:

$$G_{\alpha\beta} = \kappa T_{\alpha\beta}, \tag{2.159}$$

where

$$T^{\alpha\beta} = \frac{2}{\sqrt{-g}}\frac{\delta S^F}{\delta g_{\alpha\beta}} \tag{2.160}$$

is the energy-momentum tensor associated to the reference fluid. After the definition of the four-velocity vector

$$U^{\alpha} := -g^{\alpha\beta}T_{,\beta}, \tag{2.161}$$

it is possible to evaluate the energy-momentum tensor in order to give a clear physical interpretation of the presence model:

$$T^{\alpha\beta} = MU^{\alpha}U^{\beta} + M^{(\alpha}U^{\beta)}. \tag{2.162}$$

The Eq.(2.162) is equivalent to the Eckart energy-momentum tensor[46] that describes a heat-conducting fluid. The absence of a stress part in the energy-momentum tensor tells us that the Gaussian reference fluid behaves as a dust. In particular, if we impose only the time condition ($M^i = 0$) the Eq.(2.162) becomes:

$$T^{\alpha\beta} = MU^{\alpha}U^{\beta}, \tag{2.163}$$

which describes the behavior of an incoherent dust, where M is the rest mass density and U^{α} is the four-velocity.

If now we consider the canonical ADM form of the action (2.158) we have

$$S[h_{ij}, X^{\mu}, M, M_k] = \int_{\mathbb{R}} dt \int_{\Sigma} d^3x[\dot{h}_{ij}P^{ij} + \dot{X}^{\mu}P_{\mu} - (N^i\mathcal{H}_i + N\mathcal{H}), \tag{2.164}$$

with

$$\mathcal{H} = \mathcal{H}^G + \mathcal{H}^D \quad , \quad \mathcal{H}_i = \mathcal{H}_i^G + \mathcal{H}_i^D. \tag{2.165}$$

where $P_{\mu} = (P, P_i)$ are the conjugated momentas to $X_{\mu} = (T, X_i)$. The quantity $\mathcal{H}^D$ and $\mathcal{H}_i^D$ are respectively the superHamiltonian and supermomentum contribution due to the reference fluid and, when we take into account the case of an incoherent dust, they simply becomes:

$$\mathcal{H}^D = P \quad , \quad \mathcal{H}_i^D = X^j_{,i}P_j = 0. \tag{2.166}$$

As before, the variation with respect to N and N^i gives us the constraints:

$$\mathcal{H} = \mathcal{H}^G + \mathcal{H}^D = \mathcal{H}^G + P = 0, \tag{2.167}$$

$$\mathcal{H}_i = \mathcal{H}_i^G + \mathcal{H}_i^D = \mathcal{H}_i^G = 0. \tag{2.168}$$

The quantization procedure of the system composed by an incoherent dust coupled with gravity[64] consists to associate to the canonical variables the following operator representations

$$\hat{h}_{ij} = h_{ij}\times \quad , \quad \hat{P}^{ij} = -i\frac{\delta}{\delta h_{ij}}, \tag{2.169}$$

$$\hat{X}^{\mu} = X^{\mu}\times \quad , \quad \hat{P}_{\mu} = -i\frac{\delta}{\delta X^{\mu}}, \tag{2.170}$$

and to evaluate the action of the quantum version of the constraints (2.167),(2.168) on the physical states identified as the functional $\Psi[X^{\mu}, h_{ij}]$, *i.e.* the wave function of the Universe.

First of all, the condition $\mathcal{H}_i^D = X^j_{,i}P_j = 0$ tells us that

$$\frac{\delta}{\delta X^i}\Psi[X^{\mu}, h_{ij}] = 0, \tag{2.171}$$

so the wave function of the Universe does not depend on the spatial fluid variables X^i

but only on the time fluid variable T. Furthermore, the quantum version of the constraint (2.168),

$$\hat{\mathcal{H}}_i \Psi[T, h_{ij}] = 0, \tag{2.172}$$

ensures us that $\Psi[T, h_{ij}]$ does not depend on the particular metric representation, but only on 3-geometries.

Remembering the definitions of the operators (2.169),(2.170), the application of the constraint (2.167) on the physical states $\Psi[T, h_{ij}]$ leads us to the Wheeler-DeWitt(WDW) equation that resembles a Schrodinger-like equation:

$$\hat{\mathcal{H}}\Psi[T, h_{ij}] = \left[\hat{\mathcal{H}}^G - i\frac{\delta}{\delta T}\right]\Psi[T, h_{ij}] = 0 \rightarrow i\frac{\delta}{\delta T}\Psi[T, h_{ij}] = \hat{\mathcal{H}}^G\Psi[T, h_{ij}], \tag{2.173}$$

which determines the evolution of the system with respect to the time variable T. It is easy to verify that a general solution for the Eq.(2.173) is

$$\Psi(T, h_{ij}) = \int dE\psi(E, h_{ij})e^{-iET}, \tag{2.174}$$

leading to the time independent eigenvalue problem

$$\hat{\mathcal{H}}^G\psi = E\psi. \tag{2.175}$$

From the Eq.(2.175) we can see that E is the eigenvalue of the superHamiltonian, and it is associated to the dust energy density via the relation $\rho_{dust} = -\frac{E}{\sqrt{h}}$.

The Kuchař and Torre approach is clearly a promising point of view for addressing the problem of time, viewed as a necessary weakening of the General Relativity Principle. Indeed, although the general covariance is preserved via a general reparametrization, the time evolution of the quantum gravitational field comes out from the privileged character of the Gaussian reference frame. But the real critical point of the formulation presented above is that the super-Hamiltonian spectrum is not positive defined and consequently the dust fluid has to possess a non-positive energy density: a really unpleasant physical property, which is a serious shortcoming of the formulation. In [21], it has been demonstrated that a real incoherent dust coupled to gravity play the role of a physical clock and this issue constitutes a complementary approach to the present one.

A part from the non-trivial question about how it is possible to make the Gaussian frame compatible with the energy conditions [64] (*i.e.* its energy momentum tensor does not fulfill the condition to represent a physical fluid), we can see that a dualism exists between a physical clock for the gravitational field and a fluid of reference coupled to the gravitational field dynamics, see also [80],[72],[73]. From a more general point of view, we can infer that the coupling of the gravitational field to a given physical fluid is equivalent to induce a no longer vanishing super-Hamiltonian and/or super-momentum constraints. From a field theory point of view, we are arguing that the quantization of the gravitational field is affected by the choice of a specific gauge, *i.e.* of a real system of reference, by restoring a time evolution. In quantum gravity, the distinction between a real reference frame (a physical system) having a non-zero energy-momentum tensor, and a simple system of coordinates (a mathematical reparametrization of the dynamics) is deep: while in General Relativity the two concepts overlap, as soon as, we take the real fluid as a test system, on the quantum level, the energy-momentum tensor of the reference frame participate the gravitational field dynamics via the super-Hamiltonian spectrum.

2.8 Vilenkin Interpretation of the Wave Function of the Universe

The behavior of the Universe in quantum cosmology is described by the wave function of the Universe ψ, which represents the solution of the WDW equation. One of the main issues related to the wave function of the Universe is its probabilistic interpretation. In a generic quantum mechanics system described by a wave function $\psi(x_i, t)$, where x_i are coordinates and t is the time, the probability to find the system in a particular configuration space element $d\Omega_x$ is:

$$dP = |\psi(x_i, t)|^2 d\Omega_x. \tag{2.176}$$

The definition above provides in any case a semi definite probability, $dP \geq 0$, and a well-normalized system:

$$\int |\psi(x_i, t)|^2 d\Omega_x = 1. \tag{2.177}$$

In quantum cosmology the wave function of the Universe, defined on the super-space, depends on the configuration of the three-metrics $h_{ij}(x)$ and the matter fields $\phi(x)$ without an explicit time dependence. To discuss the problem in a simple way, let us consider the homogeneous minisuperspace models, in which the three-metrics and the matter fields does not depend on the position x. The action for this class of model is

$$S = \int dt\{p_\alpha \dot{h}^\alpha - N[h^{\alpha\beta} p_\alpha p_\beta + U(h)]\}, \tag{2.178}$$

where h^α represent the superspace variables, p_α are the conjugated momenta to h^α, $N = N(t)$ is the lapse function, $h^{\alpha\beta}$ is the superspace metric and $U(h)$ takes into account the spatial curvature and the potential energy of matter field.

If we decide to proceed in analogy with the Eq.(2.176), a straightforward extension for the probability is:

$$dP = |\psi(h_\alpha)|^2 \sqrt{h} d^n h. \tag{2.179}$$

The problem with the definition (2.179) is the "time" dependence of the variables h_α. The consequence is that the probability is not normalizable. In fact, taking into account the term $\sqrt{h} d^n h$ is equivalent to consider, in a generic quantum mechanics systems, the quantity $d\Omega_x dt$. For the latter case we have

$$\int |\psi(x_i, t)|^2 d\Omega_x dt = \infty, \tag{2.180}$$

and proceeding by analogy in quantum cosmology we have

$$\int |\psi(h_\alpha)|^2 \sqrt{h} d^n h = \infty. \tag{2.181}$$

A way to avoid this consists to provide an alternative definition of probability based on the conserved current[92]

$$J^\alpha = -\frac{i}{2} h^{\alpha\beta} [\psi^* \nabla_\beta \psi - \psi \nabla_\beta \psi^*] \quad , \quad \nabla_\alpha J^\alpha = 0. \tag{2.182}$$

This way, the probability to find the Universe in a particular state is

$$dP = J^\alpha d\Sigma_\alpha, \tag{2.183}$$

where dΣ_α represents the separation between the three-dimensional surfaces on which the current is defined. These surfaces play a role similar to that of constant-time surfaces in conventional quantum mechanics. Furthermore, if we consider the conservation of the current (2.182), than the conservation of the probability is ensured.

The problem with the probability (2.183) is that it can be negative, as it is easy to show considering a given wave function ψ and then the complex-conjugate ψ^*. The situation is the same that happens for the negative probabilities in the Klein-Gordon equation (the WDW equation resembles a Klein-Gordon equation with a variable mass).

The Vilenkin interpretation of the wave function of the Universe[92] appears as a solution to solve this issue. Such approach consists in the separation, for the configuration variables, in two classes: *semiclassical* and *quantum*. Following this prescription, the quantum variables represent a small subsystem of the Universe and the semiclassical variables act as an external observer for the quantum dynamics, or in other words the effects of the quantum variables on the semiclassical ones are negligible. We choose to describe for the configuration space the notation q_α for the semiclassical variables and ρ_ν for the quantum variables. The WDW equation for the action (2.178) takes the form

$$(\nabla^2 - U - H_\rho)\psi = 0 \quad , \quad \nabla^2 = \frac{1}{\sqrt{h}}\partial_\alpha(\sqrt{h}h^{\alpha\beta}\partial_\beta)\psi, \tag{2.184}$$

where $h = |\det h_{\alpha\beta}|$ and $\partial_\alpha = \frac{\partial}{\partial h^\alpha}$. The operator $\nabla^2 - U$ that appears in the WDW equation, is the part that survives when we neglect all the quantum variables ρ_ν and their conjugated momenta. For this reason, the other part H_ρ is due to the presence of the quantum subsystem and its smallness is ensured by the existence of a small parameter ϵ for which

$$\frac{H_\rho\psi}{(\nabla^2 - U)\psi} = O(\epsilon), \tag{2.185}$$

where ϵ is a small parameter proportional to $\hbar$. Also the superspace metric can be expanded in terms of ϵ as

$$h_{\alpha\beta} = h^0_{\alpha\beta}(q) + O(\epsilon) \tag{2.186}$$

and the wave function of the Universe can be written as

$$\psi = A(q)e^{iS(q)}\chi(q,\rho). \tag{2.187}$$

In order to perform a WKB expansion as an expansion series in ϵ in a properly way, we point out that the potential term $U(q)$ is of the order ϵ^{-2} and the action $S(q)$ is of the order ϵ^{-1}. This way, if we consider the wave function (2.187) inside the Eq.(2.184) we obtain, at the lowest order in ϵ, the Hamilton-Jacobi equation for S:

$$h_{\alpha\beta}\nabla_\alpha S\nabla_\beta S + U = 0. \tag{2.188}$$

At the next order we obtain the Equation:

$$2\nabla A\nabla S + A\nabla^2 S + 2i\nabla S\nabla\chi - H_\rho\chi = 0. \tag{2.189}$$

The terms of the Eq.(2.189) can be decoupled in a pair of equations making use of the *Adiabatic Approximation*. It consists in requiring that the semiclassical evolution be principally contained in the semiclassical part of the wave function, while the quantum part depends on it only parametrically. The adiabatic approximation is therefore expressed by the condition

$$|\partial_q A(q)| \gg |\partial_q\varphi(q,\rho)|. \tag{2.190}$$

Using the relation (2.190) in the Eq.(2.189) we obtain that:

$$\frac{1}{A}\nabla(A^2\nabla S)=0 \quad , \quad 2i\nabla S\nabla\chi - H_\rho\chi = 0. \tag{2.191}$$

The first equation represents the conservation of the current defined in Eq.(2.182) obtained neglecting the quantum part of the wave function, or in other words using a wave function

$$\psi = A(q)e^{iS(q)}. \tag{2.192}$$

The explicit form of the current is

$$j_0^\alpha = |A|^2\nabla^\alpha S. \tag{2.193}$$

Being the conjugated momenta to q_α equals to $p_\alpha = \nabla_\alpha S$, the tangent vector to the classical trajectory can be obtained starting from the variational principal $\delta_{p_q} S = 0$, in order to obtain:

$$\dot{q}^\alpha = 2N\nabla^\alpha S. \tag{2.194}$$

It is possible to show that, by requiring that the three-dimensional surfaces Σ_α on which we defined the probability (2.183) are crossed only one time by all the classical trajectories, the sign of the element $\dot{q}^\alpha d\Sigma_\alpha$ is always the same for any choice of the surface elements $d\Sigma_\alpha$. Being the initial sign arbitrary ,we can choose

$$\dot{q}^\alpha d\Sigma_\alpha > 0. \tag{2.195}$$

The classical current conservation law

$$\nabla(A^2\nabla S) = 0 \tag{2.196}$$

can be recasted in a continuity equation form. The first step is the identification of the classical probability distribution $\sigma_0 = |A|^2$. Furthermore, using the relation (2.194) and performing a coordinate transformation for one coordinate of the superspace as $q_n = t$, the Eq.(2.196) takes the form

$$\frac{\partial\sigma_0}{\partial t} + \partial_a\mathcal{J}^a = 0 \tag{2.197}$$

where $\mathcal{J}^a = \sigma_0\dot{q}^a$ and the index a runs from 1 to $(n-1)$. From the continuity equation (2.197) a conserved charge can be identified integrating both sides over a $d\Sigma_0$ volume, where $d\Sigma_0$ is the surface element of the subspace defined from the $(n-1)$ remaining classical variables q^α, and making use of the Gauss Theorem on the current term. This procedure allow to normalize the classical probability distribution as

$$\int \sigma_0(q)d\Sigma_0 = 1. \tag{2.198}$$

The second equation in (2.191) can be recast in a Schrodinger-like equation for the quantum subsystem using the relation (2.194):

$$i\frac{\partial\chi}{\partial t} = NH_\rho\chi. \tag{2.199}$$

In order to find the total (classical and quantum) probability distribution we consider the wave function (2.187) for the current (2.182). This brings to:

$$J = \sigma_\chi j_0^\alpha + \frac{1}{2}|A|^2 j_\chi^\nu, \tag{2.200}$$

where we defined the quantum current j^{ν}_{χ} and probability distribution σ_{χ} as:

$$j^{\nu}_{\chi} = -\frac{i}{2}[\chi^*\nabla_{\beta}\chi - \chi\nabla_{\beta}\chi^*] \quad , \quad \sigma_{\chi} \equiv |\chi|^2. \tag{2.201}$$

From the previous definition of the quantum part of the current and from the Schrodinger equation (2.199), a continuity equation for the quantum probability distribution can be written as

$$\frac{\partial\sigma_{\chi}}{\partial t} + N\nabla_{\nu}j^{\nu}_{\chi} = 0, \tag{2.202}$$

To complete the scheme we need to analyze if the total probability distribution is normalizable. It can be written as

$$\sigma(q,\rho) = \sigma_0(q)\sigma_{\chi}(q,\rho), \tag{2.203}$$

where $\sigma_0(q)$ is the probability distribution relates to the semiclassical variables. In this case it is possible to show that the surface element of the constant-time surfaces can be written in the form $d\Sigma = d\Sigma_0 d\Omega_{\rho}$, where $d\Sigma_0$ provides the normalization for the classical system:

$$\int \sigma_0(q)d\Sigma_0 = 1, \tag{2.204}$$

while $d\Omega_{\rho}$ gives the normalization for the quantum subsystem:

$$\int \sigma_{\chi}(q,\rho)d\Omega_{\rho} = 1. \tag{2.205}$$

As a consequence, the entire probability distribution is normalizable as

$$\int \sigma_0(q)\sigma_{\chi}d\Sigma_0 d\Omega_{\rho} = 1 \tag{2.206}$$

Chapter 3

Chaos removal in the $R + qR^2$ gravity: the Mixmaster model

The chaotic dynamics of the Mixmaster Universe [14],[74],[75] is a basic prototype of the local (sub-horizon) behaviour of the generic cosmological solution (the so-called BKL conjecture[13]). Investigating the stability of such a chaotic picture with respect to the presence of matter [11],[81],[79] and space-time dimensions number has seen a great effort over the last four decades and the most significant issue was the proof of the chaos removal when a massless scalar field is involved in the dynamics. Such a result is a consequence of the capability manifested by the scalar field kinetic energy of affecting the second (quadratic) Kasner condition, easily restated in the Hamiltonian picture, as shown in [17]. This property of the massless scalar field acquires intriguing perspectives when $f(R)$ modified theory of gravity are considered [26],[30],[85],[84],[50]. In fact, these alternative formulation of the gravitational field dynamics can be represented by an equivalent scalar-tensor picture: the scalar degree of freedom associated to the form of the function f is expressed via a self-interacting scalar field, coupled to the ordinary General Relativity [6],[8],[7],[42]. When implementing this scalar-tensor scheme to the Mixmaster Universe dynamics, a natural question arise: the kinetic term of the scalar field removes the chaotic behavior, but the presence of a potential term could restore it? Thus we can study, for specific modified theories of gravity, if the Mixmaster chaos survives or not, simply characterizing the corresponding scalar field potential. Here we analyze the modified gravity theory corresponding to a quadratic correction in the Ricci scalar to the ordinary Einstein-Hilbert Lagrangian, both because it is the simplest viable deviation from General Relativity (apart from a cosmological constant term), as well as the first correction emerging from a Taylor expansion of a $f(R)$ theory for very small values of the space-time Ricci scalar, i.e. for very law curvatures, like we observe today in the Solar System[87]. The quadratic term in the Ricci scalar provides an exponential-like potential term for the self-interacting scalar field, when a scalar-tensor reformulation of the model is considered. This case is particularly appropriate to the analysis we pursue of the Mixmaster dynamics in terms of the Misner-Chitré-like variables [79],[62],[56],[32]. In fact, the kinetic term of the scalar field is on the same footing of the anisotropy term contribution and, for the considered Lagrangian, also the potential term is isomorphic to the spatial curvature of the model, i.e. the total potential term is constituted by equivalent exponential profile. In the asymptotic limit toward the initial singularity the total potential takes the form of four potential walls, whose morphology determines if the configuration domain is closed or not. Indeed, we demonstrate how the whole domain, available in principle, is a constant negative curvature space (half-Poincarè space). Thus, if the domain defined on such a space by the total potential is closed, we can easily conclude that the Mixmaster Universe dynamics has a chaotic evolution toward the singularity. We first analyze the case of the Mixmaster Universe in the presence of a massless scalar field, demonstrating the open nature of its configuration space and the implied existence of a stable Kasner regime to the initial singularity. Then, we face a detailed study of the dynamics in the presence of the total potential and the still open structure of the configuration domain. Thus, we demonstrate the non-chaotic nature of the Mixmaster Universe behavior, as it is described by the scalar-tensor version of the R^2-gravity. Since, the applicability of the BKL conjecture to the scalar-tensor formulation is straightforward as in the simpler Einsteinian case [14], our result is expected to shed light to the non-chaotic nature of the asymptotic behaviour of a generic Universe near the cosmological singularity, as far as a quadratic correction in the Ricci scalar is included in the gravitational action. This issue has to be joint to the already well-known cosmological implication of such a modified theory of gravity [30],[85] in order to provide a consistent picture of the Universe birth in such a revised dynamical scheme.

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3.1 Mixmaster Universe in the R^2-gravity

In Section 1.6, we demonstrate the main feature of the Mixmaster model: the presence of the chaos. In the framework of the Poincarè-half plane illustrated in Section 1.6.4, as shown by [56], the asymptotic evolution towards the singularity is covariantly chaotic because it is isomorphic to a billiard on the Lobachevsky plane. This demonstration is based essentially on three points:i)the Jacobi metric in the u, v plane has a negative constant curvature; ii)the Lyapunov exponent, defined as in [86], are greater than zero; iii)the configuration space is (dinamically) compact. The occurrence of the these three properties ensures that the geodesic trajectories cover the whole configuration space, *i.e.* the chaotic behavior . As shown in Section 1.6.2, considering the Mixmaster model coupled with a free scalar field leads to the removal of the oscillatory behavior when we approach the singularity. We want to study if a quadratic correction in the gravitational Lagrangian are able to affect the chaotic structure of the Mixmaster model. Now we analyze the case of the gravitational Lagrangian (1.38), associated to a Scalar-Tensor action (1.36) with the scalar potential term (1.39), when the Bianchi IX model is considered. Differently from the presence of a scalar field in the Mixmaster model studied in Section 1.6.2, here we consider the whole problem, included the potential term, due to the fact that it naturally emerges in the scalar tensor framework of an $f(R)$ theory. As starting point we consider the configuration variables in terms of the Misner variables plus the scalar field $\{\alpha, \beta_+, \beta_-, \phi\}$. In this way, the action (1.36) can be rewritten through a Legendre transformation as

$$S = S_{IX} + S_\phi = \int \Big[p_\alpha \dot{\alpha} + p_+ \dot{\beta}_+ + p_- \dot{\beta}_- + p_\phi \dot{\phi} - N(\mathcal{H}) \Big] \, dt. \tag{3.1}$$

This time the variation of the action with respect to the lapse function leads to the super-Hamiltonian constraint

$$\mathcal{H} = -p_\alpha^2 + p_+^2 + p_-^2 + p_\phi^2 + 12\pi^2 e^{4\alpha} V_{IX} + 4e^{6\alpha} U = 0 \tag{3.2}$$

in which is present the potential term of the scalar field $U = U(\phi)$. In order to simplify the notation, in this chapter we have chosen to use the geometric unit system for which $(c = G = \hbar = 1)$. Furthermore, without loss of generality, in Eq.(3.2), we rescaled the zero point of $\alpha \to \alpha - \alpha_0$, so that the spatial metric factor $e^{3\alpha} \to \frac{1}{(6\pi)} e^{3\alpha}$, and we redefined the scalar field amplitude $\phi \to \sqrt{2}(6\pi)\phi$, so that the relative factor between p_α^2 and p_ϕ^2 is the unity. Solving the scalar constraint with respect to the momenta p_α brings to the reduced Hamiltonian

$$H \equiv \sqrt{p_+^2 + p_-^2 + p_\phi^2 + 12\pi^2 e^{4\alpha} V_{IX} + 4e^{6\alpha} U}. \tag{3.3}$$

Looking at the reduced Hamiltonian (3.3), it is evident that the whole potential term (curvature plus scalar field), in the context of the Misner variables, reproduces the usual dynamic of an infinitely steep potential well, with the position of the walls that depends on the time variable α. A way out from this problem, as demonstrated in Section **??** for the vacuum Mixmaster model, is represented by the introduction of the Misner-Cithrè variables.

Keeping in mind the conceptual steps that brings from the Misner variables to the Misner-Cithrè variables described in the Poincarè half-plane, we individuate a natural parametrization that consider the presence of the scalar field in the model. It reads as:

$$\begin{aligned}
\alpha &= -e^\tau \xi, \\
\beta_+ &= e^\tau \sqrt{\xi^2 - 1} \cos\theta, \\
\beta_- &= e^\tau \sqrt{\xi^2 - 1} \sin\theta \cos\delta, \\
\phi &= e^\tau \sqrt{\xi^2 - 1} \sin\theta \sin\delta.
\end{aligned} \tag{3.4}$$

This modified version of the Misner-Cithrè variables contains the variable δ, which is defined in the range of values $0 \le \delta < 2\pi$ and that concerns the scalar field ϕ. In particular, in the limit $\delta \to 0$ the presence of the scalar field disappears and the relations (3.4) reduce to the standard ones (1.172). The next step is to identify the Misner-Cithrè sector $\{\xi, \theta\}$ of the latter set of variables with the Poincarè variables $\{u, v\}$. Using the relations (1.184),(1.185), we can rewrite the change of variables (3.4) in what we defined as *Poincarè half-space*

$$\begin{aligned}
\alpha &= -e^\tau \frac{1 + u + u^2 + v^2}{\sqrt{3}v}, \\
\beta_+ &= e^\tau \frac{-1 + 2u + 2u^2 + 2v^2}{2\sqrt{3}v}, \\
\beta_- &= e^\tau \frac{-1 - 2u}{2v} \cos\delta, \\
\phi &= e^\tau \frac{-1 - 2u}{2v} \sin\delta,
\end{aligned} \tag{3.5}$$

where $-\infty < \tau < \infty$, $-\infty < u < +\infty$, $0 < v < +\infty$ and $0 < \delta < 2\pi$. In this new system of variables the reduced Hamiltonian takes the form:

$$-p_\tau = H \equiv \sqrt{v^2 \left[p_u^2 + p_v^2 + 4\frac{p_\delta^2}{(1+2u)^2}\right] + e^{2\tau}\mathcal{V}}. \tag{3.6}$$

The introduction of the degree of freedom related to the scalar field implies that the point-Universe lives inside a 3-dimensional domain in the configuration space u, v, δ determined by the potential term:

$$\begin{aligned} e^{2\tau}\mathcal{V} &= e^{2\tau}[12\pi^2 e^{-4e^{\tau}\xi(u,v)}V_{IX}(u,v,\delta,\tau) + 4e^{-6e^{\tau}\xi(u,v)}U(u,v,\delta,\tau)] = \\ &= 12\pi^2 e^{2\tau}\left(e^{-\frac{12e^{\tau}}{\sqrt{3}v}(u+u^2+v^2)} + e^{-\frac{6e^{\tau}}{\sqrt{3}v}(1+(1+2u)\cos\delta)} + e^{-\frac{6e^{\tau}}{\sqrt{3}v}(1-(1+2u)\cos\delta)}\right) + \\ &+ \frac{e^{2\tau}}{8\pi q}\left(e^{-\frac{12e^{\tau}}{\sqrt{3}v}(1+u+u^2+v^2)} - 2e^{-\frac{6e^{\tau}}{\sqrt{3}v}(1+u+u^2+v^2-2\sqrt{2\pi^3}(1+2u)\sin\delta)} + \right. \\ &\left. e^{-\frac{6e^{\tau}}{\sqrt{3}v}(1+u+u^2+v^2-4\sqrt{2\pi^3}(1+2u)\sin\delta)}\right), \end{aligned} \tag{3.7}$$

where $\xi(u,v) = \frac{1+u+u^2+v^2}{\sqrt{3}v}$. Due to the exponential forms of the terms in Eq.(3.7), when the singularity is approached ($\tau \to \infty$) the point-Universe is confined to live inside a 3-dimensional domain defined as the region where all the exponents of the six terms are simultaneously greater than zero. Looking the Eq.(3.7), the potential term $\mathcal{V}$ behaves as an infinitely steep potential well as in the Poincarè variables in Section 1.6.4. So for the evolution of the point-Universe it is possible to neglect the potential everywhere in a suitable domain. As first step we study the case in absence of all the potential terms ($\mathcal{V} = 0$), i.e. we deal with the Hamiltonian problem:

$$H = v\sqrt{p_u^2 + p_v^2 + 4\frac{p_\delta^2}{(1+2u)^2}}. \tag{3.8}$$

The Hamiltonian equations for this potential-free system (Bianchi I model with the massless scalar field) are

$$\begin{aligned} \dot{u} &= \frac{\partial H}{\partial p_u} = \frac{v^2}{\epsilon}p_u \quad , \quad \dot{p_u} = -\frac{\partial H}{\partial u} = \frac{8v^2}{\epsilon}\frac{p_\delta^2}{(1+2u)^3} \\ \dot{v} &= \frac{\partial H}{\partial p_v} = \frac{v^2}{\epsilon}p_v \quad , \quad \dot{p_v} = -\frac{\partial H}{\partial v} = -\frac{\epsilon}{v} \\ \dot{\delta} &= \frac{\partial H}{\partial p_\delta} = \frac{4v^2}{\epsilon}\frac{p_\delta}{(1+2u)^2} \quad , \quad \dot{p_\delta} = -\frac{\partial H}{\partial \delta} = 0. \end{aligned} \tag{3.9}$$

It is possible to demonstrate, as we approach the singularity, that H is a constant of motion with respect to the "time" variable τ, following [56]. Thus, we perform the substitution $H \simeq \epsilon = const.$ inside Eqs.(3.9). It is now possible, by following the Jacobi procedure[93] and using the equations of motion (3.9), to write down the line element for the three-dimensional Jacobi metric in terms of the configuration variables, *i.e.*

$$ds^2 = \frac{\epsilon}{v^2}\left[du^2 + dv^2 + \frac{(1+2u)^2}{4}d\delta^2\right]. \tag{3.10}$$

By a direct calculation we see that this metric has a negative constant curvature (the associated Ricci scalar is $R = -\frac{6}{\epsilon}$) and then the point-Universe moves over a negatively curved three-dimensional space. Furthermore, we can find two singular values for the metric in correspondence to $u = -\frac{1}{2}$, $v = 0$. This feature allows us to restrict the domain of the configuration space in which we will study the trajectories of the point-Universe to the fundamental one identified by the inequalities $-\frac{1}{2} < u < +\infty$, $0 < v < +\infty$, $0 < \delta < 2\pi$. Indeed there is no way for the point-Universe trajectories to cross over the two planes $u = -\frac{1}{2}$, $v = 0$ (each choice of the Lobachevsky "half-space" is equivalent respect to the other one). The intermediate step toward the general case of the potential (3.7), corresponding to the ordinary Mixmaster model in the presence of a massless scalar field, takes place when we retain only the exponential terms due to the spatial curvature, namely $\mathcal{V} \simeq 12\pi^2 e^{-4e^{\tau}\xi(u,v)} V_{IX}(u, v, \delta, \tau)$. Then, the point-Universe lives in the region where are simultaneously satisfied the three following conditions

$$\begin{cases} 1 + (1 + 2u)\cos\delta > 0, \\ 1 - (1 + 2u)\cos\delta > 0, \\ u(u + 1) + v^2 > 0. \end{cases} \tag{3.11}$$

We now implement a numerical integration of the system (3.9) in order to analyse the

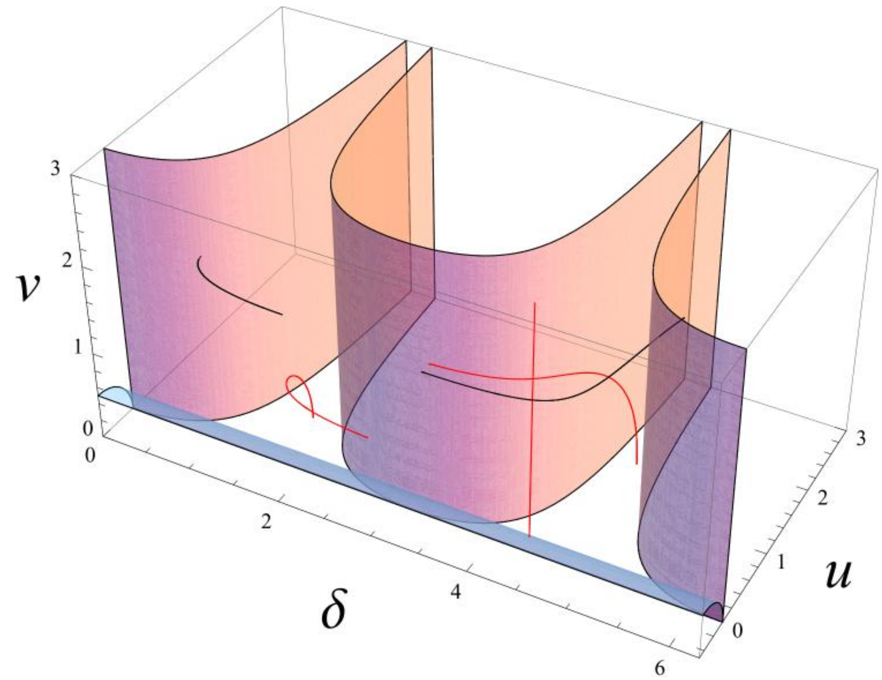

FIGURE 3.1: The black lines represent the trajectories associated to a points-Universe that bounce against the walls. Instead, the red lines describe the points-Universe witch directly approach the singularity.

behaviour of the trajectories in the potential free region and then use this result for interpreting the effect of the scalar curvature. As we can see in the Fig.3.1 an opening of the domain emerges due to the presence of the scalar field and it is possible to individuate two families of trajectories: those ones corresponding to a point-Universe that bounces against the walls and turn back inside the domain (the black ones) and those corresponding to a particle that approach the so called "absolute"[61] (the red ones), for values $v \to 0, \infty$, with no other bounces until the singularity. The presence of the trajectories of the second family shows the removal of the oscillatory behavior of the Mixmaster model coupled with a massless scalar field [13],[17]. Let us see what happen if we consider the complete potential term(3.7). This time the restrictions on the dynamics imply that the particle is confined inside a region where all the six exponential terms in Eq.(3.7) are simultaneously greater than zero. We can immediately remove one of the six conditions because the first exponent related to the potential of the scalar field $1 + u + u^2 + v^2$ is always greater than zero for any values of u, v taking in consideration. Thus, the five conditions that identify the domain are

$$\begin{cases} 1 + (1 + 2u) \cos\delta > 0 \\ 1 - (1 + 2u) \cos\delta > 0 \\ u(u + 1) + v^2 > 0 \\ 1 + u + u^2 + v^2 - 2\sqrt{2\pi^3}(1 + 2u) \sin\delta > 0 \\ 1 + u + u^2 + v^2 - 4\sqrt{2\pi^3}(1 + 2u) \sin\delta > 0 \end{cases} \tag{3.12}$$

We observe that the last of the conditions above naturally implies the validity of the fourth one too. Thus, we indeed deal with four potential walls only. As we can see in the Fig.3.2, taking into account also the potential term $U(u, v, \delta, \tau)$ implies that the available configuration space for the point-Universe is clearly reduced with respect to the case $U = 0$ (see Fig.3.1). However, trajectories yet exist(the red lines in the Fig.3.2) corresponding to a point-Universe that is able to reach the absolute for $v \to 0, \infty$. For this reason we can firmly conclude that a quadratic correction in the Ricci scalar to the Einstein-Hilbert action, that in the Scalar-Tensor theory is equivalent to the dynamics of a self-interacting scalar field (with potential terms of the form (1.39)), is able to remove the never-ending bounces of the point-Universe against the walls. As a result of the bounces against the infinite potential walls (which can be described by a reflection rule[62],[40]), soon or later the point-Universe reach a trajectory connected with the absolute. It is worth

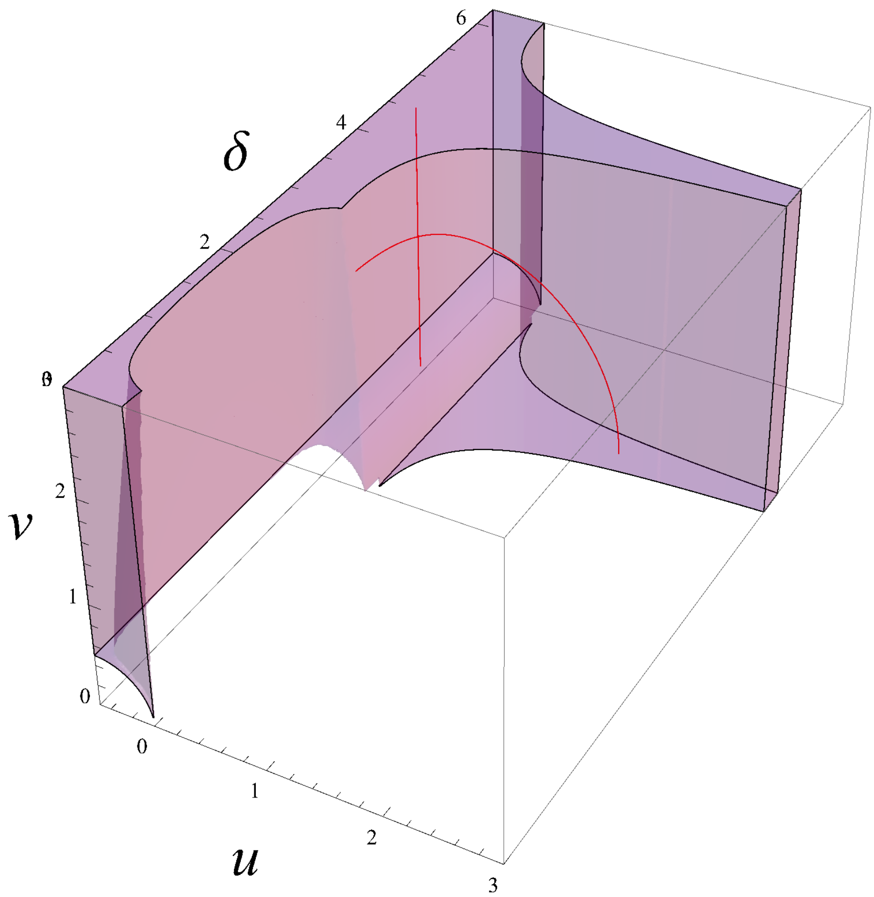

FIGURE 3.2: The point-Universe lives inside the region marked by the walls, where the conditions (3.12) are verified. We also sketch the trajectories reaching the absolute.

noting that the analysis above is referred to the choice $q > 0$, in which case the sign of the scalar field potential is the same one of the scalar curvature. This choice is forced by the request that the additional scalar mode, associated to the quadratic modification, be a real (non-tachyonic) massive one, accordingly to the original Starobinsky approach in [87] and demonstrated also in [25]. However, in the case $q < 0$, the scalar field potential would not contribute an infinite positive wall, but an infinite depression. Since in the region of zero potential, the point-Universe has always positive "energy", we can easily conclude that such a case overlaps the non-chaotic potential-free one. We now observe that, in correspondence to the configuration region $v = 0, \infty$ and $\delta = \frac{3\pi}{2}$, the scalar field acquires negative diverging values and its potential terms manifests a diverging behaviour. Such a profile of the scalar field is typical of a Bianchi I solution near the singularity [11] and the diverging character of the potential term means that General Relativity can not be asymptotically recovered. Rigorously speaking, the present result on the chaos structure applies to a quadratic correction in the Ricci scalar only, because it is the first terms of the Taylor expansion of the function $f(R)$ working nearby the singularity. Nonetheless, our analysis has a general validity, as soon as, we take into account a physical cut-off at the Planck time, where classical theory starts to fail and a quantum treatment is required. In fact, the Planckian cut-off would remove the ϕ and $U(\phi)$ divergences, allowing the Taylor expansion for $q \lesssim \frac{(ct_{cut})^2}{l_p^2}$, where t_{cut} being the cut-off time and l_P the Planck length. Since $t_{cut} > \frac{l_p}{c}$, we deal with the (non-severe) restriction $q \lesssim 1$ for preserving the general nature of our result. This estimation follows requiring $R > qR^2$ and remembering that for the case of a Kasner solution, in the presence of a potential-free scalar field, the Ricci scalar behaves as $R \sim \frac{1}{t_s^2}$, where t_s is the synchronous time. We stress that qualitatively, a similar argument is at the ground of the non-chaotic nature of the Bianchi IX Loop Quantum dynamics in the semi-classical limit [19]. However, the field $\phi(t_s)$ admits, both for $v \to 0, \infty$ and $\delta = \pi/2$, trajectories implying its positive divergence. For such behaviours, corresponding to an open region in the initial condition, the potential $U(\phi)$ approaches a constant value and ϕ is effectively massless. It is just the existence of these diverging profiles at the ground of the chaos removal in the present model. The massless nature of the potential along specific trajectories is a good criterion for determining the chaotic properties of the Mixmaster Universe in a specific non-expanded $f(R)$ model. In fact, The behavior of the free scalar field reads $\phi_f(t_s) \propto \ln t_s$ and the corresponding kinetic energy density stands as $1/t_s^2$. Then, for a given $f(R)$ model, fixing the potential $U(\phi)$, the chaos removal is ensured by the validity of the condition $\lim_{t_s \to 0} U(\phi_f(t_s))t_s^2 = 0$. Clearly, the non-chaoticity is ensured if such a limit holds for a non-zero measure set of trajectories.

3.2 Quantization in the Poincarè-half space

The main reason that pushed us to consider the Poincarè variables in the previous Section is that they provide anisotropy parameters independent from time variable 3.12 and a space of configurations with a treatable geometric structure. It is principally for those reason that we considered them for the quantization of model introduced in Section 3.1, in which we have shown that the evolution towards the singularity of the Bianchi IX model with a quadratic correction in the Ricci Scalar can be mapped, in the context of the Scalar Tensor Framework, in the dynamics of a three-dimensional particle that moves in the Poincarè-half space within a living domain determined by the presence of the potential term (due to the curvature and to the scalar field) illustrated in the Eq.(3.7). The fact that the potential term behaves as an infinitely steep potential well, suggest us that, when the particle is far from the wall, the potential can be neglect and the problem reduce to "free" particle problem.

This is exactly the starting point to attempt a quantization procedure for such a system. Let us write the superHamiltonian constraint in case of the absence of the potential term when the configuration space $\{\tau, u, v, \delta\}$ is taken into account

$$\mathcal{H} = -p_\tau^2 + v^2 \left[p_u^2 + p_v^2 + 4\frac{p_\delta^2}{(1+2u)^2} \right] = 0. \tag{3.13}$$

The canonical quantization of the system leads to the association, for the conjugate momentas, with the differential operators such that $p_j \to \widehat{p}_j = -i\partial_j$, where $i = \{\tau, u, v, \delta\}$. In this way, the action of the quantum operator $\widehat{\mathcal{H}}$ on the wave function of the Universe $\Psi(\tau, u, v, \delta)$ leads to the following WDW equation

$$\left[\partial_\tau^2 - v^2\partial_u^2 + \partial_v(v^2\partial_v) - 4v^2\frac{\partial_\delta^2}{(1+2u)^2} \right] \Psi(\tau, u, v, \delta) = 0. \tag{3.14}$$

Looking at the Eq.(3.14) is evident a specific operator-ordering in the v-part of the WDW equation. In particular, our choice is to implement that part as

$$\widehat{v}^2\widehat{p}_v^2 \to -\partial_v(v^2\partial_v). \tag{3.15}$$

Although this is not the only possibility, in this case the choice for such an operator ordering is contained in [16]. In this work is analyzed a very similar cosmological model, namely a Bianchi IX model described in the Poincare variables. What pushed the authors to consider the operator ordering (3.15) is the fact that, for this set of variables, this was the only one for which exists a correlation between a classical statistical description of the model provided from the Hamilton-Jacobi equation and a semiclassical behavior of the quantum model, thought as a WKB limit of the WDW equation. In this sense, without loss of generality, we can use the above operator-ordering also for our model.

A further look on the Eq.(3.14) allow to simplify the profile of the WDW equation. Indeed, the absence of the variables (τ, δ) means that the wave function of the Universe can be factorized as

$$\Psi(\tau, u, v, \delta) = e^{iE\tau}e^{im\delta}\psi_{E,m}(u, v) \tag{3.16}$$

and the Eq.(3.14) reduces to

$$\left[-E^2 - v^2\partial_u^2 + v^2\partial_v^2 + 2v\partial_v + 4v^2\frac{m^2}{(1+2u)^2} \right] \psi_{E,m}(u, v) = 0. \tag{3.17}$$

A redefinition of the wave function can be done in order to obtain a differential equation which is separable in the variables (u, v)[88],[89]. Redefining $\psi_{E,m}(u, v) = \frac{\phi_{E,m}(u,v)}{v}$ we can reduce the Eq.(3.17) in the form

$$\left[-\frac{E^2}{v^2} - \partial_u^2 - \partial_v^2 + \frac{4m^2}{(1+2u)^2} \right] \phi_{E,m}(u, v) = 0. \tag{3.18}$$

The latter form admits a solution with the method of the separation of variables. In terms of the wave function it means that we can write $\phi_{E,m}(u, v) = \chi(v)\varphi(u)$ and obtain

$$-\frac{E^2}{v^2}\chi(v)\varphi(u) - \chi(v)\partial_u^2\varphi(u) - \varphi(u)\partial_v^2\chi(v) + \frac{4m^2}{(1+2u)^2}\chi(v)\varphi(u) = 0. \tag{3.19}$$

Multiplying the previous relation by the factor $\frac{1}{\chi\varphi}$ and with the introduction of the separation constant k, the two dimensional differential equation (3.19) leads to a couple of one dimensional differential equation for the two components $\chi(v)$ and $\varphi(u)$ in this way

$$\partial_v^2\chi + \frac{E^2}{v^2}\chi = -k\chi, \tag{3.20}$$

$$\partial_u^2\varphi - \frac{4m^2}{(1+2u)^2}\varphi = k\varphi. \tag{3.21}$$

The Eqs.(3.20),(3.21) can be analytically solved and admit as solution

$$\chi(v) = A_1\sqrt{v}J_{\frac{1}{2}\sqrt{1-4e^2}}\left(\sqrt{k}v\right) + A_2\sqrt{v}Y_{\frac{1}{2}\sqrt{1-4e^2}}\left(\sqrt{k}v\right), \tag{3.22}$$

$$\varphi(u) = B_1 M_{0,\frac{1}{2}\sqrt{4m^2+1}}\left(2\sqrt{k}u + \sqrt{k}\right) + B_2 W_{0,\frac{1}{2}\sqrt{4m^2+1}}\left(2\sqrt{k}u + \sqrt{k}\right), \tag{3.23}$$

where $J_i(z)$ and $Y_i(z)$ are respectively the Bessel function of the first and second kind with index i, while $M_{m,n}(z)$ and $W_{m,n}(z)$ are respectively the Whittaker function of the M and W type and the values A_1, A_2, B_1, B_2 are integration constants. Unfortunately, the quantum analysis shown in this section has not been followed in our study. The main reason is that, to this today, it is still unclear how to interpret the behavior of the component $\chi(v)$ of the wave function in the vicinity of the absolute, nominally in the limit $v \to 0$. However, a further deepening regarding this issue remains a real goal for the future.

3.3 Conclusions

The analysis above demonstrated how including a quadratic correction in the Ricci scalar to the Einstein-Hilbert Lagrangian of the gravitational field gives a deep insight on the nature of the Mixmaster singularity: the evolution of the scale factors is no longer chaotic and a stable Kasner regime emerges as the final approach to the singular point.

The relevance of this result is in its generality with respect to the behavior of the cosmological gravitational field. In fact, on one hand, the result we derived in the homogeneous cosmological setting, can be naturally extended to a generic inhomogeneous Universe, simply following the line of investigation discussed in [13],[11].

The basic statement, at the ground of the BKL conjecture, is the space point decoupling in the asymptotic dynamics toward the cosmological singularity. Such a dynamical property of a generic inhomogeneous cosmological model allows to reduce the behavior of a sub-horizon spatial region [13],[77] to the prototype offered by the homogeneous Mixmaster Universe. We are actually stating that the time derivative of the dynamical variables asymptotically dominate their spatial gradients, limiting the presence of the spatial coordinates in the Einstein equation to a pure parametrical role. We are speaking of a conjecture because the chaotic features of the point-like dynamics induce a corresponding stochastic behavior of the spatial dependence and the statement above requires a non-trivial treatment for its proof. Nonetheless a valuable estimation of the spatial gradient behavior, when the space-time takes the morphology of a foam, is provided in [59]. When a scalar field is present the situation is even more simple, because, after a certain number of iterations of the BKL map, in each space point, a stable Kasner regime takes place [60] and the validity of the solution is rigorously determined [69]. Thus, we can extend our result to a generic inhomogeneous cosmological model simply considering the dynamical variables as space-time functions $u = u(\tau, x^i)$, $v = v(\tau, x^i)$ and $\delta = \delta(\tau, x^i)$, which, in each space point, live in a half-Poincarè space and are governed by an independent and morphologically equivalent dynamics. On the other hand, the extension of

General Relativity we considered here is the most simple and natural one, widely studied in literature in view of its implications on the primordial Universe features. Since the classical evolution is expected to be predictive up to a finite value of the Universe volume, i.e. up to a given amplitude of the space-time curvature, for sufficiently small coupling constant q values, the present model can be considered as the quadratic Taylor expansion of a generic $f(R)$ theory and we can then guess that the non-chaotic feature is a very general dynamical property, at least within the classical domain of validity of the $f(R)$ theory. In this sense we traced a very general and reliable properties of the cosmological gravitational field in modified theories of gravity of significant impact on the so-called billiard representation of the generic primordial Universe[62],[40].

Chapter 4

Hamiltonian dynamics and Noether symmetries in Gauss-Bonnet Cosmology

We devote this Chapter proceeding to speak about the extended theories of gravity. As said previously, the General Relativity and the SCM do not provide a complete description of the Universe as a whole, especially in the extreme regimes next to the initial singularity. This condition is underline by the absence of a clear and satisfactory Quantum theory of Gravitation. A possible way out from this pathology consists in consider non-minimally coupled scalar fields or higher-order curvature invariants into the standard Einstein-Hilbert action. In particular, in order to construct a renormalizable theory of gravity at scales closer to the Planck length, higher-order terms of curvature invariants in the Lagrangian, such as R^2,$R_{\mu\nu}R^{\mu\nu}$,$R_{\mu\nu\rho\delta}R^{\mu\nu\rho\delta}$ and the Gauss-Bonnet topological invariant, may be taken into account.

Here we consider a version of a Gauss-Bonnet gravity based on a starting modified action based that is given as a function of the Ricci Scalar R and the Gauss-Bonnet invariant $\mathcal{G}$, *i.e.* $F(R,\mathcal{G})$[30],[85]. The main strength of this kind of theories is their wide spectrum of application. Indeed, they are able to describe the acceleration of the observable Universe and the transition from different expansion phases of its history. Moreover, they can reproduce the behavior of the ΛCDM model and a lots of other cosmological solutions.

The approach that we illustrate in this Chapter is the *Noether symmetry Approach*[24]. It consists in looking if it possible to select physically interesting form for the action starting from the existence of Noether symmetries. Furthermore, such symmetries allow to individuate physical constants of motion that simplify and make treatable the dynamics.

As always, we consider the Hamiltonian formulation to describe the gravitational field and the implementation of the cosmological model will be done following the minisuperspace approach of the Section 2.3. The consideration of the minisuperspace, or in other words the choice of a particular cosmological model, brings to reduce the Lagrangian of the system to a *point-like Lagrangian*, namely the dynamics resembles the motion of an n-dimensional particle where n is the dimension of the configuration space.

Some indications about the quantum aspect for those model will be provide realizing a canonical quantization procedure, which allow to analyze the evolution of the wave function of the universe Ψ through the WDW equation.

To be more specific, let us enunciate the structure of this Chapter. We begin, in Section 4.1, speaking about the general Noether symmetry approach and the Hartle Criterion, a useful tool to select the classical trajectories from the quantum solutions of the WDW equation. Then, in Section 4.2 we review [27] the application to the homogeneous and isotropic FRW models of the Noether symmetry approach for the simple case $f(R)$. The

Section 4.3, indeed, is devoted to the original generalization of the Noether symmetry approach to the Gauss Bonnet-Cosmology, both from the classical and the quantum point of view. The final Section 4.4 about concluding remarks will close the Chapter.

The original part illustrated in Section 4.3 about the Gauss-Bonnet cosmology is now under review for future publication in an international scientific journal.

4.1 The Noether Symmetry Approach

An important role for the interpretation of the physical quantities in Quantum cosmology is played by the conserved quantities. A procedure to individuate such currents is represented by the so-called Noether Symmetry approach[24].

Let us start by considering a generic system described by a time-independent Lagrangian $\mathcal{L} = \mathcal{L}(q_i, \dot{q}_i)$. Realizing a Legendre transformation, the associated energy function is therefore obtained

$$E_{\mathcal{L}} = \pi^i_q \dot{q}_i - \mathcal{L}, \tag{4.1}$$

where $\pi^i_q = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$ are the conjugate momentas to the position variables q_i. In the Lagrangian formalism the transformations to consider are the only ones that are point transformations. Anyway, given a generic point transformation $Q^i = Q^i(q)$, this induces a modification also in the velocities as

$$\dot{Q}^i(q) = \frac{\partial Q^i}{\partial q^j} \dot{q}_j. \tag{4.2}$$

If we consider an infinitesimal parameter to characterize Q^i, the transformation is generated by a *vector field*. As examples, $\frac{\partial}{\partial z}$ represents the vector field for a translation along the z-axis while $x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}$ represents the vector field for a rotation along the z-axis. Therefore, a generic vector field that concerns also the induced transformation (4.2) is represented as

$$X = \alpha^i(q)\frac{\partial}{\partial q_i} + \dot{\alpha}^i(q)\frac{\partial}{\partial \dot{q}_i}, \tag{4.3}$$

which is also called "complete lift". In the Eq.(4.3) the dot means derivative with respect to the time and quantities $(\alpha^i, \dot{\alpha}^i)$ described the particular point transformation considered.

Considering now a generic function $f(q_i, \dot{q}_i)$, we can say that it is invariant under the transformation associated to the vector field X is the action of the Lie derivative L_X is null. In other words it is invariant if

$$L_X f \equiv \alpha^i(q)\frac{\partial f}{\partial q_i} + \dot{\alpha}^i(q)\frac{\partial f}{\partial \dot{q}_i} = 0. \tag{4.4}$$

As a particular case, useful for our purposes, choosing the function f as the Lagrangian, the condition $L_X\mathcal{L} = 0$ implies that the vector field X represents a symmetry for the Lagrangian dynamics and consequently, being valid the Noether theorem, a constant of motion exists.

The existence of such a constant of motion is evident if we consider the Euler-Lagrange equations

$$\frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial q_i} = 0. \tag{4.5}$$

The contraction of the previous one with respect to the α^i leads to

$$\alpha^i \left(\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}}{\partial q_i} \right) = \frac{d}{dt} \left(\alpha^i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right) - \dot{\alpha}^i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \alpha^i \frac{\partial \mathcal{L}}{\partial q_i} = 0. \tag{4.6}$$

If the condition (4.4) is valid for the Lagrangian, namely if $L_X \mathcal{L} = 0$, the Eq.(4.6) reduces to

$$\frac{d}{dt} \left(\alpha^i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right) = 0, \tag{4.7}$$

and the quantity

$$\Sigma_0 = \alpha^i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \tag{4.8}$$

is a constant of motion.

The Eq.(4.8) can be recasts in terms of the *Cartan one-form*:

$$\theta_{\mathcal{L}} = \frac{\partial \mathcal{L}}{\partial \dot{q}_i} dq^i. \tag{4.9}$$

For a generic vector field $Y = y^i \frac{\partial}{\partial x^i}$ and a one form $\beta = \beta_i dx^i$, the action of the inner derivative is $i_Y \beta =< \beta, Y >= y^i \beta_{i,} <,>$. In terms of the inner derivative, the Eq.(4.8) becomes

$$i_X \theta_{\mathcal{L}} = \Sigma_0, \tag{4.10}$$

while, under a point transformation, the new complete lift $\tilde{X}$ assumes the form

$$\tilde{X} = i_X Q^k \frac{\partial}{\partial Q^k} + \frac{d}{dt} \left[\frac{d}{dt} \left(i_X Q^k \frac{\partial}{\partial Q^k} \right) \right] \frac{\partial}{\partial \dot{Q}^k}. \tag{4.11}$$

Being X a symmetry for the system, $\tilde{X}$ is a symmetry too. This means that we have the freedom to choose a coordinate transformation such that

$$i_X Q^0 = 1 \quad , \quad i_X Q^i = 0 \quad , \quad i \neq 0. \tag{4.12}$$

Therefore,

$$\tilde{X} = \frac{\partial}{\partial Q^0} \quad , \quad \frac{\partial \mathcal{L}}{\partial Q^0} = 0. \tag{4.13}$$

From the above equation is evident the independence of the Lagrangian with respect to the variables Q^0 and so that variable represent a cyclic coordinate. Of course, the identification of such a propriety induced a deep simplification in the dynamics. It is important to underline that, with respect of this new change of variables, from the Euler-Lagrangian equations we can obtain that

$$\frac{\partial \mathcal{L}}{\partial Q^0} \Longleftrightarrow \frac{\partial \mathcal{L}}{\partial \dot{Q}^0} = \Sigma_0. \tag{4.14}$$

Let us see what happen if we apply the Noether symmetry approach to a generic n-dimensional minisuperspace model of the Quantum Cosmology. First of all, the energy function (4.1) is nothing else that the superHamiltonian, for which the scalar constraint is valid:

$$\mathcal{H} = \pi_q^i \dot{q}_i - \mathcal{L} = 0. \tag{4.15}$$

As discussed in Chapter 2, the canonical quantization procedure consists in the association of multiplicative and differential operators to the configuration variables and to consider the application of the quantum counterpart of the superHamiltonian constraint on the state of the system (the wave function of the Universe) as

$$\mathcal{H}\psi = 0, \tag{4.16}$$

known as the WDW equation.

Let us suppose now the existence of one Noether symmetry. Therefore, from Eq.(4.14) we have that the conjugate momenta π_0 to the coordinates Q_0 is a conserved quantity.

$$\pi_0 = \frac{\partial \mathcal{L}}{\partial \dot{Q}^0} = \Sigma_0 \tag{4.17}$$

If the canonical quantization substitution $\pi \to -i\frac{\partial}{\partial q}$ is taken into account for the direction associated to the symmetry, the application on the wave function give us that

$$-i\frac{\partial}{\partial Q_0}\psi = \Sigma_0\psi. \tag{4.18}$$

The integration of the Eq.(4.18) is immediate and with a clear physical interpretation. Being the constant of motion Σ_0 a real number, the solution for differential equation provides an oscillatory exponential behavior in the direction of the symmetry, in such a way that the total wave function of the Universe can be factorize as

$$\psi(Q) = e^{i\Sigma_0 Q^0}\varphi(Q^j) \quad , \quad 0 < j \leq n, \tag{4.19}$$

where the wave function $\varphi(Q^j)$ represents the wave function of the Universe related to the part orthogonal to the direction of the symmetry. It is important to stress the importance of such a method when it is applied to the cosmological minisuperspace models with low dimensions, for example one or two. In this case, the individuation of the first integrals of motion allow a complete resolution of the system and the selection of the classical trajectory that brings to have a properly defined semi-classical limit of the Quantum Cosmology. The existence of a class of solutions of the WDW equation that exhibits an oscillatory behavior is extremely important in the sense of the *Hartle Criterion*.

The Hartle criterion[23] is an interpretative scheme for the solutions of the WDW equation. Hartle[31] proposed to look for peaks of the wave function of the universe: If it is strongly peaked, we have correlations among the geometrical and matter degrees of freedom; if it is not peaked, correlations are lost. In the first case, the emergence of classical trajectories is expected. In this sense, the approach of the Noether symmetries can be used as a useful tool to select the solution associated to the classical Universes that emerge from the WDW equation.

4.2 Higher-order gravity minisuperspaces: $f(R)$ cosmologies

We consider in this Section a specific cosmological application of the Noether symmetry approach. In particular, here we consider the flat FRW model with no matter contribution for a $f(R)$ theory based on the action[37]

$$\frac{1}{2k}\int d^4x\sqrt{-g}f(R). \tag{4.20}$$

The line element for a FRW model is expressed in the Hamiltonian formulation in Eq.(1.52), in which t is the cosmic time, $a(t)$ is the scale factor and $N(t)$ is the lapse function. The scalar curvature R can be evaluated for such a model and this brings to the expression

$$R = 6\left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right). \tag{4.21}$$

In the previous relation and in the following we use the temporal gauge $N(t) = 1$.

If we insert directly the expression of the Ricci scalar in the action (4.20), we obtain a system described by a higher Lagrangian theory. The way to deal with a canonical Lagrangian system consists in using the method of the Lagrangian multipliers. In particular, given λ as a Lagrangian multiplier, the action (4.20) for the flat FRW model becomes

$$S = \frac{\pi^2}{k}\int dt\left\{a^3 f(R) - \lambda\left[R - 6\left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right)\right]\right\}. \tag{4.22}$$

The Lagrangian multiplier can be evaluated performing a variation of the above action with respect of the scalar curvature R. This gives

$$\delta_R S = 0 \to \lambda \propto a^3\frac{df(R)}{dR} \equiv a^3 f'(R). \tag{4.23}$$

If now one makes the substitution of the above Lagrangian multiplier in the action (4.22) and performs an integration by parts, the equivalent system obtained is described by a corresponding *point-like Lagrangian*

$$\mathcal{L} = \mathcal{L}(a, \dot{a}, R, \dot{R}) = -6\dot{a}^2 a\frac{df(R)}{dR} - 6\dot{a}a^2\dot{R}\frac{d^2f(R)}{dR^2} + a^3\left[f(R) - R\frac{df(R)}{dR}\right]. \tag{4.24}$$

The rewritten Lagrangian assumes a fascinating form if we redefine the derivative of $f(R)$ with an auxiliary field

$$p = \frac{df(R)}{dR}. \tag{4.25}$$

The Lagrangian (4.24) then becomes

$$\mathcal{L} = \mathcal{L}(a, \dot{a}, p, \dot{p}) = -6\dot{a}^2 ap - 6\dot{a}a^2\dot{p} + a^3[f(R) - Rp]. \tag{4.26}$$

From the structure of the Lagrangian is evident that in this scheme the configuration space is $\mathcal{Q} = \{a, p\}$, so we deal with a two-dimensional minisuperspace[27]. The "potential" term can be recast through the expression

$$W(p) \equiv h(p)p - r(p), \tag{4.27}$$

where

$$h(p) = R \quad , \quad r(p) = \int p dR = f(R), \tag{4.28}$$

in order to obtain the Lagrangian

$$\mathcal{L} = \mathcal{L}(a, \dot{a}, p, \dot{p}) = -6\dot{a}^2 ap - 6\dot{a}a^2\dot{p} - a^3 W(p) \tag{4.29}$$

From the configuration variables $\{a, p\}$, the existence of symmetries occurs if the action of vector field

$$X = \alpha\frac{\partial}{\partial a} + \beta\frac{\partial}{\partial p} + \dot{\alpha}\frac{\partial}{\partial \dot{a}} + \dot{\beta}\frac{\partial}{\partial \dot{p}} \tag{4.30}$$

on the Lagrangian (4.29) is such that the condition $L_X\mathcal{L} = X\mathcal{L} = 0$ is verified and at least one of the coefficients that characterizes X is different from zero. The contribution of the terms $\dot{\alpha}$ and $\dot{\beta}$ can be estimated using the relation among the coefficients $\{\alpha, \beta\}$ and the configuration variables $\{a, p\}$ that are

$$\dot{\alpha} = \frac{\partial \alpha}{\partial a}\dot{a} + \frac{\partial \alpha}{\partial R}\dot{R} \quad , \quad \dot{\beta} = \frac{\partial \beta}{\partial a}\dot{a} + \frac{\partial \beta}{\partial R}\dot{R}. \tag{4.31}$$

Substituting these in the condition $X\mathcal{L} = 0$ leads to a system of differential equation, each of which corresponds to the request that each term of a different order is equal to zero. Explicitly, we get a system of four differential equation

$$p\left[\alpha + 2a\frac{\partial \alpha}{\partial a}\right] + a\left[\beta + a\frac{\partial \beta}{\partial a}\right] = 0 \tag{4.32}$$

$$a^2\frac{\partial \alpha}{\partial p} = 0 \tag{4.33}$$

$$2\alpha + a\frac{\partial \alpha}{\partial a} + 2p\frac{\partial \alpha}{\partial p} + a\frac{\partial \beta}{\partial p} = 0 \tag{4.34}$$

$$a^2\left[3\alpha W(p) + \beta a\frac{\partial W(p)}{\partial p}\right] = 0 \tag{4.35}$$

The solution of the above system of differential equations it is satisfied for

$$\alpha = \alpha(a) \quad , \quad \beta(a,p) = \beta_0 a^s p, \tag{4.36}$$

where β_0 is an integration constant and s is an arbitrary parameter. Two cases of the parameter s are of particular interest: $s = 0$ and $s = -2$. In the first case the solutions for the coefficients are

$$s = 0 \rightarrow \alpha(a) = -\frac{\beta_0}{3}a \quad , \quad \beta(p) = \beta_0 p \quad , \quad W(p) = W_0 p \tag{4.37}$$

while in the second case

$$s = -2 \rightarrow \alpha(a) = -\frac{\beta_0}{a} \quad , \quad \beta(p) = \beta_0\frac{p}{a^2} \quad , \quad W(p) = W_1 p^3. \tag{4.38}$$

It is worth nothing that the value of parameter s implies different representation for the potential term $W(p)$. In the next Section examines in detail what the implementation of the canonical quantization implies in the two cases.

4.2.1 Case $s = 0$

Here we consider the case in Eq.(4.37). In order to deal with a Lagrangian dynamics in which a cyclic variable is present, it is necessary to individuate a particular change of variable. For this particular case the new set of variables $\{\omega, z\}$ such that

$$\omega(a,p) = a^3 p \quad , \quad z(p) = \ln p, \tag{4.39}$$

modify the Lagrangian (4.29) as

$$\tilde{\mathcal{L}} = \dot{\omega}\dot{z} - 2\omega\dot{z}^2 + \frac{\dot{w}^2}{\omega} - 3W_0\omega, \tag{4.40}$$

in which is clear that the new variable z is a cyclic variable. From the Eq.(4.40) it it possible to evaluate the conjugate momentas

$$\pi_z = \frac{\partial \tilde{\mathcal{L}}}{\partial \dot{z}} = \dot{w} - 4\dot{z} = \Sigma_0 \tag{4.41}$$

$$\pi_\omega = \frac{\partial \tilde{\mathcal{L}}}{\partial \dot{\omega}} = \dot{z} + 2\frac{\dot{\omega}}{\omega}. \tag{4.42}$$

The last equality in the Eq.(4.41) identify the conjugate momenta to the cyclic variable z as the conserved quantity associated to the Noether symmetry, as illustrated in the Eq.s(4.14), (4.17). The conjugate momentas allow to write the superHamiltonian constraint of the system with respect to them

$$\mathcal{H} = \pi_\omega \pi z - \frac{\pi_z^2}{\omega} + 2\omega\pi_\omega^2 + 6W_0\omega = 0. \tag{4.43}$$

The canonical quantization of the system consists in considering the action of the operator $\widehat{\mathcal{H}}$ on the wave function $\psi = \psi(\omega, z)$ via the WDW equation.

$$[\partial_z^2 - 2\omega^2\partial_\omega^2 - \omega\partial_\omega\partial_z + 6W_0\omega^2]\psi(\omega, z \tag{4.44}$$

The existence of the Noether symmetry gives a hint about the z-part of the wave function. Indeed, from the relation (4.41), we have that

$$-i\frac{\partial}{\partial z}\psi(\omega, z) = \Sigma_0\psi(\omega, z) \tag{4.45}$$

and therefore

$$\psi(\omega, z) \propto e^{i\Sigma_0 z}\chi(\omega). \tag{4.46}$$

Inserting the previous form of the wave function in the WDW equation $\widehat{\mathcal{H}}\psi = 0$ leads to a one-dimensional differential equation for the $chi(\omega)$

$$\left[\omega^2\partial_\omega^2 + i\frac{\Sigma_0}{2}\omega\partial_\omega + \left(\frac{\Sigma_0^2}{2} - 3W_0\omega^2\right)\right]\psi(\omega) = 0, \tag{4.47}$$

whose solution is a combination of Bessel functions $Z_\mu(\omega)$

$$\chi(\omega) = \omega^{\frac{1}{2} - i\frac{\Sigma_0}{4}} Z_\mu(\lambda\omega), \tag{4.48}$$

with

$$\mu = \pm\frac{1}{4}\sqrt{4 - 9\Sigma_0^2 - 4i\Sigma_0} \quad , \quad \lambda = \pm 9\sqrt{\frac{W_0}{2}}. \tag{4.49}$$

The whole wave function becomes

$$\psi(\omega, z) \propto \omega^{1/2} e^{i\Sigma_0[z - \frac{1}{4}\ln\omega]} Z_\mu(\lambda\omega) \tag{4.50}$$

The behavior of the Bessel function can resembles an oscillatory regime if the parameters μ and λ assume real values and for large values of ω. When it happens the solution (4.50) turns into the form

$$\psi(\omega, z) \propto e^{i[\Sigma_0 z - \frac{1}{4}\Sigma_0 \ln\omega \pm \lambda\omega]}. \tag{4.51}$$

The oscillatory behavior of the wave function in (4.51) immediately confirm the Hartle criterion and the identification of the exponent with the classical action S_0 allow to identify the conserved momenta $\pi_\omega = \frac{\partial S_0}{\partial \omega}$, $\pi_z = \frac{\partial S_0}{\partial z}$ and the classical trajectories. Turning back to the physical variables $\{a, p\}$ we get the following cosmological solutions

$$a(t) = a_0 e^{\frac{\lambda}{6}t} e^{-\frac{z_1}{3}e^{(-2\lambda/3)t}}, \tag{4.52}$$

$$p(t) = p_0 e^{\frac{\lambda}{6}t} e^{z_1 e^{(-2\lambda/3)t}}, \tag{4.53}$$

with z_1, a_0, p_0 are integration constants. The exponential profile for the scale factor asimptotically recover an inflationary behavior in which without any doubt λ plays the role of a cosmological constant.

4.2.2 Case $s = -2$

The subsection is devoted to the analysis of the particular solutions that appear in the Eq.(4.38). For those solutions the choice for the change of variables is

$$\omega(a, p) = ap \quad , \quad z(a) = a^2, \tag{4.54}$$

that modify the Lagrangian (4.29) as

$$\tilde{\mathcal{L}} = 3\dot{\omega}\dot{z} - W_1\omega^3. \tag{4.55}$$

As in the previous case, is clear that the new variable z is a cyclic variable. From the Eq.(4.55) the conjugate momentas are

$$\pi_z = \frac{\partial \tilde{\mathcal{L}}}{\partial \dot{z}} = 3\dot{w} = \Sigma_1, \tag{4.56}$$

$$\pi_\omega = \frac{\partial \tilde{\mathcal{L}}}{\partial \dot{\omega}} = 3\dot{z}. \tag{4.57}$$

Again, in the Eq.(4.41), being z a cyclic variable, the conjugate momenta is the conserved quantity associated to the Noether symmetry. The superHamiltonian constraint can now be written as

$$\mathcal{H} = \frac{1}{3}\pi_\omega \pi z + W_1\omega^3. \tag{4.58}$$

First of all, the canonical quantization of the system is simplified by the cyclic variable z. As a matter of fact, from the relation (4.56),

$$-i\frac{\partial}{\partial z}\psi(\omega, z) = \Sigma_1\psi(\omega, z) \tag{4.59}$$

and therefore

$$\psi(\omega, z) \propto e^{i\Sigma_1 z}\chi(\omega). \tag{4.60}$$

The wave function profile (4.60) entails that the WDW equation falls into a differential equation for $\chi(\omega)$:

$$[\partial_\omega + 3i\Sigma_1 W_1\omega^3]\chi(\omega) = 0. \tag{4.61}$$

The solution of Eq.(4.61) can be easily evaluated and the whole function is therefore

$$\psi \propto e^{i[\Sigma_1 z - \frac{3}{4}\Sigma_1 W 1\omega^4]}. \tag{4.62}$$

Also in this case the Hartle criterion is verified and in the same way it is possible to extract the classical trajectories. In terms of the cosmological variables we obtain

$$a(t) = \pm\sqrt{h(t)}, \tag{4.63}$$

$$p(t) = \pm\frac{c_1 + (\Sigma_1/3)t}{\sqrt{h(t)}}, \tag{4.64}$$

where

$$h(t) = \left(\frac{W_1\Sigma_1^3}{36}\right)t^4 + \left(\frac{W_1\Sigma_1\omega_1}{6}\right)t^3 + \left(\frac{W_1\Sigma_1\omega_1^2}{2}\right)t^2 + 6\omega_1^3 W_1 t + h_1 \tag{4.65}$$

and h_1, c_1, ω_1 are integration constants.

The profile obtained for the scale factor can be interpreted, in the limit for large t, as a power law inflationary behavior

$$a(t) \propto t^2 \quad , \quad p(t) \propto \frac{1}{t}. \tag{4.66}$$

4.3 Gauss-Bonnet minisuperspace models

The main goal of this Chapter is to generalize the application of the Noether symmetry approach described in Section 4.2 to the Gauss-Bonnet cosmology. In particular, we focus on the flat FRW metric and consider an action with no matter contribution that concerns the presence of the Gauss-Bonnet invariant $\mathcal{G}$ as well as the Ricci scalar R. Such an action have the form

$$S = -\frac{1}{2k}\int d^4x\sqrt{-g}F(R,\mathcal{G}) \tag{4.67}$$

In this new class of theory is necessary to estimate the value of the Gauss-Bonnet invariant for the FRW metric. Remembering the definition (1.41), for a flat homogeneous and isotropic model it reads as

$$\mathcal{G} = 24\left(\frac{\ddot{a}\dot{a}^2}{a^3}\right) \tag{4.68}$$

This expression, together with the expression for the Ricci scalar

$$R = 6\left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right), \tag{4.69}$$

grants to rewrite the Lagrangian in a treatable order derivatives way making use of the Lagrangian multipliers method as

$$S = \frac{\pi^2}{k}\int dt\left\{a^3F(R,\mathcal{G}) - \lambda_1\left[R - 6\left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right)\right] - \lambda_2\left[\mathcal{G} - 24\left(\frac{\ddot{a}\dot{a}^2}{a^3}\right)\right]\right\}. \tag{4.70}$$

The Lagrangian multipliers can be evaluated performing a variation of the action (4.70) with respect of the scalar curvature R and the Gauss-Bonnet invariant $\mathcal{G}$. This gives

$$\delta_R S = 0 \to \lambda_1 \propto a^3\frac{dF(R,\mathcal{G})}{dR}. \tag{4.71}$$

$$\delta_{\mathcal{G}} S = 0 \to \lambda_2 \propto a^3\frac{dF(R,\mathcal{G})}{d\mathcal{G}}. \tag{4.72}$$

Considering the expressions for the Lagrangian multipliers in the action and performing a similar integration by part with respect to the $f(R)$ case, on arrives to a point-like Lagrangian of this form

$$\mathcal{L} = 6a\dot{a}^2 \frac{\partial F(R,\mathcal{G})}{\partial R} + 6a^2\dot{a}\frac{d}{dt}\left(\frac{\partial F(R,\mathcal{G})}{\partial R}\right) - 8\dot{a}^3\frac{d}{dt}\left(\frac{\partial F(R,\mathcal{G})}{\partial \mathcal{G}}\right) + \\ + a^3\left[F(R,\mathcal{G}) - R\frac{\partial F(R,\mathcal{G})}{\partial R} - \mathcal{G}\frac{\partial F(R,\mathcal{G})}{\partial \mathcal{G}}\right] \quad (4.73)$$

Let us introduce the auxiliary variables $p = \frac{\partial F(R,\mathcal{G})}{\partial R}$, $q = \frac{\partial F(R,\mathcal{G})}{\partial \mathcal{G}}$. In this way the previous Lagrangian becomes

$$\mathcal{L} = 6a\dot{a}^2 p + 6a^2\dot{a}\dot{p} - 8\dot{a}^3\dot{q} - a^3 W(p,q), \quad (4.74)$$

where $W(p,q)$ is the potential term. The configuration space is defined as $\mathcal{Q} = (a,p,q)$ and the conjugated momentas to the configuration variables are

$$\pi_a = 12ap\dot{a} + 6a^2\dot{p} - 24\dot{a}^2\dot{q} \quad , \quad \pi_p = 6a^2\dot{a} \quad , \quad \pi_q = -8\dot{a}^3. \quad (4.75)$$

Taking into account the Legendre transform for the point-Lagrangian it is possible to evaluate the Hamiltonian

$$\mathcal{H} = \frac{1}{6a^2}\left[\pi_a\pi_p - \frac{p}{a^2}\pi_p^2\right] + a^3 W(p,q) = 0 \quad (4.76)$$

The existence of a Noether symmetry is guaranteed if the condition $X\mathcal{L} = 0$ is satisfied, where X represent the Noether vector and in this case takes the form:

$$X = \alpha\frac{\partial}{\partial a} + \beta\frac{\partial}{\partial p} + \gamma\frac{\partial}{\partial q} + \dot{\alpha}\frac{\partial}{\partial \dot{a}} + \dot{\beta}\frac{\partial}{\partial \dot{p}} + \dot{\gamma}\frac{\partial}{\partial \dot{q}}, \quad (4.77)$$

where α, β, γ are generic functions of (a, p, q). The condition $X\mathcal{L} = 0$ gives explicitly a system of eleven partial differential equation:

$$\begin{aligned}
&\alpha p + \beta a + 2ap\frac{\partial \alpha}{\partial a} + a^2\frac{\partial \beta}{\partial a} = 0\\
&a\frac{\partial \alpha}{\partial a} + 2p\frac{\partial \alpha}{\partial p} + 2\alpha + a\frac{\partial \beta}{\partial p} = 0\\
&3\frac{\partial \alpha}{\partial a} + \frac{\partial \gamma}{\partial q} = 0\\
&a^2\frac{\partial \alpha}{\partial p} = 0\\
&\frac{\partial \alpha}{\partial p} = 0\\
&2p\frac{\partial \alpha}{\partial q} + a\frac{\partial \beta}{\partial q} = 0\\
&a^2\frac{\partial \alpha}{\partial q} = 0\\
&\frac{\partial \alpha}{\partial q} = 0\\
&\frac{\partial \gamma}{\partial a} = 0\\
&\frac{\partial \gamma}{\partial p} = 0\\
&3\alpha W(p,q) + a\left[\beta\frac{\partial W}{\partial p} + \gamma\frac{\partial W}{\partial q}\right] = 0
\end{aligned} \tag{4.78}$$

The equations from fourth to tenth say to us that $\alpha = \alpha(a), \beta = \beta(a,p), \gamma = \gamma(q)$. This means that the first three equation becomes

$$\begin{aligned}
&\alpha p + \beta a + 2ap\frac{\partial \alpha}{\partial a} + a^2\frac{\partial \beta}{\partial a} = 0\\
&a\frac{\partial \alpha}{\partial a} + 2\alpha + a\frac{\partial \beta}{\partial p} = 0\\
&3\frac{\partial \alpha}{\partial a} + \frac{\partial \gamma}{\partial q} = 0,
\end{aligned} \tag{4.79}$$

with solutions

$$\alpha(a) = -\frac{\beta_0}{3}a \quad , \quad \beta(p) = \beta_0 p \quad , \quad \gamma(q) = \beta_0 q \tag{4.80}$$

After this it is possible, from the eleventh equation, to individuate the value of $W(p,q)$:

$$W(p,q) - p\frac{\partial W(p,q)}{\partial p} - q\frac{\partial W(p,q)}{\partial q} = 0 \Longrightarrow W(p,q) = W_0 p + W_1 q \tag{4.81}$$

In order to individuate the presence of a cyclic variables it is useful to perform the following change of variables

$$w = a^3 p \quad , \quad u = a^3 q \quad , \quad z = \ln a. \tag{4.82}$$

In this way the Lagrangian (4.74) takes the form

$$\tilde{\mathcal{L}}(w,u,\dot{z},\dot{w},\dot{u}) = 6\dot{z}\dot{w} - 12w\dot{z}^2 + 24u\dot{z}^4 - 8\dot{u}\dot{z}^3 - W_0 w - W_1 u, \tag{4.83}$$

where the absence of z means that it is a cyclic variable. The conjugated momentas are

$$\pi_z = \frac{\partial \tilde{\mathcal{L}}}{\partial \dot{z}} = 6\dot{w} - 24w\dot{z} + 96u\dot{z}^3 - 24\dot{u}\dot{z}^2 = \Sigma_0 \tag{4.84}$$

$$\pi_w = \frac{\partial \tilde{\mathcal{L}}}{\partial \dot{w}} = 6\dot{z} \tag{4.85}$$

$$\pi_u = \frac{\partial \tilde{\mathcal{L}}}{\partial \dot{u}} = -8\dot{z}^3 \tag{4.86}$$

Taking into account the Legendre transformation the Hamiltonian takes the form

$$\begin{aligned}\tilde{\mathcal{H}} = \pi_z\dot{z} + \pi_w\dot{w} + \pi_u\dot{u} - \tilde{\mathcal{L}} = 6\dot{z}\dot{w} - 12w\dot{z}^2 + 72u\dot{z}^4 - 24\dot{u}\dot{z}^3 + W_0 w + W_1 u = \\ = \frac{1}{6}\pi_z\pi_w + \frac{1}{3}w\pi_w^2 + \frac{1}{2}u\pi_u\pi_w + W_0 w + W_1 u\end{aligned} \tag{4.87}$$

Now it is possible to use the energy condition, or the so-called superHamiltonian constraint, $\tilde{\mathcal{H}} = 0$ and the presence of a constant of motion $\pi_z = \Sigma_0$ and write down the quantum correspondence, trough a canonical quantization, over the wave function of the universe $\Psi(z, u, w)$.

$$[-2w\partial_w^2 - 3u\partial_u\partial_w - \partial_z\partial_w + 6(W_0 w + W_1 u)]\Psi(z, u, w) = 0 \tag{4.88}$$

$$-i\partial_z\Psi(z, u, w) = \Sigma_0\Psi(z, u, w) \tag{4.89}$$

The relation (4.89) allows to individuate the z-component of the wave function. In particular it means that

$$\Psi(z, u, w) = e^{i\Sigma_0 z}\psi(u, w) \tag{4.90}$$

When the shape (4.90) is considered in the WDW equation (4.88) we have

$$[-2w\partial_w^2 - 3u\partial_u\partial_w - i\Sigma_0\partial_w + 6(W_0 w + W_1 u)]\psi(u, w) = 0. \tag{4.91}$$

It is possible to remove one of the derivatives term by introducing this change of variables:

$$r = -(i\Sigma_0)\ln\left(\frac{2w}{i\Sigma_0}\right) \quad , \quad t = \ln u. \tag{4.92}$$

When we do this the Eq.(4.91) takes the form

$$\left[-k^2\partial_r^2 + 3\partial_t\partial_r + \left(3W_0 e^{-\frac{2r}{k}} + \frac{6W_1}{k}e^{t-\frac{r}{k}}\right)\right]\psi(r, t) = 0, \tag{4.93}$$

where we define $k = i\Sigma_0$. As a next step it is possible to eliminate the presence of derivative mixing term through a further change of variables:

$$x = \frac{4k}{3\sqrt{5}}\left(t + \frac{3r}{2k^2}\right) \quad , \quad y = -\frac{2r}{k}. \tag{4.94}$$

When we do this the Eq.(4.93) takes the form

$$\left[\frac{1}{5}\partial_x^2 - \partial_y^2 + \left(\frac{3}{4}W_0 e^y + \frac{3W_1}{2k}e^{x+\left(\frac{1}{\sqrt{5}}+\frac{2k}{3\sqrt{5}}\right)y}\right)\right]\psi(x, y) = 0. \tag{4.95}$$

In order to find particular solutions, we analyze all the cases for which is possible to solve the Eq.(4.95) with the method of the separation of variables. For all the following cases we argue if the Hartle Criterion is verified or not and by the identification of the classical if it is possible to individuate classical cosmological solutions.

4.3.1 $W_0 = 0, W_1 = 0$

The first and the most simple case to analyze is when the values of the two constants W_0 and W_1 are equal to zero. When we do this the differential equation Eq.(4.95) becomes:

$$\left[\frac{1}{5}\partial_x^2 - \partial_y^2\right]\psi(x,y) = 0. \tag{4.96}$$

We can find a solution via the separation of variables method for the wave function of the form $\psi(x,y) = \xi(x)\phi(y)$ in this way:

$$\frac{1}{5}\partial_x^2\xi(x) = -c^2\xi(x) \quad , \quad \partial_y^2\phi(y) = -c^2\phi(y), \tag{4.97}$$

where c represents the separation constant. The previous differential equation admits as solutions:

$$\xi(x) \propto e^{i\sqrt{5}cx} \quad , \quad \phi(y) \propto e^{icy}, \tag{4.98}$$

The entire wave function in the configuration space $\{z, x, y\}$ takes the form

$$\Psi(z,x,y) \propto e^{i\Sigma_0 z} e^{i\sqrt{5}cx} e^{icy}, \tag{4.99}$$

while in the starting configuration space $\{a, p, q\}$ we have

$$\Psi(a,p,q) \propto e^{i\Sigma_0 \ln a - \frac{4c\Sigma_0}{3}\ln(a^3 q)} \tag{4.100}$$

It is now clear that the Hartle criterion in this case is verified if we choose the separation constant c as a pure imaginary number $c = ij \quad , \quad j \in \mathbb{R}$. In this case the Hartle Criterion is recovered and the classical action S_0 is equal to

$$S_0 = \Sigma_0 \ln a - \frac{4j\Sigma_0}{3}\ln(a^3 q) \quad , \quad j \in \mathbb{R}. \tag{4.101}$$

If we try to determinate the classical cosmological solutions starting by the previous action, we have to consider the relations $\partial_i S_O = \pi_i$, with $i = \{a, p, q\}$. Unfortunately, also taking into account the relations for the momenta in the Eqs.(4.75), we obtain an undetermined system of differential equations.

4.3.2 $W_1 = 0$

The second case that we analyze is when only one of the two constants is equal to zero, specifically $W_1 = 0$. When we do this, the differential equation becomes:

$$\left[\frac{1}{5}\partial_x^2 - \partial_y^2 + \frac{3}{4}W_0 e^y\right]\psi(x,y) = 0. \tag{4.102}$$

We can find a solution for the wave function of the form $\psi(x,y) = \xi(x)\phi(y)$, and this leads, via the separation of variables method, to two differential equations

$$\frac{1}{5}\partial_x^2\xi(x) = -c^2\xi(x) \quad , \quad \partial_y^2\phi(y) - \frac{3}{4}W_0 e^y\phi(y) = -c^2\phi(y), \tag{4.103}$$

where c represents the separation constant. The previous differential equations can be solved analytically, and the solutions are

$$\xi(x) \propto e^{i\sqrt{5}cx} \quad , \quad \phi(y) \propto I_{2ic}[\sqrt{3W_0}e^{y/2}], \tag{4.104}$$

where I is the first kind modified Bessel function. The whole function in the configuration space $\{z, x, y\}$ takes the form:

$$\Psi(z, x, y) \propto e^{i\Sigma_0 z} e^{i\sqrt{5}cx} I_{2ic}[\sqrt{3W_0}e^{y/2}]. \tag{4.105}$$

When we turn back to the initial configuration space $\{a, p, q\}$ the wave function takes the form:

$$\begin{aligned} \Psi(a,p,q) &\sim e^{i\Sigma_0 \log a} e^{-\frac{2}{3}c\left(2\Sigma \log\left(a^3 q\right) + 3i \log\left(-\frac{2ia^3 p}{\Sigma}\right)\right)} I_{2ic}\left[\frac{2i\sqrt{3W_0}a^3 p}{\Sigma}\right] \sim \\ &\sim e^{i\Sigma_0 \log a} e^{-\frac{2}{3}c\left(2\Sigma \log\left(a^3 q\right) + 3i \log\left(-\frac{2ia^3 p}{\Sigma}\right)\right)} J_{2ic}\left[\frac{-2\sqrt{3W_0}a^3 p}{\Sigma}\right] \sim \\ &\sim e^{i\Sigma_0 \log a} e^{-\frac{1}{3}c\left(2\Sigma \log\left(a^3 q\right) + 3i \log\left(-\frac{2ia^3 p}{\Sigma}\right)\right)} \left(\frac{-2\sqrt{3W_0}a^3 p}{\Sigma}\right)^{-1/2} e^{i\left[\frac{2\sqrt{3W_0}a^3 p}{\Sigma_0}\right]} \sim \\ &\sim e^{i\left[\Sigma_0 \log a + i\frac{2}{3}c\Sigma_0 \log(a^3 q) - c \log\left(\frac{-2a^3 p}{\Sigma_0}\right) + \frac{i}{2}\log\left(-\frac{2a^3 p}{\Sigma_0}\right) + \frac{2\sqrt{3W_0}a^3 p}{\Sigma_0}\right]}. \end{aligned} \tag{4.106}$$

In the previous equalities we used the relation between the first order Bessel function J_c and the modified first order Bessel function

$$I_\alpha[ix] = i^{-\alpha} J_\alpha[-x] \tag{4.107}$$

and the expansion for large argument of the Bessel function:

$$J_\alpha[-x] \simeq \frac{e^{ix}}{\sqrt{x}}. \tag{4.108}$$

The exponent that appears in the last line of the (4.106) corresponds in the semiclassical approach to the action S_0. So, we can recover the classical dynamics, remembering the identities $\partial_i S_0 = \pi_i$, with $i = \{a, p, q\}$. Taking into account the relations (4.75), we can obtain the following system of differential equations

$$\begin{cases} 3\xi a p = 2p\dot{a} + a\dot{p} - 4\frac{\dot{a}^2 \dot{q}}{a} \\ \xi a = \dot{a} \\ \frac{\Sigma_0}{24q} = \dot{a}^3, \end{cases} \tag{4.109}$$

where we set the value of the arbitrary separation constant $c = \frac{i}{2}$ and we define the constant $\xi = \sqrt{\frac{W_0}{3\Sigma_0^2}}$. With this choice of the separation variable the action that appear to the exponent in the last line of (4.106) is a pure real number:

$$S_o = \Sigma_0 \ln a - \frac{\Sigma_0}{3}\ln(a^3 q) + 2\sqrt{3W_0}\frac{a^3 p}{\Sigma_0} \tag{4.110}$$

and so the Hartel Criterion is verified. We can solve the system (4.109) to obtain the classical trajectories

$$\begin{cases} a(t) = C_1 e^{\xi t} \\ q(t) = \frac{\Sigma_0}{24\xi^3 C_1^3} e^{-3\xi t} \\ p(t) = C_2 e^{\xi t} + \frac{\Sigma_0}{8\xi C_1^3} e^{-3\xi t}, \end{cases} \tag{4.111}$$

where C_1 and C_2 are arbitrarily constants. The cosmological solutions obtained in Eqs. (4.111) exhibit an inflationary behavior, due to the exponential profile that characterizes the scale factor of the Universe. In some sense, we recover with this solution a generalization for the Gauss-Bonnet cosmology of the inflationary behavior founded in the Eqs. (4.52),(4.53) for the $f(R)$ theory, where the role of a cosmological constant is assumed by the quantity ξ.

4.3.3 $W_0 = 0$, $\Sigma_0 = \frac{3i}{2}$

In this case we assign the value $W_0 = 0$ and, in order to apply the separation of variable method, we choose the value $\Sigma_0 = \frac{3i}{2}$. In this way the Eq.(4.95) becomes:

$$\left[\frac{1}{5}\partial_x^2 - \partial_y^2 - W_1 e^x\right]\psi(x,y) = 0. \tag{4.112}$$

As before, we choose a form for the wave function $\psi(x,y) = \xi(x)\phi(y)$ and we obtain

$$\frac{1}{5}\partial_x^2\xi(x) - W_1 e^x \xi(x) = -c^2\xi(x) \quad , \quad \partial_y^2\phi(y) = -c^2\phi(y), \tag{4.113}$$

where c represents the separation constant. The previous differential equations can be solved analytically, and the solutions are

$$\xi(x) \propto I_{2i\sqrt{5}c}[2\sqrt{5W_1}e^{x/2}] \quad , \quad \phi(y) \propto e^{icy}, \tag{4.114}$$

where I is the first kind modified Bessel function. The whole function in the configuration space $\{z, x, y\}$ takes the form:

$$\Psi(z,x,y) \propto e^{-\frac{3}{2}z} e^{icy} I_{2i\sqrt{5}c}[2\sqrt{5W_1}e^{x/2}]. \tag{4.115}$$

When we turn back to the initial configuration space $\{a, p, q\}$ the wave function takes the form:

$$\Psi(a,p,q) \propto e^{-\frac{3}{2}\ln a} e^{2ic\ln\left(\frac{4a^3 p}{3}\right)} J_{2i\sqrt{5}c}\left[2i\sqrt{5W_1}\left(\frac{3}{4a^6 pq}\right)^{\frac{1}{\sqrt{5}}}\right] \simeq$$

$$\simeq e^{-\frac{3}{2}\ln a} e^{2ic\ln\left(\frac{4a^3 p}{3}\right)} e^{2ic\ln\left(\frac{3A}{4a^6 pq}\right)} = e^{-\frac{3}{2}\ln a} e^{i2c\ln\left(\frac{A}{a^3 q}\right)}, \tag{4.116}$$

where we used again the relation (4.107) for the Bessel functions and this time, in order to see what happen in the semiclassical limit, we used the expansion for the Bessel function for small argument

$$J_\alpha[x] \simeq \left(\frac{x}{2}\right)^\alpha. \tag{4.117}$$

Furthermore, the constant A that appears in the Eq. (4.116) is defined as $A = (20W_1)^{\frac{\sqrt{5}}{2}}$.

From the solution (4.116) is clear that we can select a semiclassical form for the wave function with a purely imaginary Action if we define the separation constant as an imaginary number $c = ij$, with $j \in \mathbb{R}$. In this way we obtain

$$\Psi(a,p,q) \propto e^{-\frac{3}{2}\ln(a)-2j\ln\left(\frac{A}{a^3 q}\right)}. \tag{4.118}$$

The previous solution represent a soliton solution, and it is not possible to connect this with a classical cosmological solution through the conjugated momentas definition (4.75).

However we can define the separation constant as a real number $c = l$, with $l \in \mathbb{R}$. In this way, the solution (4.116) becomes

$$\Psi(a,p,q) \propto e^{-S_I+iS_O} = e^{-\frac{3}{2}\ln(a)+i\left[2l\ln\left(\frac{A}{a^3 q}\right)\right]}. \tag{4.119}$$

If we take into account the case in which the real part e^{-S_I} varies slowly and the imaginary part e^{iS_O} varies rapidly[1], we can claim that the classical trajectories are identified by $\partial_i S_O = \pi_i$, with $i = \{a,p,q\}$. Unfortunately, also taking into account the relations for the momenta in the Eqs.(4.75), we obtain a undetermined system of differential equations.

4.3.4 $\Sigma_0 = \frac{3i}{2}$

Let us now see what happen if we assign only the value $\Sigma_0 = \frac{3i}{2}$, leaving generically values for W_0 and W_1. In this way we have the following:

$$\left[\frac{1}{5}\partial_x^2 - \partial_y^2 + \frac{3}{4}W_0 e^y - W_1 e^x\right]\psi(x,y) = 0. \tag{4.120}$$

As in the previous cases, we can solve the differential equation via the separation of variables method. By defining again the wave function $\psi(x,y) = \xi(x)\phi(y)$ we arrive to a couple of equations

$$\frac{1}{5}\partial_x^2\xi(x) - W_1 e^x \xi(x) = -c^2\xi(x) \quad , \quad \partial_y^2\phi(y) - \frac{3}{4}W_0 e^y = -c^2\phi(y), \tag{4.121}$$

that admit as solutions

$$\xi(x) \propto I_{2i\sqrt{5}c}[2\sqrt{5W_1}e^{x/2}] \quad , \quad \phi(y) \propto I_{2ic}[\sqrt{3W_0}e^{y/2}], \tag{4.122}$$

In the configuration space $\{a,p,q\}$ the whole wave function is[2]

$$\Psi(a,p,q) \propto e^{-\frac{3}{2}\ln a} J_{2ic}\left[4i\sqrt{\frac{W_0}{3}}a^3|p|\right] J_{2i\sqrt{5}c}\left[2i\sqrt{5W_1}\left(\frac{3}{4a^6|p|q}\right)^{\frac{1}{\sqrt{5}}}\right] \simeq$$
$$\simeq e^{-\frac{3}{2}\ln a} e^{-4\sqrt{\frac{W_0}{3}}a^3|p|} e^{-\frac{1}{2}\ln\left(-4\sqrt{\frac{W_0}{3}}a^3|p|\right)} e^{i2c\ln\left(\frac{3A}{4a^6|p|q}\right)}, \tag{4.123}$$

As in the previous section, if we define the separation constant $c = l$, with $l \in \mathbb{R}$, the wave function can be recast as:

$$\Psi(a,p,q) = e^{-S_I+iS_O}, \tag{4.124}$$

[1]This is exactly our case, because for late times it is easy to verify that it is true.

[2]We choose the restriction $p < 0$ in order to have a well-defined logarithmic function

where

$$S_I = \frac{3}{2}\ln a + 4\sqrt{\frac{W_0}{3}}a^3|p| + \frac{1}{2}\ln\left(-4\sqrt{\frac{W_0}{3}}a^3|p|\right) \quad , \quad S_O = 2l\ln\left(\frac{3A}{4a^6|p|q}\right) \tag{4.125}$$

Also in this case the real part varies slowly respect to the imaginary part, so we identify the classical trajectories by the equalities $\partial_i S_O = \pi_i$, with $i = \{a, p, q\}$. We obtain the following system of differential equations:

$$\begin{cases} -l = a^2 p\dot{a} + \frac{1}{2}a^3\dot{p} - 2a\dot{a}^2\dot{q} \\ \frac{l}{p} = -3a^2\dot{a} \\ \frac{l}{q} = 4\dot{a}^3, \end{cases} \tag{4.126}$$

The previous system of differential equations admit the following cosmological classical solutions

$$\begin{cases} a(t) = C_1[8t - 5C_2]^{\frac{5}{8}} \\ p(t) = -\frac{l}{15C_1^3}[8t - 5C_2]^{-\frac{7}{8}} \\ q(t) = \frac{l}{500C_1^3}[8t - 5C_2]^{\frac{9}{8}}, \end{cases} \tag{4.127}$$

where C_1 and C_2 are integration constants. The Eqs.(4.127) show a power-law solution for the scale factor of the Universe.

4.4 Collection of solutions and concluding remarks

Before to conclude the Chapter, in order to summarize what founded, It is useful to collect all the results obtained in the previous Sections in a Table, in order to analyze in which particular cases we founded classical cosmological solutions and when the Hartle Criterion is recovered or not.

W_0	W_1	Σ_0	c	Wave Function type	Classical solution
0	0	$\mathbb{R}$	$\mathbb{R}$	$e^{-S_I+iS_O}$	-
0	0	$\mathbb{R}$	$\mathbb{I}$	e^{iS_O}	No
$\neq 0$	0	$\mathbb{R}$	$\frac{i}{2}$	e^{iS_O}	Yes
$\neq 0$	0	$\mathbb{R}$	$\mathbb{I}$	$e^{-S_I+iS_O}$	-
0	$\neq 0$	$\frac{3i}{2}$	$\mathbb{R}$	e^{-S_I}	-
0	$\neq 0$	$\frac{3i}{2}$	$\mathbb{I}$	$e^{-S_I+iS_O}$	No
$\neq 0$	$\neq 0$	$\frac{3i}{2}$	$\mathbb{R}$	e^{-S_I+iSO}	Yes
$\neq 0$	$\neq 0$	$\frac{3i}{2}$	$\mathbb{I}$	e^{-S_I}	-

As mentioned earlier, the original part of what is shown in this chapter consists in the generalization of the Noether symmetry approach to the minisuperspace to the Gauss-Bonnet cosmologies. The starting point for such a generalization was the paper [27], in which many aspects of the minisuperspace approach to Quantum Cosmology are treated.

Although this approach does not give a fully solution to the Quantum Gravity problem, anyway it stands as a useful tool to individuate the emerging classical universes, which in principle are observable with the standard astrophysical measurements. As we have shown, also in the Gauss-Bonnet cosmology, the identification of constants of motion, associated to the Noether symmetries of the theory, is fundamental to select peaked wave function of the universe. In this sense, the Noether symmetries can be considered as a restriction that imply a less complex dynamics in order to restore classical solutions.

The existence of Noether symmetry implies that the Lie derivative of the point like Lagrangian associated to the Noether vector field vanishes. As we have shown previously, from this application one can obtain the explicit form of the potential term and, in some sense, information about the shape of the $F(R, G)$ taken into account. The absence of an explicit cyclic variable in the Lagrangian requires, in order to simplify the quantization of the model, a point transformation for the configuration variables such that the new phase space admits a cyclic variable.

We have then quantized the model and shown that the corresponding WDW equation admits some exact solutions that, due to the existence of Noether symmetry, can be traced in the form e^{iS_O}, where S_O is the semiclassical action. In semiclassical approximation for quantum gravity, this type of state represents the . The main result of this original work is the individuation, through this correlation between classical trajectories and the peaks of the wave function, of a particular solution in which an exponential behavior for the scale of the Universe associated to an inflationary regime occurs.

Chapter 5

Big-bounce cosmology from quantum gravity: the case of cyclical Bianchi I Universe

The WDW approach[43],[44],[45] to quantum cosmology [75],[79] has two main relevant shortcomings, i.e. the absence of a unique definition of time [57] and the difficulty in removing or properly interpreting the primordial singularity [18],[53],[27].

Such problem, mainly characterizing all the canonical metric approaches, is essentially addressed by the LQC [3],[4],[5], where, adopting a scalar field as a relational time, it is shown the existence of a big bounce that remove the singularity.

However, this important result does not overcome some subtleties concerning its derivation and which are relevant on a general ground too. First of all, it is not clear if the choice of any relation time and, in particular the scalar field one, is suitable to describe the early Universe quantum dynamics[36],[90]. Then it calls for attention the question concerning weather or not the symmetry preservation, characterizing LQC, is the correct quantization procedure of a cosmological model [34].

As we have seen in the previous speaking about the polymer quantum cosmology, its main feature consists in the regularization of the physical quantities in the proximity of the initial singularity. In particular, the introduction of a physical cut-off in the spatial scale induces the most evident effect of a theory based on the presence of a fundamental lattice, *i.e.* the substitution of the big-bang singularity in favor of a big-bounce. Nevertheless, considering a polymer paradigm it is not the only way to formulate a bouncing cosmology. Many different approaches that consider for example the presence of matter scalar field with non-trivial potential and non-standard kinetic term [22],[49] can be considered in order to arrive at the same conclusion.

Another approach, very similar to the one followed in [71], consists in studying the quantum cosmological problem in the presence of a "clock" dust contribution, in the spirit of the Brown and Kuchař approach [21].

Keeping this in mind, in analogy with the paper cited above, in the present chapter we analyze a cosmological model that contains features interesting for the deep understanding of the two points mentioned above. In fact, we consider a canonical minisuperspace model using a dust fluid as external time, according to the time-dust dualism discussed in [64]. The very important feature of the obtained quantum cosmology is the emergence of a non-singular cyclical Universe, which is characterized by a quantum Big-Bounce and a classical turning point, associated to the existence of a small negative cosmological constant, i.e. small enough to ensure that such a re-collapsing feature be in the far future of the actual Universe.

An important aspect of such a cosmological scenario, which legitimate the idea of cyclical Universe is the possibility to link the quantum evolution to the standard isotropic behaviour via a well-defined classical limit (see also [30],[29], for this problem in alternative theories of gravity). In fact the presence of a negative cosmological constant induces an harmonic oscillator morphology to the system Hamiltonian (a part a global minus sign) and this is responsible both for the existence of a classical limit and of the positive nature of the dust energy density. This latter fact solves, in our cosmological implementation, the basic problem of the approach discussed in [64].

More in detail, we consider the evolutionary quantum dynamics of a Bianchi I model in the presence of a negative cosmological constant, as represented in Misner-like variables [74],[76]. Clearly, the classical limit corresponds to an increasingly isotropic Universe, although we do not address here the role of the matter and then the reproduction of Standard Cosmology. This is because, we aim to determine a cosmological behavior which be able to mimic a very general cosmological scenario near the singularity, according to the idea that the natural isotropization mechanism must be recogniced in the inflationary scenario[62].

To this end, we investigate the implications of our dynamical model on the evolution of the Bianchi IX cosmology, which is, accordingly to the BKL conjecture, the prototype for the evolution of a generic inhomogeneous Universe on a sufficiently small spatial scale [15]. We demonstrate that, along the dynamics of the stable expectation values of the configurational variables, the presence of the Bianchi IX potential can be neglected, as soon as the value of the dust energy density is sufficiently large. Thus, for such a (non-severe) restriction, the Bianchi I and Bianchi IX model quantum dynamics overlap nearby the primordial singularity and our result acquires a high degree of generality, i.e. our picture of a cyclical Universe could have a very general implementation in the generic cosmological problem. Finally, we investigate which ingredient of our model is relevant in determining a cut-off physics and we show that there exists a direct relation between the negative cosmological constant presence and an effective semiclassical polymer dynamics [39],[38], in which that constant is removed but the discrete nature of the Universe volume is included.

Summarizing, in this work we discuss a cosmological scenario containing a number of very peculiar properties, suggesting that its features are physically meaningful and are not formal coincidences. In particular, we stress how, in the present canonical evolutionary quantum context, the emergence of a Big-Bounce and of a cyclical Universe is at all natural and general in its structure, so much to encourage more general implementations.

This Chapter is organized as follows.

In Section 5.1 we describe the Bianchi I model in presence of a negative cosmological constant from the classical and from the quantum point of view. The first part of the Section is devoted to analyze the classical trajectories of the Misner-like variables near the singularities while in the second part we compare this classical behaviors with the related quantum expectation values.

In Section 5.2 we generalize, in a qualitatively way, the properties founded for the Bianchi I model to the more general Bianchi IX model, shedding light on the role playing by the potential term.

The Section 5.3 is dedicated to the cosmological interpretation of the results obtained in the previous, giving in particular a phenomenological explanation of how to extend the features of the Bianchi I and Bianchi IX model to the generic inhomogeneous Universe.

Then, in Section 5.4, we see how the role of the negative cosmological constant is related to a cut-off physics, making use of a polymer quantization for the variable connected to the Universe volume.

Brief concluding remarks complete the Chapter.

The work illustrated in this Chapter was published on the international journal **Physical Review D** in **July 2016**[82].

5.1 Bianchi I quantum dynamics in the Kuchař and Torre Approach

The cosmological scenario we are going to implement can be applied also to the isotropic Universe [35], as soon as the role played here by the anisotropy variables is supplied by a massless (or even self-consistent) scalar field. Indeed, the kinetic term in the Hamiltonian of a scalar field on the isotropic Universe dynamics is at all isomorphic to that one of an anisotropic variable in the Misner representation (*i.e.* β_+ or β_-) in the Hamiltonian of a Bianchi Model, in particular for the type I and IX we will address in this work. The motivation to consider the present more general scheme than the isotropic Universe must be individualized in the natural presence of the anisotropy terms near the cosmological singularity, in comparison to the necessity of postulating the presence of a kinetic scalar field contribution asymptotically to the singularity (a reasonable but not rigorously proved feature associated to the pre-inflationary inflaton dynamics [79]). Furthermore, the morphology of the Bianchi I and IX models outlines a high degree of generality with respect to the Robertson-Walker geometry since, as shown in [15], the generic cosmological solution, near the singularity, is an infinite series of Kasner epochs (periods of time in which the dynamics is Bianchi I-like), one for each space point (physically for each cosmological horizon). Such a basic result, known as the BKL conjecture, suggests that the analysis here addressed can be implemented to a very general picture and we can infer that the discussed scenario removes the cosmological singularity for a generic inhomogeneous Universe, as far as its evolution admits the Bianchi IX oscillatory regime as a homogeneous prototype. In what follows, we prefer to deal with minisuperspace models, in order to avoid the non-trivial question of how can be rigorously implemented the conjecture above on a quantum level: the spatial decoupling of the space point in the asymptotic dynamics of an inhomogeneous Universe towards the singularity is demonstrated in the classical sector, on the base of statistical arguments [58], but it remains an open issue in a metric quantum dynamics. Let us consider a Universe described by a Bianchi I model in the presence of a negative cosmological constant $-\Lambda$, with $\Lambda > 0$.

Before to analyze the dynamical properties of the model, it is important to underline some phenomenological aspects. If we taking in consideration the actual acceleration of the observed Universe, associated to a dark energy contribution in the energy spectrum, this behavior can be described, for example, when a positive cosmological constant is present within the Einstein equations. In this view, considering the presence of this positive cosmological constant coupled with the negative one introduced in our model, called them Λ_+ and Λ_-, it brings inevitably to consider the action of an effective cosmological constant defined as $\Lambda_{eff} = |\Lambda_+| - |\Lambda_-|$. This means, in the optic of the actual observations, that in the future the only effective contribution will be due to the positive cosmological constant, the Universe will continue to accelerate and the effect of the negative cosmological constant will never be observed. For this reason, the model described in this chapter becomes meaningless if a dark energy contribution is associated to a positive cosmological constant.

Nevertheless, the fact that an accelerated Universe can be described not only with a positive cosmological constant term allows to make compatible our model with a dark energy contribution. Indeed, given an equation of state $P = \omega\rho$, with P and ρ respectively pressure and energy density, the state parameter for an accelerated Universe have to respect the condition $\omega_{DE} < -\frac{1}{3}$. If now we restrict the range of the possible values for the parameter state to $-1 < \omega_{DE} < -\frac{1}{3}$ this means that the behavior of the energy density $\rho < a^{-3(1+\omega)}$ can never become constant (because the parameter state is strictly greater than -1) and it is limited from above by the behavior $\rho_{DE} < a^{-2}$. For this reason, when the Universe expands (namely in the limit $a \to \infty$), the effect of the dark energy density goes to zero and the contribution of a small negative cosmological constant can emerge as the dominant one in the future. In the light of what has been said, given the above restriction on the parameter state, the present model can maintain its validity also in the context of the actual phenomenological observations.

It is useful to describe the model with respect to the Misner variables $\{\alpha, \beta_\pm\}$, where α expresses the isotropic volume of the universe (the initial singularity is reached for $\alpha \to -\infty$) while $\beta_\pm$ accounts for the anisotropies of this model. The associated minisuperspace superHamiltonian takes the form[1]

$$\mathcal{H} = \frac{e^{-3\alpha}}{24\pi}\left[-p_\alpha^2 + p_+^2 + p_-^2\right] - \pi e^{3\alpha}\Lambda, \tag{5.1}$$

where $\{p_\alpha, p_+, p_-\}$ are the conjugated momenta related to the Misner variables. In view of a later quantization of the model, it is convenient to introduce the auxiliary variable ρ such that:

$$\rho = e^{\frac{3}{2}\alpha} \quad\longrightarrow\quad p_\rho = \frac{2}{3}e^{-\frac{3}{2}\alpha}p_\alpha. \tag{5.2}$$

In terms of this new conjugated variables the superHamiltonian (6.1) takes the form

$$\mathcal{H} = -\frac{3}{32\pi}p_\rho^2 + \frac{p_+^2 + p_-^2}{24\pi\rho^2} - \pi\rho^2\Lambda. \tag{5.3}$$

We now perform a canonical quantization of the system, after the definition of a suitable Hilbert space, by replacing the space-phase variables with multiplicative operators for variables $\{\rho, \beta_+, \beta_-\}$ and differential operators for $\{p_\rho, p_+, p_-\}$, so that:

$$p_i \to -i\frac{d}{dq_i} \quad , \quad q_i = \{\rho, \beta_+, \beta_-\}. \tag{5.4}$$

If now we introduce the wave function of the Universe $\psi(\rho, \beta_\pm)$ we can apply to it the quantum version of the superHamiltonian (5.3) in order to obtain the Wheeler-DeWitt operator

$$\hat{\mathcal{H}}\psi(\rho, \beta_\pm) = \left[\frac{3}{32\pi}\partial_\rho^2 - \frac{\partial_+^2 + \partial_-^2}{24\pi\rho^2} - \pi\rho^2\Lambda\right]\psi(\rho, \beta_\pm). \tag{5.5}$$

For the Bianchi I model that we are taking into account the superHamiltonian $\mathcal{H}^G$ is of the form (5.3), which in the quantum version $\hat{\mathcal{H}}^G$ correspond to the Eq.(5.5), and the eigenvalue problem (2.175) takes the explicit form:

$$\left[\frac{3}{32\pi}\partial_\rho^2 - \frac{\partial_+^2 + \partial_-^2}{24\pi\rho^2} - \pi\rho^2\Lambda\right]\psi(\rho, \beta_\pm) = E\psi(\rho, \beta_\pm). \tag{5.6}$$

The present study addresses the question concerning the positive character of the dust energy density, since we construct a quantum cosmology model for which such property definitely holds. It is actually relevant that from such a regularization of the Kukhař and Torre model the relevant issues described below come out: the emergence of a cyclical

[1] In this Chapter we use the $(-, +, +, +)$ signature of the metric and the geometric unit system ($c = G = \hbar = 1$).

Universe, possessing a Big-Bounce feature and the proper classical limit. The basic ingredient for such a physical implementation of the clock-dust dualism is the presence of a small negative cosmological constant (also ensuring the Universe turning point), while the evolutionary quantum dynamics is then crucial for the emergence of a cyclical picture. The physical meaning of our cosmological time consists of the possibility to restate the Bianchi I super-Hamiltonian eigenvalue as the energy density of a physical fluid, co-moving with the synchronous reference system and, de facto, identified with the latter. In the classical limit, our Universe possesses a dust contribution (non-relativistic matter) which is redshifted by the inflationary paradigm [79],[63] up to so much small values that its present day contribution to the Universe critical parameter is at all negligible, see [35],[9]. By other words, our physical dust is a valuable clock to describe the considered model evolution, but it is today so much diluted across the Universe that the difference with a formal system of coordinates is no longer appreciable and the General Relativity Principle is fully restored.

5.1.1 Semiclassical limit

Before to deal with the full quantum problem, it is interesting for our porpoises to study the associated classical problem to the Eq.(2.175), namely the zero-th order of a WKB expansion of the evolutionary quantum system[10]. The constraint that we obtain is

$$\mathcal{H} = -\frac{3}{32\pi}p_\rho^2 + \frac{p_+^2 + p_-^2}{24\pi\rho^2} - \pi\rho^2\Lambda = E \tag{5.7}$$

We can solve the classical dynamics making use of the Hamiltonian equations and the constraint (5.7). We can find solution for the isotropic variable ρ taking into account the Hamiltonian equations[2]

$$\begin{cases} \dot{\rho} = \frac{d\rho}{dt} = \frac{\partial\mathcal{H}}{\partial p_\rho} = -\frac{3}{16\pi}p_\rho \\ \dot{p_\rho} = \frac{dp_\rho}{dt} = -\frac{\partial\mathcal{H}}{\partial\rho} = \frac{p_+^2+p_-^2}{12\pi\rho^3} + 2\pi\rho\Lambda, \end{cases} \tag{5.8}$$

in order to obtain

$$\ddot{\rho} + \frac{p_+^2 + p_-^2}{64\pi^2\rho^3} + \frac{3}{8}\rho\Lambda = 0. \tag{5.9}$$

Recalling that $p_\rho = -\frac{16\pi}{3}\dot{\rho}$, the superHamiltonian constraint become

$$\dot{\rho}^2 - \frac{p_+^2 + p_-^2}{64\pi^2\rho^2} + \frac{3}{8}\rho^2\Lambda + \frac{3}{8\pi}E = 0. \tag{5.10}$$

It is possible to show that a solution for Eqs. (5.9) and (5.10) is given by

$$\rho(t) = \sqrt{\left(\frac{-E}{2\pi\Lambda}\right)\left[1 \pm \sqrt{1 + \frac{\Lambda(p_+^2 + p_-^2)}{6E^2}}\sin\left(\sqrt{\frac{3\Lambda}{2}}t + \varphi\right)\right]}. \tag{5.11}$$

The solution (5.11) exhibits the usual initial singularity in the past for which $\rho = 0 \rightarrow \alpha = -\infty$ and furthermore a singularity in the future exists too, namely a *big crunch* singularity. The value of the integration constant φ can be chosen in such a way that the initial

[2] In the following we label the Gaussian time variable T as t.

singularity happen for the value $t = 0$, to give us:

$$\varphi_0 = \arcsin\left(\mp\frac{1}{\sqrt{1+\frac{\Lambda(p_+^2+p_-^2)}{6E^2}}}\right). \tag{5.12}$$

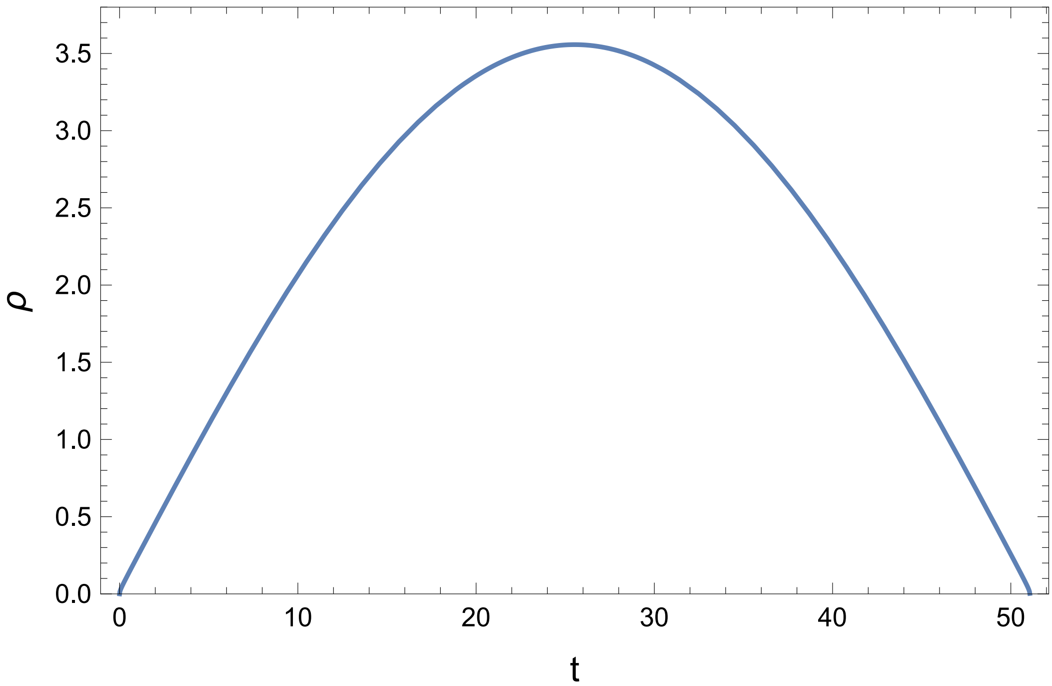

FIGURE 5.1: The classical trajectory for the isotropic variable ρ exhibit a singularity in the past and another one in the future. The solution is sketched for the parameters: $\Lambda = 0.01, p_+ = p_- = 0.1, E = -0.397$.

The classical behaviour of the isotropic variable ρ is sketched in Fig. 5.1. Analogously, The classical dynamics of the anisotropies $\beta_\pm$ can be solved, including the solution (5.11) inside the Hamiltonian equations. This way, we have

$$\begin{cases} \dot{\beta_\pm} = \frac{\partial\mathcal{H}}{\partial p_\pm} = \frac{p_\pm}{12\pi\rho^2} = -\frac{\Lambda p_\pm}{6E}\left[1 \pm \sqrt{1+\frac{\Lambda(p_+^2+p_-^2)}{6E^2}}\sin\left(\sqrt{\frac{3\Lambda}{2}}t+\varphi_0\right)\right]^{-1} \\ \dot{p_\pm} = -\frac{\partial\mathcal{H}}{\partial\beta_\pm} = 0 \end{cases} \tag{5.13}$$

The solution reads as

$$\beta_\pm(t) = \frac{p_\pm}{3\sqrt{p_+^2+p_-^2}}\ln\left|\frac{1+\frac{\sqrt{6}E}{\sqrt{\Lambda(p_+^2+p_-^2)}}\left(\sqrt{1+\frac{\Lambda(p_+^2+p_-^2)}{6E^2}}+\tan\left(\frac{1}{2}\sqrt{\frac{3\Lambda}{2}}t+\frac{\varphi_0}{2}\right)\right)}{1-\frac{\sqrt{6}E}{\sqrt{\Lambda(p_+^2+p_-^2)}}\left(\sqrt{1+\frac{\Lambda(p_+^2+p_-^2)}{6E^2}}+\tan\left(\frac{1}{2}\sqrt{\frac{3\Lambda}{2}}t+\frac{\varphi_0}{2}\right)\right)}\right| + const.. \tag{5.14}$$

As we can see in Fig. 5.2, at the classical level the anisotropies of the model become important in magnitude towards the singularities in the past and in the future. So, the presence of a negative cosmological constant in the semiclassical evolution case do not mine the divergence of the anisotropies towards the singularities, typical of the anisotropic models.

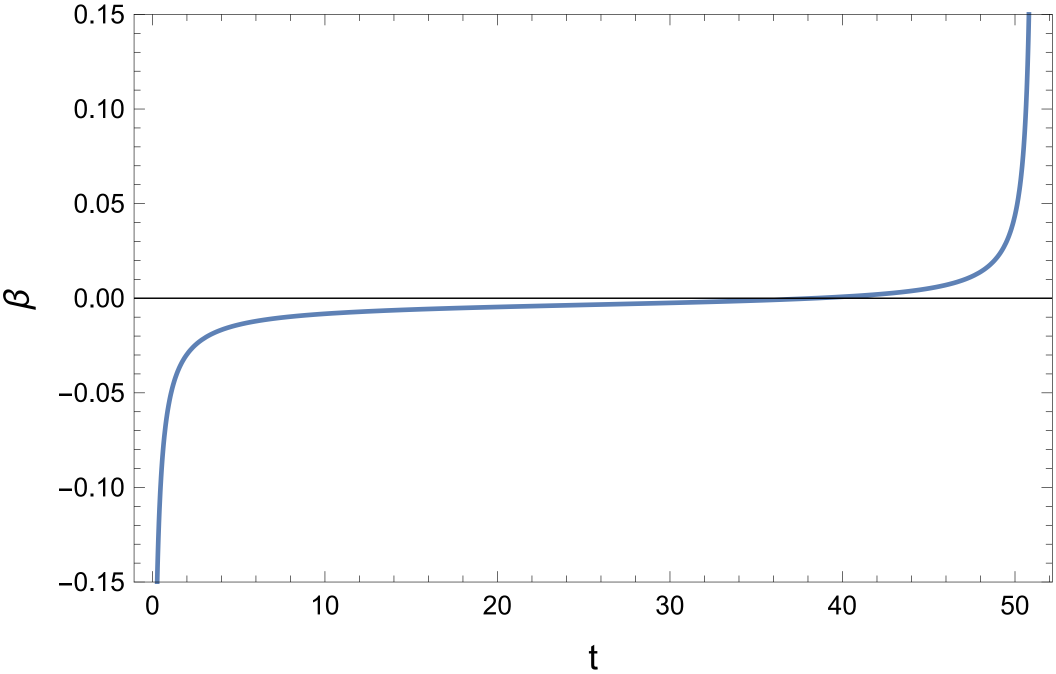

FIGURE 5.2: The classical trajectory for the anisotropies $\beta_\pm$. Next to the singularities the anisotropies diverge. The solution is sketched for the parameters: $\Lambda = 0.01, p_+ = p_- = 0.1, E = -0.397$.

5.1.2 Dynamics of the quantum expectation values

Let us consider now the full quantum evolution case (5.6). The absence of a potential term for the anisotropies suggests to us to consider for them a plane-waves solution, so that

$$\psi(\rho,\beta_\pm) = \frac{1}{2\pi} e^{ik_+\beta_+} e^{ik_-\beta_-}\chi(\rho), \tag{5.15}$$

where $\{k_+, k_-\}$ are the quantum numbers associated to $\{\beta_+, \beta_-\}$. Taking into account this shape of the wave function in the Eq.(5.6) brings to the following differential equation:

$$\left[\partial_\rho^2 + \frac{k_*^2}{\rho^2} - \Lambda_*\rho^2\right]\chi(\rho) = E_*\chi(\rho), \tag{5.16}$$

where

$$k_*^2 = \frac{4}{9}(k_+^2 + k_-^2) \quad , \quad \Lambda_* = \frac{32\pi^2\Lambda}{3} \quad , \quad E_* = \frac{32\pi E}{3}. \tag{5.17}$$

Looking at Eq.(5.16) we can observe a formal analogy with the problem of the 3-D harmonic oscillator, where the angular momentum l is in correspondence with the continuous values $k_*^2 = -l(l+1)$. Following the analogy, we choose a solution for $\chi(\rho)$ of the form[94]:

$$\chi(\rho) = e^{-\frac{\sqrt{\Lambda_*}\rho^2}{2}} \rho^{\frac{1}{2}+\frac{\sqrt{1-4k_*^2}}{2}} \xi(\rho). \tag{5.18}$$

The motivation of this choice is due to the fact that the terms $e^{\frac{\sqrt{\Lambda_*}\rho^2}{2}}$ and $\rho^{\frac{1}{2}+\frac{\sqrt{1-4k_*^2}}{2}}$ represent respectively the solutions of Eq.(5.16) in the limit $\rho \to \infty$ and $\rho \to 0$. The solution (5.18) should takes into account these two limit behaviours. We assume a finite power series expansion for the function $\xi(\rho)$ of the form:

$$\xi(\rho) = \sum_{k=0}^{k'} c_{k,k'}\rho^k \quad , \quad k, k' \in 2\mathbb{N}. \tag{5.19}$$

The reason is due to the fact that this is the only way to obtain a physical acceptable solutions. Indeed, if we take into account a solution $\sum_{k=0}^{\infty} c_k \rho^k$ for the problem (5.16) we obtain a non-converging series and then a diverging solution. To obtain a finite solution, as it is done in Eq.(5.19), we must required the series to be truncated at a certain power associated to k'. Including expansion (5.19) in Eq.(5.16) we arrive to the following difference equation

$$c_{k+2,k'}(k+2)\left[\sqrt{1-4k_*^2}+k+2\right] - c_{k,k'}\left[E_* + \sqrt{\Lambda_*}\left(\sqrt{1-4k_*^2}+2k+2\right)\right] = 0. \tag{5.20}$$

In order to obtain a finite solution we must set $c_{k+2,k'} = 0$. This restriction allows us to determine the behavior of the eigenvalue E, making use of the definitions (5.17):

$$E_* + \sqrt{\Lambda_*}\left(\sqrt{1-4k_*^2}+2k'+2\right) = 0 \Longrightarrow E_{k',k_\pm} = -\frac{1}{4}\sqrt{\frac{3\Lambda}{2}}\left[\sqrt{1-\frac{16}{9}(k_+^2+k_-^2)}+2k'+2\right]. \tag{5.21}$$

In order to deal with a real eigenvalues, we consider a restriction for the values of $\{k_+, k_-\}$ of the form

$$(k_+^2+k_-^2) \leq \frac{9}{16}. \tag{5.22}$$

This way we obtain a spectrum for the eigenvalues that assumes only negative real values and then the associated dust-energy density is always positive. Finally, always following the analogy with the 3-D harmonic oscillator, we can evaluate the coefficients $c_{k,k'}$ in terms of the Γ-function:

$$c^s_{k,k'} = \frac{(-1)^{\frac{k}{2}}((-1)^k+1)\Gamma\left[1+\frac{1}{2}\sqrt{1-\frac{16}{9}(k_+^2+k_-^2)}\right]\left(\frac{32\pi^2\Lambda}{3}\right)^{\frac{k}{4}}\frac{k'}{2}!}{\Gamma\left[1+\frac{k}{2}\right]\Gamma\left[1+\frac{n}{2}+\frac{1}{2}\sqrt{1-\frac{16}{9}(k_+^2+k_-^2)}\right](\frac{k'}{2}-\frac{k}{2})!}. \tag{5.23}$$

Now we can obtain the shape of the entire wave function, solution to the problem (5.6), that is

$$\psi(\rho,\beta_\pm) = Ae^{ik_+\beta_+}e^{ik_-\beta_-}e^{-\frac{\sqrt{\Lambda_*}\rho^2}{2}}\rho^{\frac{1}{2}+\frac{\sqrt{1-4k_*^2}}{2}}\sum_{k=0}^{k'}c^s_{k,k'}\rho^k, \tag{5.24}$$

where A is a normalization constant. Now we want to perform a comparison between the classical trajectories (5.11),(5.14) and the expectation values of the associated operator $\hat{\rho}$ and $\hat{\beta}_\pm$. The states on which we evaluate them can be constructed taking into account the wave packets associated to the wave function (5.24) peaked around classical values $\{k'^*, k_+^*, k_-^*\}$,*i.e.*

$$\Psi_{k'^*,k_\pm^*}(\rho,\beta_\pm) = A\int\int_R dk_\pm e^{-\frac{(k_+-k_+^*)^2}{2\sigma_+^2}}e^{-\frac{(k_--k_-^*)^2}{2\sigma_-^2}}\sum_{k'=1}^{\infty}e^{-\frac{(k'-k'^*)^2}{2\sigma^2}}e^{-iE_{k',k_\pm}t}\psi(\rho,\beta_\pm), \tag{5.25}$$

where the integration on $\{k_+, k_-\}$ are restricted over the region $R = \{k_+, k_- \in \mathbb{R}|(k_+^2 + k_-^2) \leq \frac{9}{16}\}$ and we choose Gaussian weights to peak the wave packets. The evolution in time of the expectation value of the operator $\hat{\rho}$ is evaluated over such states:

$$< \hat{\rho} >_t = \int_0^\infty d\rho \int_{-\infty}^\infty d\beta_\pm (\Psi_{k'^*,k_\pm^*})^* \rho \Psi_{k'^*,k_\pm^*}. \tag{5.26}$$

As we can see in Fig. 5.3 we have an overlap between the expectation value (black points) and classical trajectory (red continuous line) only for late time t. When we approach $t = 0$, the expectation value moves away from the classical trajectory and it does not exhibit a singular behavior. As a consequence, we can argue that in the evolutionary quantum model the singularity is avoided and it is replaced by a bounce. The validity of this argument is supported by the analysis of the uncertainty:

$$< \Delta\rho^2 >_t = \int_0^\infty d\rho \int_{-\infty}^\infty d\beta_\pm (\Psi_{k'^*,k_\pm^*})^* \rho^2 \Psi_{k'^*,k_\pm^*} - < \hat{\rho} >_t^2, \tag{5.27}$$

essentially for two reasons. The first one is, as we can see in Fig. 5.4, that when we are near the singularity the uncertainty $< \Delta\rho^2 >$ has a maximum value but it remains always small compared to the expectation value and it does not diverge in correspondence of the singularity. Thus we can conclude that the expectation value (5.26) is a good indicator for the system next to the singularity. The second reason is the late times behavior. It is clear from Fig. 5.4 that as we get farther away from the singularity, the uncertainty becomes smaller and smaller and approaches zero in the region of the overlap between expectation value and classical trajectory, guaranteeing that the Universe becomes always more and more classical at late times.

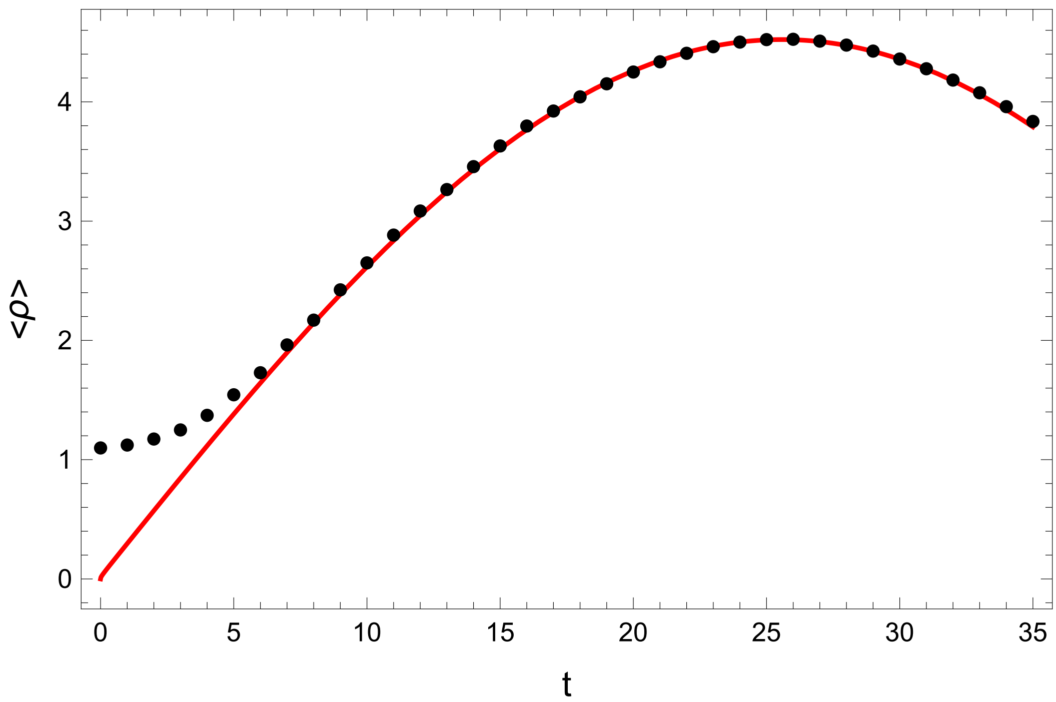

FIGURE 5.3: The black points represent the expectation value $< \rho >_t$ evaluated via numerical integration for the following choose of the integration parameters: $\Lambda = 0.01, k'^* = 5, k_+^* = k_-^* = 0.1, \sigma_+ = \sigma_- = 0.01, \sigma = 0.88$. The continuous red line represents the classical trajectory evaluated with the same classical parameters.

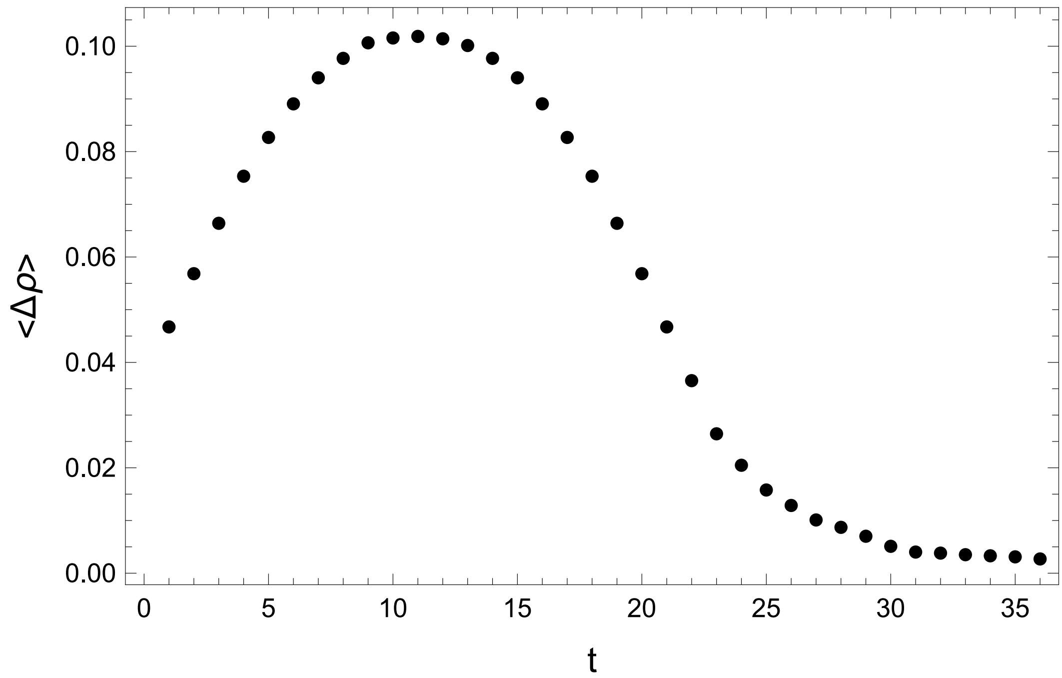

FIGURE 5.4: The uncertainty of ρ as a function of time t that confirm how the expectation value $<\rho>_t$ is a genuine quantity.

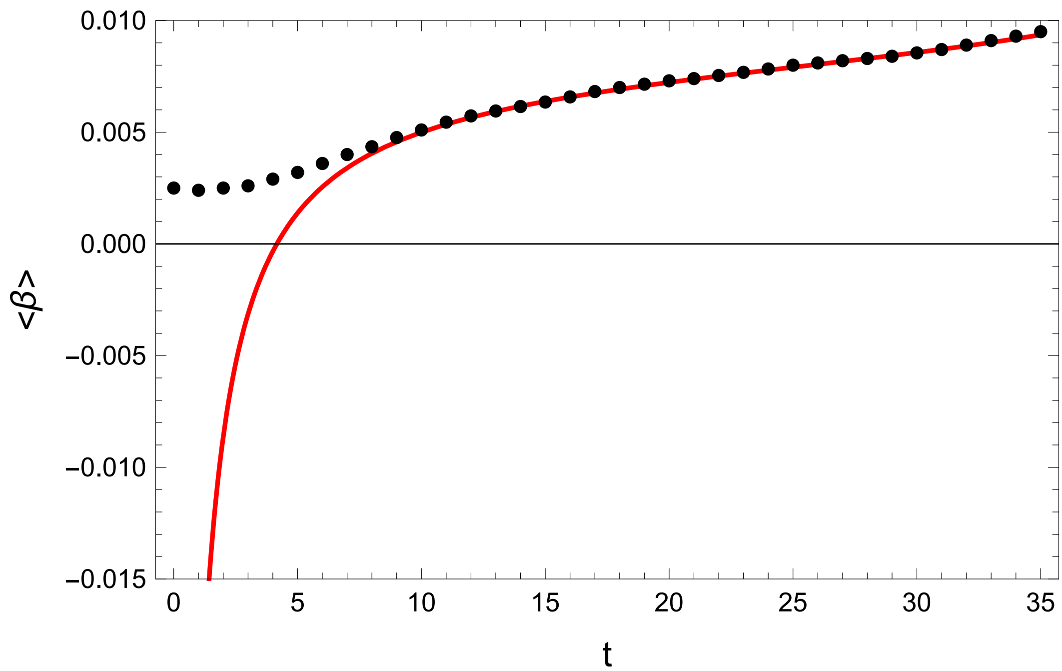

FIGURE 5.5: The black points represent the expectation value $<\beta_{\pm}>_t$ evaluated via numerical integration for the following choose of the integration parameters: $\Lambda = 0.01, k^{'*} = 5, k^*_+ = k^*_- = 0.1, \sigma_+ = \sigma_- = 0.01, \sigma = 0.88$. The continuous red line represents the classical trajectory evaluated with the same classical parameters.

The same approach can be used to compare expectation values related to the anisotropies with the corresponding classical trajectories. The evolution in time is:

$$< \hat{\beta_{\pm}} >_t = \int_0^{\infty} d\rho \int_{-\infty}^{\infty} d\beta_{\pm} (\Psi_{k'^*,k^*_{\pm}})^* \beta \Psi_{k'^*,k^*_{\pm}} \tag{5.28}$$

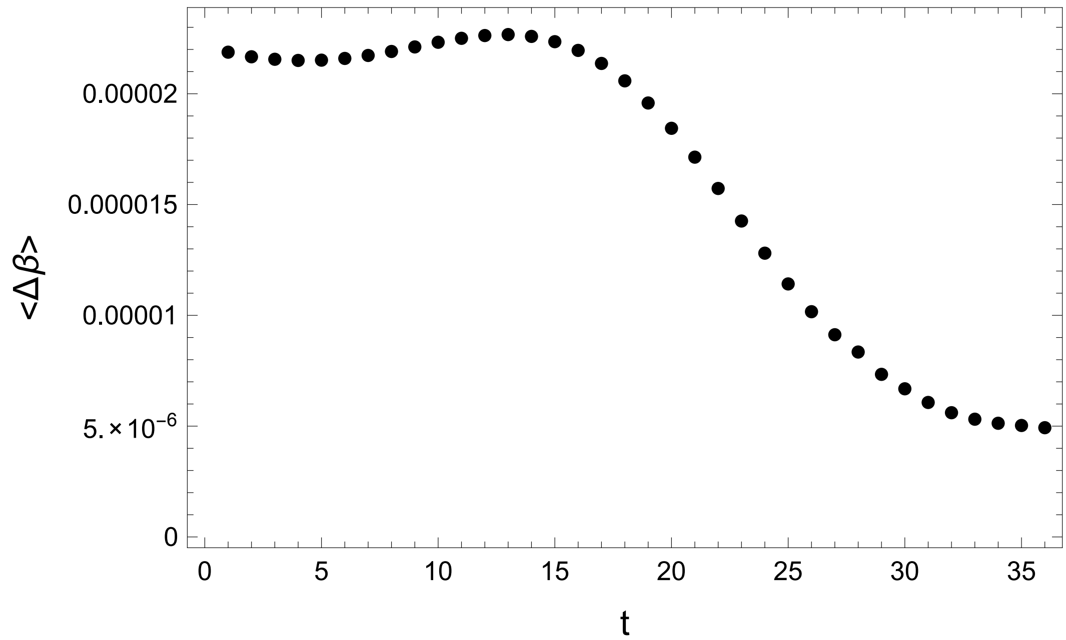

FIGURE 5.6: The uncertainty of β as a function of time t that confirm how the expectation value $<\beta>_t$ is a genuine quantity.

As we can see in Fig. 5.5 again we have an overlap between the expectation value (black points) and the classical trajectory (red continuous line) only for late time t. At early times, the diverging behavior exhibited by the anisotropies at the classical level disappears in the quantum model. Indeed, when we approach the limit $t \to 0$ the anisotropies remain small and finite. As before, the validity of this argument is supported by the analysis of the uncertainty $\Delta\beta_\pm$, defined as

$$< \Delta\beta^2 >_t = \int_0^\infty d\rho \int_{-\infty}^{\infty} d\beta_\pm (\Psi_{k'^*,k^*_\pm})^* \beta^2 \Psi_{k'^*,k^*_\pm} - < \hat{\beta} >_t^2 \,. \tag{5.29}$$

As it is shown in Fig. 5.6, the situation is exactly the same with respect to the case of the variable ρ, and this bring us to conclude in an analogous way that the (5.28) is a genuine quantity to describe the system next to the singularity and to recover the classical limit for late times. We conclude this section by noting how all the considerations here discussed for the initial singularity must remain valid when we consider the Bianchi I singularity in the future. By other words also the existing Big-Crounch is removed in favour of a bounce and our model acquires a cyclical feature. The non-diverging character of the anisotropies in this scenario can have intriguing implications for the so-called Big-Bounce cosmologies [20] in view of the possibility to minimize the effect on anisotropic evolution.

5.2 Implication on the Bianchi IX model

Now, in order to implement the proprieties founded before to a general one model, we analyze the Bianchi IX cosmology in presence of a negative cosmological constant in the context of the evolutionary model. With respect to the configurational variables $\{\rho, \beta_+, \beta_-\}$ the superHamiltonian constraint takes the form

$$\mathcal{H} = -\frac{3}{32\pi} p_\rho^2 + \frac{p_+^2 + p_-^2}{24\pi\rho^2} + \frac{\pi}{2}\rho^{2/3} V_{IX}(\beta_\pm) - \pi\rho^2\Lambda = E, \tag{5.30}$$

where the potential term, which accounts for the spatial curvature of the model, reads as

$$V_{IX}(\beta_\pm) = e^{-8\beta_+} - 4e^{-2\beta_+}\cosh(2\sqrt{3}\beta_-) + 2e^{4\beta_+}\left[\cosh(4\sqrt{3}\beta_-) - 1\right]. \tag{5.31}$$

This potential is obtained selecting the three constants of structure $(\lambda_l, \lambda_m, \lambda_n) = (1, 1, 1)$. As it is well known, in the context of the Misner-like variables, it is clear that the difference between the Bianchi I model and the Bianchi IX model is the presence of the potential term $\frac{\pi}{2}\rho^{2/3}V_{IX}(\beta_\pm)$. For this reason we want to see if exists a regime in which the potential term of the Bianchi IX model is negligible with respect to the kinetic plus the cosmological constant term. In other words, we want to see when it is possible to argue that the properties founded in the previous section for the Bianchi I model are valid also for the Bianchi IX model. The importance to find a regime of this kind is due to presence of the BKL conjecture, which it allows to extend such conclusion to the generic cosmological solution. To this aim, we now want to assess the importance of the potential term $V^*_{IX} = \frac{\pi}{2}\rho^{2/3}V_{IX}(\beta_\pm)$ evaluated at the bounce as the dust energy E, estimated in the (5.21), changes. As we can see in Fig. 5.7, the potential term of the Bianchi IX

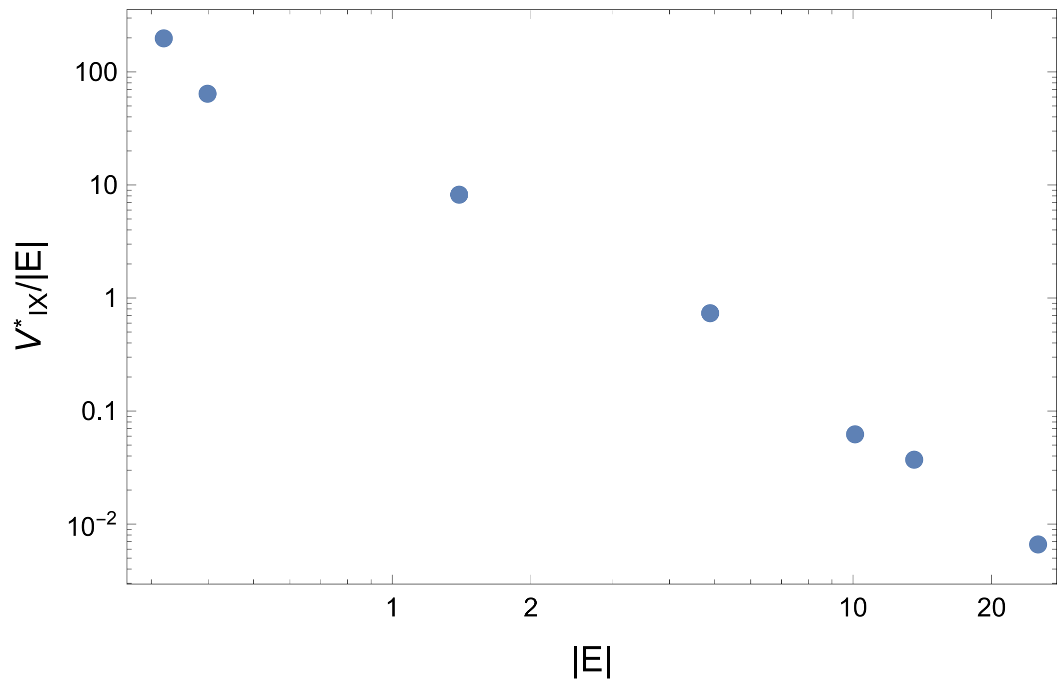

FIGURE 5.7: The behavior of the quantity $V^*_{IX}/|E|$ as a function of $|E|$ evaluated in correspondence of the bounce. The role of the Bianchi IX potential term became more and more marginal with the increase of the dust-energy.

model becomes more and more negligible as the magnitude of the dust energy density increases. This means that, following the trajectory of a Bianchi IX cosmology the relevant contribution comes from the kinetic plus cosmological constant term because the potential is more and more negligible as far as the parameter E becomes large. In this sense we can conclude, provided that the dust energy density is large enough to neglect the potential term, that the Bianchi IX model in presence of a negative cosmological constant in the evolutionary context possesses the same qualitatively features of the Bianchi I model previously founded.

5.3 Phenomenological considerations

Let us now provide a proper cosmological interpretation to the results we obtained in the previous sections and to outline the main merits of the proposed scenario.

We considered a cosmological model which corresponds to the type I of the Bianchi classification, i.e. having zero spatial curvature and we included in the dynamics a small negative cosmological constant. The quantization of the model, to account for its behavior nearby the cosmological singularity, has been performed accordingly to the Kuchař-Torre approach, relaying on a basic dualism between an external clock and the presence of a real dust fluid in the model evolution. The weak point of such a viable perspective to construct a physical time in quantum gravity, consists, in general, of the non positive definite nature of the dust energy density, emerging from the implementation of an external time (this fact reflects the non positive character of the super-Hamiltonian eigenvalue). However, in the considered model, this shortcoming of the dualism time-dust is fully overcome, since the energy of the dust is always positive and this is a consequence of the negative value of the cosmological constant, which, from a purely formal point of view, allows to compare the Universe volume quantum dynamics to an harmonic oscillator, but having a global minus sign.

Then, studying the behavior of quantum expectation values and uncertainties, we get the very surprising and valuable issue of a Big-Bounce cosmology. What makes our model physically meaning is the existence of a spontaneous classical limit, associated to the same harmonic structure removing the singularity. The quadratic potential, associated to the negative cosmological constant is responsible for a localization of the physical quantum states nearby the classical trajectory, as the Universe has a sufficiently large volume.

This two important features of the model, i.e. the presence of a Big-Bounce nearby the classical location of the singularity and the natural classical limit of the expanded Universe, together with the turning point in the Universe late time evolution that the negative cosmological constant induces in the classical dynamics, suggests that our Bianchi I cosmology is an intriguing candidate for a cyclic Universe.

This issue would be in itself a remarkable scenario, but our interest for the constructed picture is actually for the potential degree of generality it could represent. In fact, in section 5.2, we have inferred that the behavior of the Bianchi type I model can be extended, under suitable conditions (i.e. a sufficiently large value of the parameter E) to the most general Bianchi type IX cosmology, which is a good prototype for the generic cosmological Universe. By other words, it is a natural guess that the implementation of an evolutionary quantum gravity in the presence of a small negative cosmological constant can lead to a non-singular cyclic Universe even when we are referring it to a generic inhomogeneous Universe. According to the BKL conjecture [14] and to its quantum implementation (the so-called long-wavelength assumption), for each sufficiently small neighbor of a space point, physically corresponding to the cosmological horizon, the dynamical evolution is qualitatively that one of a Bianchi IX Universe. Thus, we trace in the present analysis the basic dynamical features that could regularize the cosmological problem, without explicitly including an ultraviolet cut-off in the canonical Wheeler-DeWitt quantization of the system. Now, we should get light on the physical mechanism at the ground of such dynamical picture traced above and, in this respect, we investigate which of our ingredients is related in the model to a cut-off physics.

5.4 Physical interpretation of the Big Bounce

In this section we want to show how is central the presence of the negative cosmological constant for the appearance of the Big Bounce. To this aim we analyse here an evolutionary Bianchi I model without the negative cosmological constant and we consider a cut-off polymer dynamics that makes discrete the isotropic variable ρ in order to show how the behaviour of the quantum expectation values of the previous section and the behaviour of the polymer semiclassical dynamics are equivalent. This equivalence testifies the fact that the negative cosmological constant plays the role of a cut-off physics. The model will be analysed in the same configurational space variables $\{\rho, \beta_+, \beta_-\}$ and the physical choice is to define the isotropic variable ρ as a discrete variable and to leave unchanged the anisotropies $\{\beta_+, \beta_-\}$. We consider the polymer modification at a semiclassical level. It means that we are working with a modified superHamiltonian constraint obtained as the lowest order term of a WKB expansion for $\hbar \to 0$ of the full polymer quantum problem[39],[38]. This procedure formally consists in the replacement

$$p_\rho^2 \to \frac{2}{\mu^2}[1-\cos(\mu p_\rho)], \tag{5.32}$$

where μ is the polymer scale, or equivalently the lattice spacing for the variable ρ. From the substitution (5.32) the superHamiltonian becomes

$$\mathcal{H}_p = -\frac{3}{16\pi\mu^2}[1-\cos(\mu p_\rho)] + \frac{p_+^2+p_-^2}{24\pi\rho^2}, \tag{5.33}$$

and again the superHamiltonian constraint is

$$\mathcal{H}_p = E. \tag{5.34}$$

As in the previous case, we can solve the semiclassical polymer dynamics making use of the Hamiltonian equations

$$\begin{cases} \dot{\rho} = \frac{\partial \mathcal{H}_p}{\partial p_\rho} = -\frac{3}{16\pi\mu}\sin(\mu p_\rho) \\ \dot{p_\rho} = -\frac{\partial \mathcal{H}_p}{\partial \rho} = \frac{p_+^2+p_-^2}{12\pi\rho^3} \end{cases} \tag{5.35}$$

and of the constraint (5.34). This way we obtain the following second order differential equation:

$$\ddot{\rho} + \frac{(p_+^2+p_-^2)\left(1-\frac{2\mu^2(p_+^2+p_-^2)}{9\rho^2}+\frac{16}{3}\pi\mu^2 E\right)}{64\pi^2\rho^3} = 0 \tag{5.36}$$

It is not possible to individuate an analytical solution for the differential equation above, and then we perform a numerical integration. In order to find a link between the presence of a negative cosmological constant and the polymer scale we make a comparison between the classical and the quantum models analyzed in Section 5.1 and this new semiclassical polymer model. We impose that the initial condition for the numerical integration of the differential equation (5.36) is exactly equal to $<\rho>_0$ adopted in Fig. 5.3, *i.e* we are arguing that the initial condition for the semiclassical evolutionary polymer problem matches the expectation value of the quantum evolutionary model in the correspondence of the bounce determined in the previous section. In order to perform this comparison we obviously choose the same classical values for the parameters $\{p_+, p_-, E\}$ and the same corresponding parameters $\{k'^*, k_+^*, k_-^*\}$ around which we have built the wave packets that we have used in Section 5.1. The only free parameter that we can fix is the polymer scale μ.

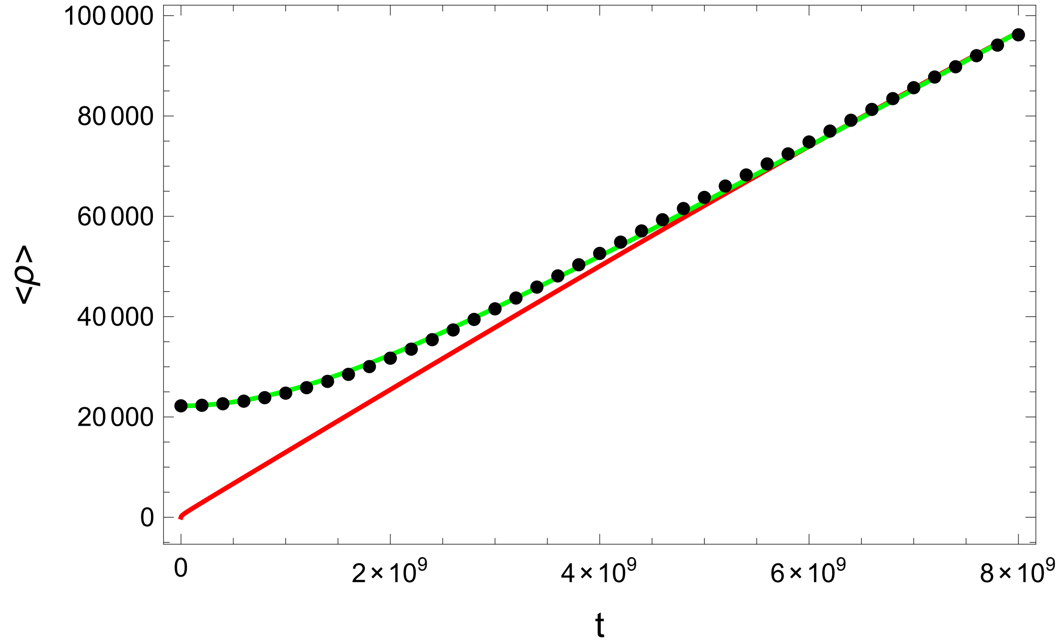

FIGURE 5.8: The black points represent the expectation value $<\rho>_t$ evaluated via numerical integration for the following choose of the integration parameters: $\Lambda = 10^{-20}, k'^* = 20, k_+^* = k_-^* = 0.1, \sigma_+ = \sigma_- = 0.01, \sigma = 0.88$. The continuous red line represents the classical trajectory while the green line represents the semiclassical polymer trajectory, where the polymer scale is fixed with the choice $\mu = 3.08 \cdot 10^5$.

As we can see in Fig.5.8 it is possible to individuate a special value for the parameter μ for which the behavior of $\rho(t)$ in the semiclassical polymer approach overlaps the expectation value $<\rho>_t$ in the quantum evolutionary theory. Furthermore, as it is expected for every kind of polymer approach, for late times the semiclassical polymer trajectory overlaps the classical one. This way we show that near the singularity in the context of the evolutionary theory, a negative cosmological constant acts the same way as a polymer modification related to the isotropic variable, *i.e.* a cut-off physics.

It is possible to deepen the connection between the negative cosmological constant and the polymer scale making use of several numerical integrations related to different choice of the parameters values and seeing, time after time, if there is a general law. In Fig.5.9 it is shown the behavior of $\log \mu$ as a function of $\log \sqrt{\Lambda}$, where the values of the numerical integration parameters $\{k', k_+, k_-\}$ used for evaluating the expectation value (5.26)(and obviously the correspondent polymer integration parameters $\{p_+, p_-, E\}$) are fixed for each line. As we can see, the slope of the lines is always the same, independently from the choice of the parameters, and it is equal to $-\frac{1}{2}$. It means that a universal law exists such that:

$$\log \mu = \log \alpha_k - \frac{1}{2} \log \sqrt{\Lambda} \longrightarrow \mu^2 \sqrt{\Lambda} = \alpha_k^2, \tag{5.37}$$

where the constant $\alpha_k = \alpha_{k',k_+,k_-}$ depends on the values assigned to the parameters.

5.5 Concluding remarks

The main merit of the present work is in demonstrating how a rather general scenario for a cyclical Universe can be recovered even within the metric canonical quantum approach,

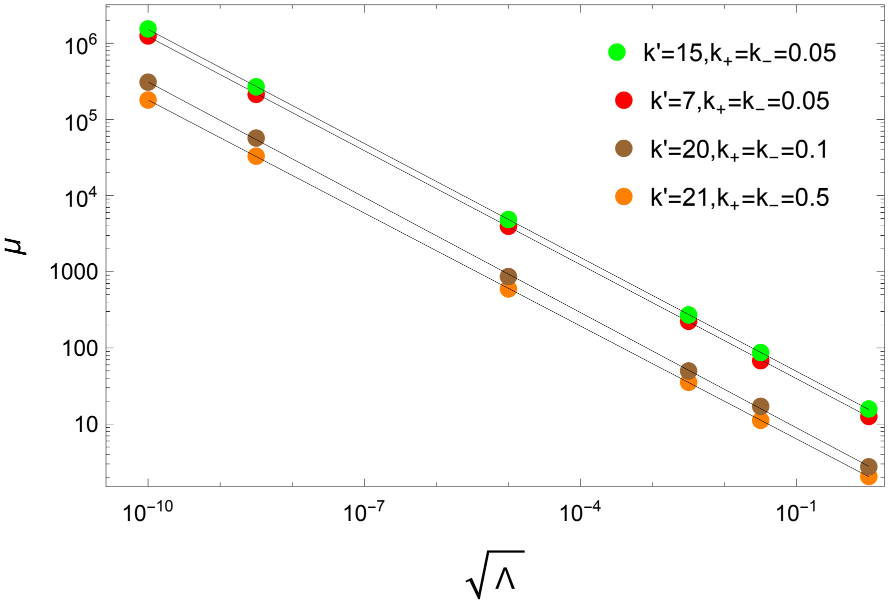

FIGURE 5.9: The behavior of the polymer scale μ as a function of $\log\sqrt{\Lambda}$. It is evident the existence of a law between the polymer scale and the negative cosmological constant, independently from the choice of the parameters.

as far as a well-defined evolutionary theory is taken into account.

The basic ingredient of our approach is the small negative cosmological constant, which is responsible for the classical turning point, but overall, it induces an harmonic oscillator morphology in the quantum universe volume dynamics. The Bianchi I cosmology we addressed here allows the simultaneous manifestation of significant properties, like the Big-Bounce, the existence of well-defined classical limit and the positive character of the dust energy density, playing the role of a clock. However, what makes the present issues of intriguing cosmological meaning is the possibility to extend this picture to the Bianchi IX Universe. In fact, this property suggests that the considered minisuperspace scheme can be generalized to the generic inhomogeneous cosmological problem. As far as we implement the long-wavelength approximation to the inhomogeneous quantum dynamics, we can factorize the Wheeler superspace into the local minisuperspaces, associated to space point neighbours. From a physical point of view, we can speak of causal regions evolving, independently of each other, according to the non-singular cyclic dynamics we traced above. The implementation of the present ideas to a generic inhomogeneous Universe, as well as, the characterization of the role played by the matter, especially the radiation component, during the classical evolution, constitutes the natural perspective of the present analysis.

Chapter 6

Vilenkin Interpretation of the wave function of the Universe for a Polymer Bianchi I universe

The Bianchi cosmological models are the simplest generalization of the isotropic Universe and they are possible candidate to describe the nature of the initial singularity [14],[65],[79].

Two Bianchi model are of particular dynamical interest, the type I, because it contains the metric time derivatives dominating near the singularity, and the type IX, which generalizes the closed Robertson-Walker dynamics and thus having a space curvature, responsible for a chaotic behavior near the singularity [76].

Indeed, the Bianchi types VIII and IX (however the type VIII does not admit an isotropic limit) are the most general models allowed by the homogeneity and their chaotic features are typical of the generic inhomogeneous cosmological solution.

The anisotropic components of the metric tensor can be easily separated for the Bianchi models from the isotropic component, which is associated to the Universe volume and this separation takes place in a very elegant representation, by using the so-called Misner variables [75].

Near the initial singularity, the Universe volume vanishes and the Bianchi model anisotropies typically diverges.

However, it is a common belief that the cosmological singularity must be replaced by a Big-Bounce of the Universe, *i.e.* the volume reaches a minimum and then re-expands. This picture has been reproduced in many quantum approaches to the early Universe dynamics, especially in the so-called Loop Quantum Cosmology [3],[4], see also [big bounce,pittorino]. Such a reliable prediction of the quantum cosmology has given rise to a new theoretical framework to interpret the Universe history, dubbed Big-Bounce Cosmology [20]. In fact, some important aspects of the Universe dynamics, especially in its early stages, like the basic paradoxes of the Standard cosmological Model [63], could be differently addressed in view of the pre-Big-Bounce history.

A crucial point in the direction of a revised point of view on the primordial Universe, once the existence of a Big-Bounce is postulated, requires a precise understanding of the role played by the anisotropies degrees of freedom near the primordial turning point of the Universe: by other words, which is the behavior of the Universe anisotropies across the Big-Bounce. The most natural arena in which testing such a feature of the primordial cosmology is given by the Bianchi model, especially the type I and IX respectively. In this paper, we address exactly this problem, by reproducing the Big-Bounce via a Polymer quantum approach [39],[38]. However, to provide a clear physical meaning to the anisotropy variable wavefunction, we combine the polymer technique with the original Vilenkin semiclassical approach to the Wheeler-DeWitt equation [92],[**halliwell**]. More specifically, we describe the Bianchi models via the Misner variables [75]and we retain the volume as a quasi-classical coordinate, although obeying to the modified Hamilton-Jacobi equation, due to the polymer discretization. The anisotropies Misner variables are instead treated as pure quantum degrees of freedom.

The main technical merit of the present analysis is just to reconcile two different, but complementary points of view, as the mentioned above, in order to provide a consistent and regularized Big-Bounce cosmology, in which the behavior of the anisotropies near and far from the turning point can be discussed in detail.

We observe how, the dynamics of the semi-classical Universe volume is analyzed in the presence of stiff matter. This choice actually underlying technical reasons, but it is also cosmologically relevant since the stiff matter equation of state mimic the dynamics of a free massless scalar field, whose energy fills the Universe and determines its evolution: this is just the case of an inflaton field at sufficiently high temperature, where the potential term, responsible for the inflation scenario, can be neglected (actually the cut-off energy density is supposed to be at the Planck scale, well above with respect to the inflation threshold).

We study in detail the behavior of the wave packets, comparing it with the prediction of the Ehrenfest theorem [47]. We recall that the Vilenkin approach allows to deal with an ordinary Schroedinger equation for the anisotropy variables, although the translation of the dynamical picture in the synchronous reference involves the details of the polymer Hamilton-Jacobi equation, describing the leading order dynamics of the Universe volume.

We first address a careful analysis of the Bianchi I model, demonstrating that the anisotropies mean values and variances remain finite near the singularity, differently from the Einsteinian classical behavior, associated to a divergence of the Universe anisotropy near the singularity.

As far as the WKB Vilenkin approximation holds, we can claim that the anisotropy of the Universe remains finite across the Big-Bounce, its limit valued being dependent on the initial conditions, fixed far from the turning point. It is worth noting that WKB assumption is reliable since the Universe volume is essentially a time-like variable in the minisuperspace, more than a real physical degree of freedom. The anisotropy variables behavior tends also to become more and more classical near the Big-Bounce, in the sense that the ratio between the variance to the mean value decreases. This feature could be also recovered in a non-polymer representation of the Universe volume quasi-classical dynamics, but, in that case, it remains meaningless due to the intrinsic divergence of the anisotropies mean value, as we discuss in some detail.

Then, we extend the same analysis to the Bianchi IX model, estimating the relative behavior of the kinetic term of the Hamiltonian (present in both the Bianchi I and IX types) versus the potential term of the Bianchi IX model, due to its non-vanishing spatial curvature(for Bianchi I the three-dimensional Ricci scalar identically vanishes).

This study demonstrate that, for a non-zero set of initial conditions (fixed far from the Big-Bounce), the potential term is negligible in the Bianchi IX dynamics, with respect to the kinetic one: all the considerations developed for the Bianchi I model can be applied to the Bianchi IX one too. We estimate the behavior of the potential term on the mean values of the anisotropic variables, but, their increasing classical behavior to the Big-Bounce ensures the predictivity of this quantity toward the average value of the potential (rigorously involved in the Ehrenfest theorem).

The study of the Bianchi IX dynamics and the possibility to claim a regular behavior of the Universe anisotropies across the Bounce, provides our results with a an high degree of generality, since the Bianchi IX model is the homogeneous prototype for the generic inhomogeneous cosmological solution [15],[79]. The most relevant conceptual progress contained in the present analysis concerns the possibility, on a different regularized framework, to elucidate the original result of Misner about the existence of semiclassical states off the Universe anisotropies, near enough to the singularity [75]. The Misner conclusion involves only high occupation numbers of the anisotropy degrees of freedom and its physical interpretation remains obscure, due to the diverging character of the anisotropy variables according to the Ehrenfest theorem. The proper interpretation of that Misner result comes out, as soon as, a Big-Bounce and WKB cosmology is implemented for the Universe volume.

The structure of the Chapter is organized as follows.

The Section 6.1 is dedicated to the application of the Vilenkin approach to a specific cosmological model: the Bianchi I model in presence of a stiff matter. Firstly, we faced the semiclassical dynamics by studying the Hamilton-Jacobi equation and evaluating the evolution of the variable related to the Universe volume near the initial singularity. Then, the WKB expansion due to the Vilenkin form of the wave function, allow to describe the behaviour of the pure quantum degrees of freedom of the system: the anisotropies. For the description of such a variables, a Schrodinger-like equation is resemble whose solution represents the quantum states of the system. Starting from this states it is possible to build the wave packets associated to the wave function of the Universe and compare their evolution with the trajectories of the mean values obtained from the Ehrenfest theorem. Furthermore, both from the semiclassical and the quantum point of view, is stressed the equivalence in the obtained results making the two different polarization choices for the isotropic component of the wave function.

Moreover, the polymer generalization of the latter model is illustrated in Section 6.2. In particular, we consider the modifications induced in the configuration variables dynamics towards the initial singularity when a polymer discretization of the Universe volume occurs.

The polymer modification applied to the Bianchi I model is then extended to the more general Bianchi IX model in Section 6.3. The main focus in this section is devoted to the importance of the curvature potential term of the Bianchi IX model next to the turning point.

Brief concluding remarks complete the Chapter.

The work illustrated in this Chapter is now under revision on the international journal **Physical Review D** for publication.

6.1 Bianchi I model in the Vilenkin approach

In this Section we introduce a simple and instructive model for which it is possible to individuate a separation in the configuration space between classical and quantum variables. Let us consider a universe described by a Bianchi I model filled with a stiff matter. The description of the model will be done with respect to the Misner-like variables $\{a, \beta_\pm\}$[1], where a expresses the isotropic volume of the universe (the initial singularity is reached for $a \to 0$) while $\beta_\pm$ accounts for the anisotropies of this model. The associated superHamiltonian constraint takes the form[2]

$$\mathcal{H} = \frac{l_p^2}{24\pi\hbar}\left[-\frac{p_a^2}{a} + \frac{p_+^2 + p_-^2}{a^3}\right] + \frac{8\pi^2\mu^2}{\hbar a^3} = 0 \tag{6.1}$$

[1]The original isotropic Misner variable α is just $\alpha = \ln a$.

[2]In this Chapter we use the $(-,+,+,+)$ signature of the metric, the unit system with $(c = 1)$ and we explicit the Einstein constant as $k = 8\pi G = \frac{8\pi l_p^2}{\hbar}$ where l_p is the Planck length.

where $\{p_a, p_+, p_-\}$ are the conjugated momenta related to the Misner-like variables and the constant μ represents the stiff matter contribution. The canonical quantization of the model will be done at first in the a-polarization, following the prescription of the Section 2.8, and then in the p_a-polarization. In both cases the quantization of the anisotropies will be in the position polarization. Through the realization of such a comparison we shall show how the semiclassical and quantum solutions obtained will be equivalent in both cases. This result will be very useful in respect of the implementation of the polymer paradigm.

6.1.1 a-polarization

Here we perform a canonical quantization imposing that the physical states ψ being annihilated by the operator $\mathcal{H}$, *i.e.* the quantum version of the superhamiltonian constraint (6.1). If we choose to describe all the configuration variables in the position polarization, this means that $\{\widehat{a}, \widehat{\beta}_+, \widehat{\beta}_-\}$ act as a multiplicative operators and $\{\widehat{p}_a, \widehat{p}_+, \widehat{p}_-\}$ as a derivative operators in this way:

$$\widehat{p}_a = -i\hbar\frac{\partial}{\partial a} = -i\hbar\partial_a \quad , \quad \widehat{p}_\pm = -i\hbar\frac{\partial}{\partial \beta_\pm} = -i\hbar\partial_\pm. \tag{6.2}$$

Therefore, the WDW equation for the superhamiltonian (6.1) can be written as

$$\left[\hbar^2 a^2\partial_a^2 - \hbar^2\left(\partial_+^2 + \partial_-^2\right) + \frac{3(4\pi)^3\mu^2}{l_p^2}\right]\psi(a,\beta_\pm) = 0. \tag{6.3}$$

Starting from the equation (6.3), it is possible to individuate a corresponding current of this form

$$J^\mu = \begin{bmatrix} J^a \\ J^+ \\ J_- \end{bmatrix} = -\frac{i}{2}\hbar^2 \begin{bmatrix} a^2(\psi^*\partial_a\psi - \psi\partial_a\psi^*) \\ -(\psi^*\partial_+\psi - \psi\partial_+\psi^*) \\ -(\psi^*\partial_-\psi - \psi\partial_-\psi^*) \end{bmatrix},$$

for which the conservation law $\nabla_\mu J^\mu = 0$ is valid. Here ∇_i is the covariant derivative built with the superspace metric $g^{\mu\nu} = diag(\hbar^2 a^2, -\hbar^2, -\hbar^2)$ and its action on a generic vector v^ν is

$$\nabla_\mu v^\nu = \partial_\mu v^\nu + \Gamma^\nu_{\mu\rho}v^\rho. \tag{6.4}$$

For our superspace metric $g_{\mu\nu}$, the only non-vanishing Christoffel symbol is $\Gamma^a_{aa} = -\frac{2}{a}$. Therefore, the conservation of the current in Eq.(6.3) takes the form:

$$\nabla_\mu J^\mu = \partial_\mu J^\mu + \Gamma^\mu_{\mu\rho}j^\rho = \left(\partial_a - \frac{2}{a}\right)J^a + \partial_+ J^+ + \partial_- J^- = 0. \tag{6.5}$$

Following the Vilenkin interpretation of the wave function discussed in the Section 2.8, as it is natural we choose to assign the character of *semiclassical* to the isotropic variable a, while the anisotropies $\{\beta_+, \beta_-\}$ characterize the *quantum* subsytem. With this prescription we choose the wave function of the Universe as:

$$\psi(a,\beta_\pm) = \chi(a)\varphi(a,\beta_\pm) = A(a)e^{\frac{i}{\hbar}S(a)}\varphi(a,\beta_\pm). \tag{6.6}$$

Considering the previous wave function inside the WDW equation (6.3) we obtain, at the lowest order in $\hbar$, the Hamilton-Jacobi equation:

$$-a^2(S')^2 + \frac{3(4\pi)^3\mu^2}{l_p^2} = 0, \tag{6.7}$$

where $(\bullet)' \equiv \frac{\partial}{\partial a}$. In the Eq.(6.7) does not appear the anisotropies or their conjugate momenta. In fact, the lowest order in the WKB performed respect to the $\hbar$ parameter takes into account the semiclassical behaviour of the whole system, and this regard only the isotropic variable. Furthemore, making a comparison between the Eq.(6.7) and the superhamiltonian constraint (6.1) when the anisotropies are "frozen"[3] , we can establish the connection $S' = p_a$ and rewrite the Eq.(6.7) in this way:

$$p_a^2 = \frac{3(4\pi)^3\mu^2}{l_p^2 a^2}. \tag{6.8}$$

It is possible to obtain the explicit solution for $a = a(t)$ making use of the Eq.(6.8) with the Hamiltonian Equation

$$\frac{da}{dt} = \frac{\partial \mathcal{H}}{\partial p_a} = -\frac{l_p^2}{12\pi\hbar}\frac{p_a}{a} \tag{6.9}$$

in order to achieve[4]

$$\frac{da}{dt} = \sqrt{\frac{4\pi}{3}}\frac{l_p\mu}{\hbar a^2} \Longrightarrow a(t) = \left(\frac{2\sqrt{3\pi}l_p\mu}{h}t\right)^{\frac{1}{3}}. \tag{6.10}$$

The next order in the WKB expansion gives us the following equation

$$ia^2\frac{1}{A}(A^2S')' + 2ia^2AS'\varphi' - A\left(\frac{\partial^2}{\partial\beta_+^2} + \frac{\partial^2}{\partial\beta_-^2}\right)\varphi = 0. \tag{6.11}$$

As in the Section 2.8, we can decoupled the above equation making an adiabatic approximation. Naturally, we require that the a-evolution is mainly contained in the amplitude A, while the isotropic variation of the quantum part φ is negligible. This is express by the condition

$$|\partial_a\chi(a)| \gg |\partial_a\varphi(a,\beta_\pm)|. \tag{6.12}$$

Considering the condition (6.12) in the Eq.(6.11), we obtain:

$$\frac{a^2}{A}(A^2S')' = 0 \quad , \quad 2ia^2S'\varphi' - \left(\partial_+^2 + \partial_-^2\right)\varphi = 0 \tag{6.13}$$

Looking at the first equation in (6.13), we can see that it corresponds to the conservation of the current $\nabla_a J^a = 0$ when we take into account just the semiclassical version of the wave function (6.6):

$$\psi(a) = A(a)e^{\frac{i}{\hbar}S(a)}. \tag{6.14}$$

The explicit form of the current is

$$J^a = \hbar a^2 A^2 S'. \tag{6.15}$$

The second equation in (6.13) provides the evolution of the quantum subsystem:

$$2ia^2S'\partial_a\varphi = \left(\partial_+^2 + \partial_-^2\right)\varphi \tag{6.16}$$

It is important to underline that, in analogy with the Vilenkin approach, the Eq.(6.16)

[3]In this case we mean that the term $\frac{p_+^2+p_-^2}{a^3}$ is neglected.

[4]We choose the integration's constant in such a way that $a(0) = 0$.

is consistent requiring that $\left(\partial_+^2 + \partial_-^2\right)\varphi = O(\hbar)$. It is possible to write a Schrodinger-like equation for the quantum wave function φ using the relation $\frac{\partial\varphi}{\partial a} = \frac{\partial\varphi}{\partial t}\frac{\partial t}{\partial a}$ and the Eqs.(6.8),(6.10). This way we have:

$$i\left(\frac{24\pi\hbar}{l_p^2}\right)a^3\frac{\partial\varphi(t,\beta_\pm)}{\partial t} = \left(\partial_+^2 + \partial_-^2\right)\varphi(t,\beta_\pm), \tag{6.17}$$

and with the introduction of the time-like variable τ for which $\frac{\partial}{\partial\tau} = \frac{24\pi}{l_p^2}a^3\frac{\partial}{\partial t}$ we can finally write:

$$i\hbar\frac{\partial\varphi(\tau,\beta_\pm)}{\partial\tau} = \left(\partial_+^2 + \partial_-^2\right)\varphi(\tau,\beta_\pm). \tag{6.18}$$

The Eq.(6.18) resembles a plane wave equation which solution is of the form

$$\varphi(\tau,\beta_\pm) = e^{\frac{iE\tau}{\hbar}}e^{\frac{ik_+\beta_+}{\hbar}}e^{\frac{ik_-\beta_-}{\hbar}}, \tag{6.19}$$

with $E = \frac{(k_+^2+k_-^2)}{\hbar^2}$. We can make explicit the dependence $\tau(t)$ by solving the integral:

$$\tau(t) = \int\frac{l_p^2}{24\pi a(t)^3}dt = \frac{l_p\hbar}{48\pi\sqrt{3\pi}\mu}\ln\frac{t}{t^*}, \tag{6.20}$$

where t^* is the integration constant. To conclude, the quantum part of the wave function takes the form:

$$\varphi(t,\beta_\pm) = Ce^{i\frac{l_p}{48\pi\sqrt{3\pi}\hbar^2}(k_+^2+k_-^2)\ln\frac{t}{t^*}}e^{\frac{ik_+\beta_+}{\hbar}}e^{\frac{ik_-\beta_-}{\hbar}}, \tag{6.21}$$

where the $\{k_+, k_-\}$ are the quantum numbers associated to the anisotropies, for which is valid the dispersion relation $k_\pm = p_\pm$.

From the quantum part of the wave function φ in the Eq.(6.21) can be defined a probability distribution for the quantum sub-system associated to the anisotropies as $\rho_\varphi = |\varphi|^2$. This way, the components of the current (6.1.1) assume the form:

$$J^a = \hbar a^2 A^2 S'\rho_\varphi, \tag{6.22}$$

$$J^\pm = -\frac{\hbar^2 A^2}{2}(\varphi^*\partial_\pm\varphi - \varphi\partial_\pm\varphi^*) \equiv \frac{A^2}{2}J_\varphi^\pm, \tag{6.23}$$

and the conservation law $\nabla_\mu J^\mu = 0$ can be recast as

$$2\hbar a^2 S'\frac{d\varphi}{da} + \partial_i J_\varphi^i = 0, \tag{6.24}$$

In the above rewrite of the conservation of the current the index $i = \{+,-\}$ and we used the first relation in the Eq.(6.13). Then, an explicit presence of the variable t can be include through the relation $\frac{\partial\varphi}{\partial a} = \frac{\partial\varphi}{\partial t}\frac{\partial t}{\partial a}$ and making use of the Eqs.(6.7),(6.10), in order to obtain a *continuity equation*:

$$\frac{d\rho_\varphi}{dt} = -\frac{l_p^2}{24\hbar^2\pi a^3(t)}\partial_i J_\varphi^i. \tag{6.25}$$

Integrating the both sides of the equation over a β_+,β_- volume we have that the right side can be rewritten using the Gauss Theorem:

$$\frac{l_p^2}{24\hbar^2\pi a^3(t)}\int\int d\beta_+ d\beta_-\partial_i J_\varphi^i = \int_{\partial\beta} d\sigma J_\varphi^i \tag{6.26}$$

6.1.2 p_a-polarization

This subsection is devoted to the implementation of the quantum model in the p_a-polarization. The action of the operators $\{\widehat{p}_a, \widehat{\beta}_+, \widehat{\beta}_-\}$ is multiplicative, while $\{\widehat{a}, \widehat{p}_+, \widehat{p}_-\}$ act as a derivative operators:

$$\widehat{a} = i\hbar\frac{\partial}{\partial p_a} = i\hbar\partial_{p_a} \quad , \quad \widehat{p}_\pm = -i\hbar\frac{\partial}{\partial\beta_\pm} = -i\hbar\partial_\pm. \tag{6.27}$$

The quantum counterpart of the superhamiltonian constraint (6.1), or in other words the WDW equation, in this polarization is:

$$\left[\hbar^2 p_a^2\partial_{p_a}^2 - \hbar^2\left(\partial_+^2 + \partial_-^2\right) + \frac{3(4\pi)^3\mu^2}{l_p^2}\right]\psi(p_a, \beta_\pm) = 0 \tag{6.28}$$

Also in this case, with the difference that the role of a is taken by the conjugated momenta p_a, choosing the normal operator-ordering for the isotropic part of the WDW equation from the Eq.(6.28) we can build a current term that this time is

$$J^\mu = \begin{bmatrix} J^{p_a} \\ J^+ \\ J_- \end{bmatrix} = -\frac{i}{2}\hbar^2\begin{bmatrix} p_a^2(\psi^*\partial_{p_a}\psi - \psi\partial_{p_a}\psi^*) \\ -(\psi^*\partial_+\psi - \psi\partial_+\psi^*) \\ -(\psi^*\partial_-\psi - \psi\partial_-\psi^*) \end{bmatrix},$$

that respect the conservation law $\nabla_i J^i = 0$.

The operator ∇_i, in this polarization, is the covariant derivative built with the superspace metric $h^{ij} = diag(\hbar^2 p_a^2, -\hbar^2, -\hbar^2)$. Again, there is just one non-vanishing Christoffel symbol $\Gamma^{p_a}_{p_a p_a} = -\frac{2}{p_a}$ and the conservation of the current in Eq.(**??**) takes the form:

$$\nabla_i J^i = \partial_i J^i + \Gamma^i_{ik} j^k = \left(\partial_{p_a} - \frac{2}{p_a}\right) J^{p_a} + \partial_+ J^+ + \partial_- J^- = 0. \tag{6.29}$$

As in the previous subsection, we choose to assign the role of the quantum subsystem to the anisotropies while the semiclassical variable is represented by p_a. A straightforward version of the wave function of the Universe is:

$$\psi(p_a, \beta_\pm) = \chi(p_a)\varphi(p_a, \beta_\pm) = A(p_a)e^{\frac{i}{\hbar}S(p_a)}\varphi(p_a, \beta_\pm). \tag{6.30}$$

Considering the above shape for the wave function in the WDW equation leads, to the lowest order in $\hbar$, to the Hamilton Jacobi equation:

$$-p_a^2(\dot{S})^2 + \frac{3(4\pi)^3\mu^2}{l_p^2} = 0, \tag{6.31}$$

where $(\dot{\bullet}) \equiv \frac{\partial}{\partial p_a}$. This time, a comparison between the Eq.(6.31) and the part related to the semiclassical variable of the superhamiltonian constraint establish the equality $\dot{S} = a$ and the H-J equation can be written as:

$$p_a^2 = \frac{3(4\pi)^3\mu^2}{l_p^2 a^2}, \tag{6.32}$$

exactly the same relation obained in the Eq.(6.8) for the a-polarization case. As a consequence, also the evolution of $a(t)$ is the same in the Eq.(6.10).

If we consider the successive order in the WKB expansion we obtain the equation

$$ip_a^2 \frac{1}{A}(A^2\dot{S})^{\dot{}} + 2ip_a^2 A\dot{S}\dot{\varphi} - A\left(\partial_+^2 + \partial_-^2\right)\varphi = 0. \tag{6.33}$$

Via the same consideration of the previous subsection, we can obtain from the Eq.(6.33) a pair of equations using the adiabatic approximation that, in the p_a-polarization, is expresses by the condition:

$$|\partial_{p_a}\chi(p_a)| \gg |\partial_{p_a}\varphi(p_a, \beta_\pm)|. \tag{6.34}$$

This way we obtain:

$$\frac{p_a^2}{A}(A^2\dot{S})^{\dot{}} = 0 \quad , \quad 2ip_a^2 A\dot{S}\dot{\varphi} - A\left(\partial_+^2 + \partial_-^2\right)\varphi = 0. \tag{6.35}$$

The first equation in (6.35) corresponds to the conservation of the current $\nabla_{p_a} J^{p_a} = 0$ when the semiclassical version of the wave function (6.30) is considered:

$$\psi(a) = A(a)e^{\frac{i}{\hbar}S(a)}. \tag{6.36}$$

The current obtained in this way has the form

$$J^a = \hbar p_a^2 A^2 \dot{S}. \tag{6.37}$$

The description of the quantum subsytem is contained in the second equation in (6.35):

$$2ip_a^2\dot{S}\dot{\varphi} = \left(\partial_+^2 + \partial_-^2\right)\varphi. \tag{6.38}$$

An explicit time dependence for the φ can be introduce using the relation $\frac{\partial\varphi}{\partial p_a} = \frac{\partial\varphi}{\partial t}\frac{\partial t}{\partial p_a} = \frac{\partial\varphi}{\partial t}\frac{1}{\dot{p_a}}$. The quantity $\dot{p_a}$ can be evaluated differentiating the relation (6.32) and using the Eq.(6.10) it is possible to recast the Eq.(6.38) in such a way:

$$i\left(\frac{24\pi\hbar}{l_p^2}\right)a^3\frac{\partial\varphi(t, \beta_\pm)}{\partial t} = \left(\partial_+^2 + \partial_-^2\right)\varphi(t, \beta_\pm). \tag{6.39}$$

A comparison between the last equation and the Eq.(6.17) shows that the two differential equation are the same. Furthermore we can proceed in the same way as in the previous subsection and conclude that the solution for the wave function related to the quantum subsystem is

$$\varphi(t, \beta_\pm) = Ce^{i\frac{l_p}{48\pi\sqrt{3\pi}\hbar^2}(k_+^2 + k_-^2)\ln\frac{t}{t^*}}e^{\frac{ik_+\beta_+}{\hbar}}e^{\frac{ik_-\beta_-}{\hbar}}. \tag{6.40}$$

As we expected, also in the in the implementation of the Vilenkin approach there are no differences, both from a semiclassical and the quantum point of view, when we study the problem in the position polarization respect to the momentum polarization. This aspect will be crucial in the next Section, when the discrete nature of the isotropic variable shall be taken into account in the context of the Polymer Quantum Mechanics.

Let us now say something about the application of the Vilenkin steps for the individuation of a conserved probability distribution. In the general scheme illustrated in Section 2.8, the coordinated transformation $h_n = t$ for one of the classical configuration variable allowed to rewrite the conservation law (2.196) in the continuity equation form (2.197) and to individuate a normalizable probability distribution (2.198). The crucial point in this procedure is the fact that the classical configuration space contains more than one variable, in order to define an orthogonal Σ_0 surfaces over which integrate. In our model, equally in both polarization, the classical configuration space has dimension one (we have just one variable: a or p_a). This imply that the orthogonal space over which to evaluate the probability distribution has dimension zero and therefore the Vilenkin procedure cannot be replicated.

Regarding the quantum sub-system, starting from the quantum part of the wave function φ in the Eq.(6.21), a probability distribution for the quantum variables is defined as $\rho_\varphi = |\varphi|^2$. This way, the leading terms of the components of the current (6.3), considering the entire wave function (6.21), assume the form:

$$J^a = \hbar a^2 A^2 S' \rho_\varphi, \tag{6.41}$$

$$J^\pm = -\frac{\hbar^2 A^2}{2}(\varphi^* \partial_\pm \varphi - \varphi \partial_\pm \varphi^*) \equiv \frac{A^2}{2} J^\pm_\varphi, \tag{6.42}$$

and the conservation law $\nabla_\mu J^\mu = 0$ can be recast as

$$2\hbar a^2 S' \frac{d\varphi}{da} + \partial_i J^i_\varphi = 0. \tag{6.43}$$

We provides the calculus in the a-polarization, but the conclusions will be the same also in the other one. In the above rewrite of the conservation of the current the index $i = \{+, -\}$ and we used the first relation in the Eq.(6.13). Then, an explicit presence of the variable t can be include through the relation $\frac{\partial \varphi}{\partial a} = \frac{\partial \varphi}{\partial t}\frac{\partial t}{\partial a}$ and making use of the Eqs.(6.7),(6.10), in order to obtain a *continuity equation*:

$$\frac{d\rho_\varphi}{dt} = -\frac{l_p^2}{24\hbar^2 \pi a^3(t)} \partial_i J^i_\varphi. \tag{6.44}$$

Integrating the both sides of the equation over a β_+, β_- volume we have that the right side can be rewritten using the Gauss Theorem:

$$\frac{l_p^2}{24\hbar^2 \pi a^3(t)} \int\int d\beta_+ d\beta_- \partial_i J^i_\varphi = \frac{l_p^2}{24\hbar^2 \pi a^3(t)} \int_{\partial\beta} d\sigma J^i_\varphi \tag{6.45}$$

Making the hypothesis that all the system is contained in the surface $\partial\beta$, the term in the Eq.(6.45) vanishes, being evaluated over the surfaces. Therefore, what remains in the integration of the Eq.(6.86) is

$$\frac{d}{dt}\int\int d\beta_+ d\beta_- \rho_\phi = 0, \tag{6.46}$$

which means that the integral is conserved and can be normalized as

$$\int\int d\beta_+ d\beta_- \rho_\varphi = 1 \tag{6.47}$$

All the previous steps can be replicated in the p_a-polarization simply taking in consideration the conservation of the current (6.28) with the wave function (6.40) and through the relation $\frac{\partial \varphi}{\partial p_a} = \frac{\partial \varphi}{\partial t}\frac{\partial t}{\partial p_a}$. This leads exactly to the continuity equation (6.86) and to the same final considerations.

To conclude this Section we underline how, for our specific model, it was not possible to build an entire conserved probability distribution as in the Eq.(2.206). Nevertheless, our results are not so far from the Vilenkin conclusions. Indeed, we were able to obtain a quantum normalizable probability distribution (6.47) coupled with a classical conserved quantity (6.13),(or the Eq.(6.35) in the p_a-polarization).

6.1.3 Adiabatic Approximation

We close this Subsection performing a test about the validity of the adiabatic approximation in the two polarization cases (6.12),(6.34).

First of all, considering the conservation of the classical current in the Eq.(6.13) and the H-J equation (6.7), we can argue that amplitude of the wave function of the Universe evolves as $A(a) \propto a^{\frac{1}{2}}$ and therefore $|\partial_a A(a)| \propto a^{-\frac{1}{2}}$. Furthermore, using the Eq.(6.10), for the derivative of the quantum part of the wave function (6.21) the behavior is $|\partial_a \varphi| \propto a^{-1}$. Given the identification $S' = p \propto \frac{1}{a}$, for what concerns the a-polarization case we can then conclude that the adiabatic approximation (6.12) is valid for an initial condition of the Universe in which the isotropic variable, or in other words the volume of the Universe, assumes not too small values.

Repeating the same steps in the p-polarization, from the conservation of the classical current (6.35) and the H-J equation (6.31) we can achieve that $A(p_a) \propto p_a^{\frac{1}{2}}$ and consequently $|\partial_{p_a} A(p_a)| \propto p_a^{-\frac{1}{2}}$. Using the H-J equation and the Eq.(6.10), the derivative of the wave function φ behaves as $|\partial_{p_a}\varphi| \propto p_a^{-1}$. Taking into account the founded trends, we can conclude, recalling $\dot{S} = a \propto \frac{1}{p}$, that the adiabatic approximation (6.34), is valid in the p-polarization when the conjugated momenta to the isotropic variables starts its evolution towards the singularity assuming large values.

6.1.4 Expectation values of the anisotropies: the Ehrenfest theorem

To conclude this Section let us analyze the behaviour of the quantum variables: the anisotropies. To this aim, let us introduce a useful theorem to study the evolution of a quantum operator: the *Ehrenfest Theorem*. Let $|\varphi >|$ the state of the quantum subsytem built starting by the wave function (6.21). The expectation value of the quantum operators $\{\widehat{\beta}_+, \widehat{\beta}_-\}$ corresponds to:

$$< \widehat{\beta}_\pm > = < \varphi | \widehat{\beta}_\pm | \varphi > \tag{6.48}$$

The time derivative of the expectation value of a time independent operator A is given by[5]

$$\frac{d}{dt} < A > = \frac{1}{i\hbar} < [A, H] >, \tag{6.49}$$

where H is the Hamiltonian of the system. The Ehrenfest Theorem concerns the application of the above results to the one-dimensional systems. Therefore, remembering that the only non vanishing position-momentum commutators are $[\beta_+, p_+] = [\beta_-, p_-] = i\hbar$, we can apply it to the anisotropies in order to obtain

$$\frac{d < \widehat{\beta}_\pm >}{dt} = \frac{1}{i\hbar} < [\beta_\pm, \mathcal{H}] > = \frac{l_p^2}{24 i\pi\hbar^2 a^3} < [\beta_\pm, p_\pm^2] > = \frac{l_p^2}{12\pi\hbar a^3} < p_\pm >, \tag{6.50}$$

where we used the commutation rule $[A, BC] = [A, B]C + B[A, C]$. In the previous relation the term $\frac{1}{a^3}$ was brought out to the because the expectation values is evaluated over the quantum states $|\varphi(a, \beta_\pm) >$ and the isotropic variable represent for them a fixed orbit over which the dynamics of the anysotropies occurs. Applying the Ehrenfest theorem to $p_\pm$ it is possible to show that its expectation value is a constant of motion :

$$\frac{d < \widehat{p_\pm} >}{dt} = \frac{1}{i\hbar} < [p_\pm, \mathcal{H}] > = 0 \rightarrow < \widehat{p_\pm} > = const. \tag{6.51}$$

[5]This general equality is due to a Werner-Heisenberg theorem

Using the above result in the Eq.(6.50) with the time-evolution for the isotropic variable in the Eq.(6.10) we arrive at the differential equation:

$$\frac{d < \widehat{\beta}_\pm >}{dt} = \frac{l_p p_\pm}{24\sqrt{3\pi}\pi\mu}\frac{1}{t} \tag{6.52}$$

whose solution is

$$< \widehat{\beta}_\pm >_t = \frac{l_p p_\pm}{24\sqrt{3\pi}\pi\mu}\ln\frac{t}{t^*}, \tag{6.53}$$

where t^* is an integration constant.

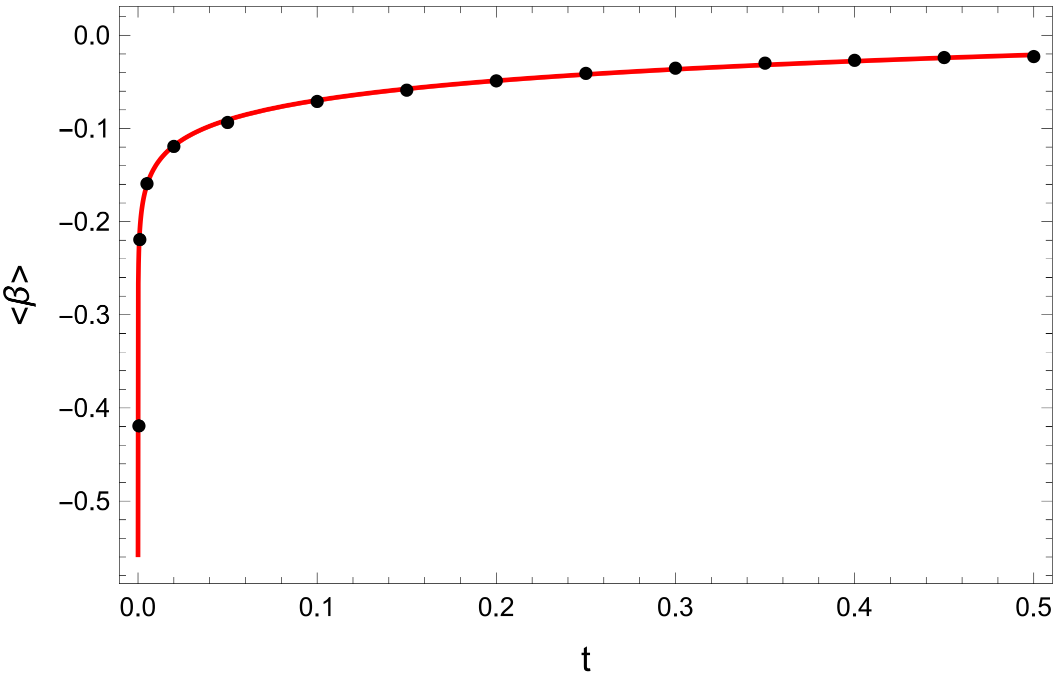

FIGURE 6.1: The black points represent the position of the maximum of the wave packet $|\Psi_{k^*_\pm}(t,\beta_\pm)|$ evaluated via numerical integration for the following choice of the integration parameters:$C = 1, k^*_+ = k^*_- = 1, \sigma_+ = \sigma - = 0.03$. The continuous red line represents the trajectory evaluated with the same parameters from the Ehrenfest theorem.

From the Eq.(6.53) we can see that the anisotropies become important in magnitude near the initial singularity and they diverge for $t = 0$, as we expected from any classical anisotropic model. From the study of the standard deviation it is possible to establish effectively if the trajectory obtained in the Eq.(6.90) differs not to much from the classical trajectory.

The application of the Ehrenfest Theorem to the operator $< \widehat{\beta}^2 >$ brings to:

$$\frac{d < \widehat{\beta}^2_\pm >}{dt} = \frac{1}{i\hbar} < [\beta^2_\pm, \mathcal{H}] >= \frac{l_p^2 < [\beta^2_\pm, p^2_\pm] >}{24 i\pi\hbar^2 a^3} = \frac{l_p^2}{12\pi\hbar a^3} < \beta_\pm p_\pm + p_\pm\beta_\pm >, \tag{6.54}$$

where we used the commutation rule $[AB, CD] = AC[B, D] + A[B, C]D + C[A, D]B + [A, C]DB$. The quantity $< \beta_\pm p_\pm + p_\pm\beta_\pm >$ can be evaluated applying again the Ehrenfest theorem:

$$\frac{d < \beta_\pm p_\pm + p_\pm\beta_\pm >}{dt} = \frac{l_p^2 < [\beta_\pm p_\pm + p_\pm\beta_\pm, p^2_\pm] >}{24 i\pi\hbar^2 a^3} = \frac{l_p^2 p^2_\pm}{6\pi\hbar a^3}. \tag{6.55}$$

The above differential equation can be solved using the time-dependence (6.10) in order to obtain:

$$< \beta_\pm p_\pm + p_\pm \beta_\pm >= \frac{l_p p_\pm^2}{12\pi\sqrt{3\pi}\mu}(\ln t + K), \tag{6.56}$$

where K is an integration constant. Inserting the latter relation in the Eq.(6.54) we obtain the solution

$$< \widehat{\beta}_\pm^2 >= \frac{l_p^2 p_\pm^2}{(12\pi)^3\mu^2}\left[\ln^2 t + 2K\log\frac{t}{t^*} - \ln^2 t^*\right]. \tag{6.57}$$

Finally, it is possible to write the standard deviation for the operator $< \widehat{\beta}_\pm >$ as

$$\sigma_\beta = \sqrt{< \widehat{\beta}_\pm^2 > - < \widehat{\beta}_\pm >^2} = \frac{l_p p_\pm}{24\sqrt{3\pi}\pi\mu}\sqrt{2\left(-\ln^2\tau + K\ln\frac{t}{\tau} + \ln t\ln\tau\right)} \tag{6.58}$$

The presence of the square root in the standard deviation (6.58) force to impose, in order to maintain a physical meaning for this quantity, particular values to the integration constant K. From the Eq.(6.58) we see that also the standard deviation shows a divergent nature in proximity of the singularity, as it clear performing the limit $t \to 0$. However, An estimate of how the expectation value (6.53) differs from the classical trajectory can be evaluated from the ratio

$$\frac{\sigma_\beta}{< \widehat{\beta}_\pm >} = \frac{\sqrt{2\left(-\ln^2\tau + K\ln\frac{t}{\tau} + \ln t\ln\tau\right)}}{\ln\frac{t}{\tau}} \tag{6.59}$$

As we can see in the Fig. 6.2, the condition $\frac{\sigma_\beta}{<\widehat{\beta}_\pm>} \ll 1$ remains always valid during

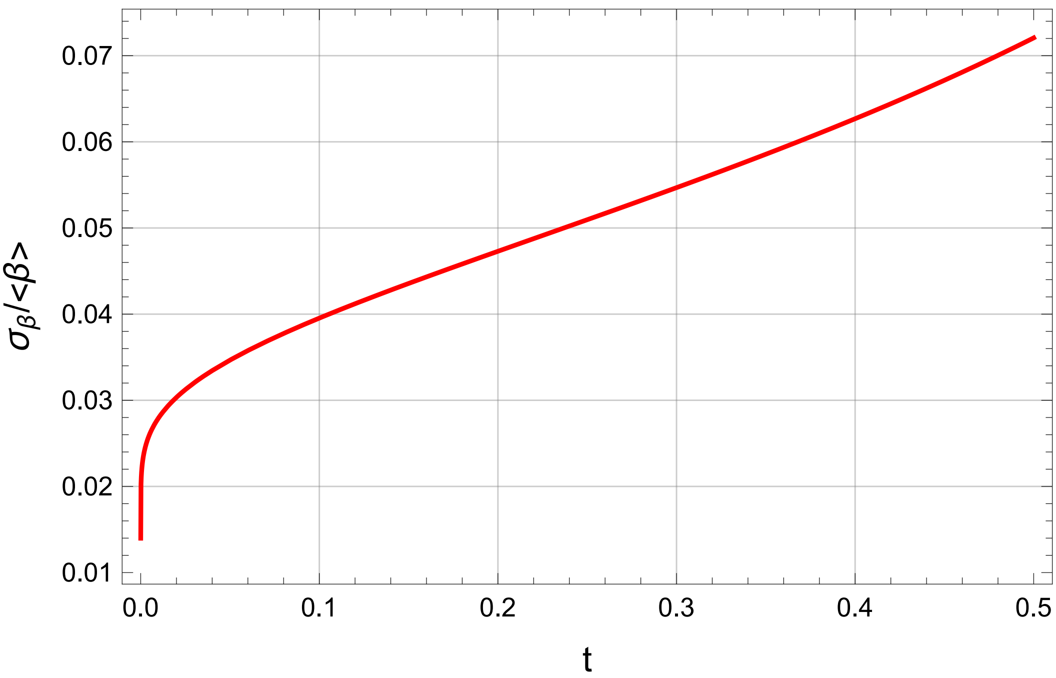

FIGURE 6.2: The evolution of the ratio $\frac{\sigma_\beta}{<\widehat{\beta}_\pm>}$ as a function of time t. The ratio becomes zero in the limit $t \to 0$, so the Universe approach the singularity "classically"

the approach to the singularity, and furthermore the ratio (6.59) goes to zero in the limit

$t \rightarrow 0$. Such occurrence tells us that the divergent behaviour of the expectation values $< \widehat{\beta}_\pm >$ are always more and more "classically ensured" as we approach the singularity.

An additional confirm on the dynamics of the anisotropies can be provide by studying the behavior of the maximum of the wave packet built from the wave function (6.21), in this way:

$$\Psi_{k^*_\pm}(t,\beta_\pm) = \int\int dk_\pm e^{-\frac{(k_+-k^*_+)^2}{2\sigma^2_+}} e^{-\frac{(k_--k^*_-)^2}{2\sigma^2_-}} \varphi(t,\beta_\pm), \tag{6.60}$$

where we choose Gaussian weights to peak the wave packets. The evolution of the wave packets has been studied through a numerical integration and as we can see in the Fig. 6.1, the position of the maximum of the wave packet $|\Psi_{k^*_\pm}(t,\beta_\pm)|$ as a function of t overlaps exactly the trajectory of the anisotropies obtained by the Ehrenfest theorem in the Eq.(6.53).

6.2 Polymer Quantization

As we have shown in the Section 2.5.3 for the one-dimensional particle case, if we consider the position variable q as a discrete variable for the conjugated momenta p it is not possible to associate a differential quantum operator. Thus, characterizing the wave function in the momentum polarization, through the polymer procedure we can identify an approximate version of the operator $\widehat{p}$ which acts multiplicatively on the states of the system.

For what concerns the Bianchi I model analysed in the Section 6.1, we make the physical choice to assign a discrete character to the isotropic variable a without modification in the anisotropy variables. Such a mixed choice for the quantization can be made typically in two cases: when the configuration variables are totally independent or when a configuration variable depends from the other one but weakly. The latter is exactly our case, where the variables $\beta_\pm$ depend parametrically only on the isotropic variable and so the effects of the variable a on the anisotropies of the Universe are negligible.

This means, following Eq.(2.76), to consider the substitution

$$p_a^2 \rightarrow \frac{2\hbar^2}{\lambda^2}\left[1-\cos\left(\frac{\hbar p_a}{\lambda}\right)\right]. \tag{6.61}$$

Since the results of the quantization procedure does not depend on the particular choice of the polarization, as it is clear from the subections 6.1.1, 6.1.2 in our model, we choose to describe the wave function of the Universe $\psi = \psi(p_a,\beta_\pm)$ in the momentum base for the isotropic part and in the position base for the anisotropies. This implies that the action of the operators are the same in Eq.(6.27) but taking into account the multiplicative action of the quantum operator associated to approximate version provided in the Eq.(6.61). It brings to the modification of the superhamiltonian constraint (6.1) and the WDW equation (6.28) in this way:

$$\mathcal{H}_p = \frac{l_p^2}{24\pi\hbar}\left\{-\frac{2\hbar^2}{\lambda^2 a}\left[1-\cos\left(\frac{\lambda p_a}{\hbar}\right)\right]+\frac{p_+^2+p_-^2}{a^3}\right\}+\frac{8\pi^2\mu^2}{\hbar a^3}=0 \tag{6.62}$$

$$\left\{\hbar^2\frac{\partial}{\partial p_a}\left(\frac{2\hbar^2}{\lambda^2}\left[1-\cos\left(\frac{\lambda p_a}{\hbar}\right)\right]\frac{\partial}{\partial p_a}\right)-\hbar^2\left(\frac{\partial^2}{\partial\beta_+^2}+\frac{\partial^2}{\partial\beta_-^2}\right)+\frac{3(4\pi)^3\mu^2}{l_p^2}\right\}\psi(p_a,\beta_\pm)=0 \tag{6.63}$$

From the Eq.(6.63) it is possible to obtain a modified polymer current as

$$J^\mu = \begin{bmatrix} J^{p_a} \\ J^+ \\ J_- \end{bmatrix} = -\frac{i}{2}\hbar^2 \begin{bmatrix} \frac{2\hbar^2}{\lambda^2}\left[1-\cos\left(\frac{\lambda p_a}{\hbar}\right)\right](\psi^*\partial_{p_a}\psi - \psi\partial_{p_a}\psi^*) \\ -(\psi^*\partial_+\psi - \psi\partial_+\psi^*) \\ -(\psi^*\partial_-\psi - \psi\partial_-\psi^*) \end{bmatrix},$$

with the associated conservation law $\nabla_i J^i = 0$. This case, the superspace metric is $h^{ij} = diag\left\{\hbar^2\frac{2\hbar^2}{\lambda^2}\left[1-\cos\left(\frac{\hbar p_a}{\lambda}\right)\right], -\hbar^2, -\hbar^2\right\}$ and being $\Gamma^{p_a}_{p_a p_a} = -\frac{\lambda}{\hbar}\frac{\sin\left(\frac{\lambda p_a}{\hbar}\right)}{1-\cos\left(\frac{\lambda p_a}{\hbar}\right)}$ the only non-vanishing Christoffel symbol, we can evaluate the explicit form of the conserved current as

$$\nabla_i J^i = \left(\partial_{p_a} - -\frac{\lambda}{\hbar}\frac{\sin\left(\frac{\lambda p_a}{\hbar}\right)}{1-\cos\left(\frac{\lambda p_a}{\hbar}\right)}\right) J^{p_a} + \partial_+ J^+ + \partial_- J^- = 0. \tag{6.64}$$

6.2.1 Semiclassical Limit

What we want to realize is the implementation of the Vilenkin approach for the polymer version of the WDW equation. In other words, we consider the wave function of the Universe (6.30) inside the Eq.(6.63). At the lowest order of the expansion in $\hbar$, namely the semiclassical level, the Hamilton-Jacobi equation obtained can be written as

$$p_a^2 = \frac{\hbar^2}{\lambda^2}\arccos\left(1 - \frac{3(4\pi)^3\mu^2\lambda^2}{2\hbar^2 l_p^2 a^2}\right)^2, \tag{6.65}$$

where we have identified again $\dot{S} = a$. From the superhamiltonian (6.62) we can write the hamiltonian equation for the isotropic variable:

$$\frac{da}{dt} = \frac{\partial\mathcal{H}_p}{\partial p_a} = -\frac{l_p^2}{12\pi\lambda a}\sin\left(\frac{\lambda p_a}{\hbar}\right) \tag{6.66}$$

Then, we introduce the the Eq.(6.65) in the Eq.(6.66) using the trigonometric relation

$$\sin(\arccos(x)) = \sqrt{1-x^2} \tag{6.67}$$

so as to obtain

$$\frac{da}{dt} = \sqrt{\frac{4\pi}{3}}\frac{l_p\mu}{\hbar a^2}\sqrt{1 - \frac{48\pi^3\mu^2\lambda^2}{\hbar^2 l_p^2 a^2}}. \tag{6.68}$$

Looking at the latter equation it is immediate to show the existence of a particular value

$$a_{min} = \sqrt{\frac{48\pi^3\mu^2\lambda^2}{\hbar^2 l_p^2}} \tag{6.69}$$

for which $\frac{da}{dt}$ changes the sign, or in other words a stationary point for the function $a(t)$. The branch of the solution that we are interested to compare with the standard behavior (6.10) can be obtained through an analytic integration of the differential equation (6.68) and its form is:

$$a(t) = \frac{1}{\hbar l_p} \frac{\sqrt{6\pi\mu^2 \left[h^2 l^4 t \left(h^2 l^4 t + \sqrt{h^4 l^8 t^2 + 36864\pi^8\lambda^6\mu^4}\right) + 18432\pi^8\lambda^6\mu^4\right]^{\frac{1}{3}} +}}{+48\pi^3\lambda^2\mu^2 \left[\left(\frac{72\pi^8\lambda^6\mu^4}{h^2 l^4 t \left(h^2 l^4 t + \sqrt{h^4 l^8 t^2 + 36864\pi^8\lambda^6\mu^4}\right) + 18432\pi^8\lambda^6\mu^4}\right)^{\frac{1}{3}} - 1\right]}, \quad (6.70)$$

where we have chosen the integration in such a way that the stationary point a_{min} is reached in correspondence to $t = 0$.

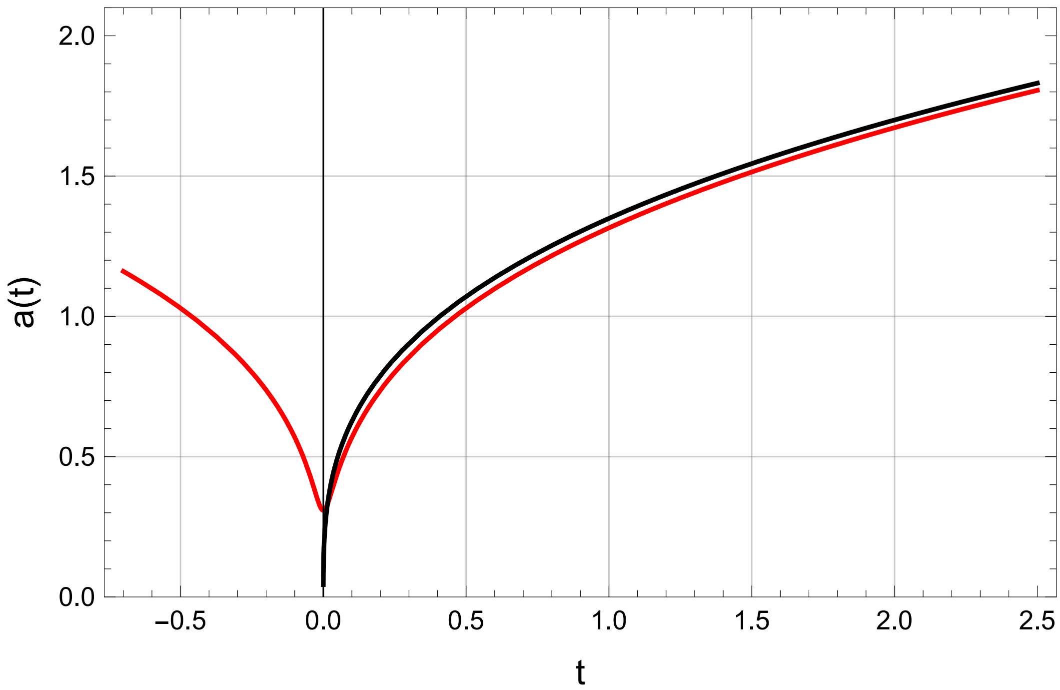

FIGURE 6.3: The black line represents the standard behavior $a(t)$ as evaluated in the Eq.(6.10) and the red line represents the polymer behavior of the isotropic variable (6.70). The solution is sketched for the parameters: $\hbar = {}_p = 1, \lambda = 0.01, \mu = 0.4$. The standard solution reaches the singularity in $t = 0$ while the polymer solution arrives at the minimum value a_{min} and then grows up for $t < 0$ after the bounce.

As it is possible to see in the Fig. 6.3, the stationary point is associated to a minimum value of the variable $a(t)$. Differently from the standard case, in the presence of a polymer structure, the isotropic variable does not reach $a = 0$ in correspondence of $t = 0$ and furthermore a collapsing phase towards the singularity is followed by a contracting phase. Let us emphasize that the obtained solution reproduce the standard results, formally it reduces to the solution (6.10), in the regimes where we expect that a polymer modification does not change the dynamics. In fact, in the limit $\lambda \to 0$ the expression (6.70) assumes the form (6.10) and for late times (namely $t \to +\infty$) the two solutions tend to be indistinguishable.

The presence of the small parameter $\lambda \neq 0$ within the theory associated to the lattice on the isotropic variable led to a cosmological model in which the initial singularity of the big bang has been avoided and it has been replaced with a bounce.

6.2.2 Quantum subsytem

In this subsection we analyse the first order in $\hbar$ obtained considering the wave function (6.40) in the WDW equation (6.63). This brings to the equation:

$$i\frac{2\hbar^2}{\lambda^2}\left[1-\cos\left(\frac{\lambda p_a}{\hbar}\right)\right]\frac{1}{A}(A^2\dot{S})^{\cdot}+2i\frac{2\hbar^2}{\lambda^2}\left[1-\cos\left(\frac{\lambda p_a}{\hbar}\right)\right]A\dot{S}\dot{\varphi}-A\left(\partial_+^2+\partial_-^2\right)\varphi=0. \tag{6.71}$$

Making use of the adiabatic approximation (6.34), the above expression provides, as in the standard case, a pair of equations. The first one is

$$i\frac{2\hbar^2}{\lambda^2}\left[1-\cos\left(\frac{\lambda p_a}{\hbar}\right)\right]\frac{1}{A}(A^2\dot{S})^{\cdot}=0 \tag{6.72}$$

and it concerns the conservation of the classical current $\nabla_{p_a}J^{p_a}=0$ which explicit form in the polymer case and with the wave function (6.30) is:

$$J^{p_a}=-\hbar\frac{2\hbar^2}{\lambda^2}\left[1-\cos\left(\frac{\lambda p_a}{\hbar}\right)\right]A^2\dot{S}. \tag{6.73}$$

The second equation gives the description of the quantum part of the wave function φ:

$$2i\frac{2\hbar^2}{\lambda^2}\left[1-\cos\left(\frac{\lambda p_a}{\hbar}\right)\right]\dot{S}\dot{\varphi}=\left(\partial_+^2+\partial_-^2\right)\varphi \tag{6.74}$$

It is possible to rewrite also in the polymer scheme a pure Schrodinger equation. First of all, from the H-J equation (6.65) we achieve the expression for the trigonometric term:

$$\frac{2\hbar^2}{\lambda^2}\left[1-\cos\left(\frac{\lambda p_a}{\hbar}\right)\right]=\frac{3(4\pi)^3\mu^2}{l_p^2a^2}. \tag{6.75}$$

Moreover, we can use the relations $\dot{S}=a$ and $\dot{\varphi}=\frac{\partial\varphi}{\partial t}\frac{\partial t}{\partial p_a}=\frac{\partial\varphi}{\partial t}\frac{1}{\dot{p_a}}$. The last step is to evaluate $\dot{p_a}$ through a differentiation of the relation (6.65) and the Eq.(6.68) in order to write

$$\dot{p_a}=\frac{16\pi^2\mu^2}{\hbar a^4} \tag{6.76}$$

Realizing all the previous substitutions the Eq.(6.74) reduces to

$$i\left(\frac{24\pi\hbar}{l_p^2}\right)a^3\frac{\partial\varphi(t,\beta_\pm)}{\partial t}=\left(\partial_+^2+\partial_-^2\right)\varphi(t,\beta_\pm). \tag{6.77}$$

It is important to note that the functional form of the equation that describes the quantum subsystem is exactly the same of the standard case in the Eq.(6.39). The real difference is in the time-dependence of the isotropic factor a that, in the polymer case, assumes the form in the Eq.(6.70). For this reason, we proceed defining the same change in the time varible $\frac{\partial}{\partial\tau}=\frac{24\pi}{l_p^2}a^3\frac{\partial}{\partial t}$ in order to arrive at the same Schrodinger equation (6.17) with solution (6.19). With respect to the standard case the distinction is in the integration of the time-like variable τ

$$\tau(t)=\int\frac{l_p^2}{24\pi}\frac{dt}{a(t)^3}. \tag{6.78}$$

In fact, it brings to a non-solvable integral in the t variable due to the special form $a(t)$ in the polymer case. We can elude this changing the integration variable this way:

$$d\tau = \frac{l_p^2}{24\pi}\frac{dt}{a^3} = \frac{l_p^2}{24\pi}\frac{1}{\dot{a}}\frac{da}{a^3} \tag{6.79}$$

The expression $\tau(a)$ can be determined integrating the latter equation and considering the relation (6.68) in order to obtain:

$$\tau(a) = \frac{\sqrt{3}l_p\hbar}{48\pi^{3/2}\mu}\int\frac{da}{\sqrt{a^2 - \frac{48\pi^3\mu^2\lambda^2}{\hbar^2 l_p^2}}}, \tag{6.80}$$

which admits the analytic solution

$$\tau(a(t)) = \frac{\sqrt{3}l_p\hbar}{48\pi^{3/2}\mu}\log\left[\frac{\left(a(t) + \sqrt{a(t)^2 - \frac{48\pi^3\mu^2\lambda^2}{\hbar^2 l_p^2}}\right)}{\left(a(t^*) + \sqrt{a(t^*)^2 - \frac{48\pi^3\mu^2\lambda^2}{\hbar^2 l_p^2}}\right)}\right]. \tag{6.81}$$

Certainly, if we implement the limit $\lambda \to 0$ and we substitute the standard time dependence of the isotropic variable (6.10) we turn back to the expression (6.20). This allow to write down the analytic version of the quantum part of the wave function φ:

$$\varphi(t, \beta_\pm) = Ce^{i(k_+^2 + k_-^2)\tau(a(t))}e^{\frac{ik_+\beta_+}{\hbar}}e^{\frac{ik_-\beta_-}{\hbar}}. \tag{6.82}$$

To find the probability distribution for the polymer Bianchi I model in presence of a stiff matter contribution, we reply the steps of the subsection 6.1.2. For what concern the classical part of the probability distribution, the situation is the same of the standard case. Indeed, the presence of just one classical configuration variable, p_a, denotes the impossibility to recast the conservation of the classical current (6.72) in a continuity equation that regards the classical probability distribution. However, also in the polymer case, for the quantum sub-system a continuity equation can be extracted. Referring to the quantum part of the wave function (6.82), the probability distribution for the quantum variables is defined as $\rho_\varphi = |\varphi|^2$. Considering the Vilenkin wave function (6.82), the leading terms of the components of the current (6.63) become

$$J^a = \hbar\frac{2\hbar^2}{\lambda^2}\left[1 - \cos\left(\frac{\lambda p_a}{\hbar}\right)\right]A^2\dot{S}\rho_\varphi, \tag{6.83}$$

$$J^\pm = -\frac{\hbar^2 A^2}{2}(\varphi^*\partial_\pm\varphi - \varphi\partial_\pm\varphi^*) \equiv \frac{A^2}{2}J^\pm_\varphi, \tag{6.84}$$

and the conservation law $\nabla_\mu J^\mu = 0$ can be recast as

$$2\hbar\frac{2\hbar^2}{\lambda^2}\left[1 - \cos\left(\frac{\lambda p_a}{\hbar}\right)\right]\dot{S}\frac{d\varphi}{dp_a} + \partial_i J^i_\varphi = 0, \tag{6.85}$$

where the index $i = \{+, -\}$. Via the relation $\frac{\partial\varphi}{\partial p_a} = \frac{\partial\varphi}{\partial t}\frac{\partial t}{\partial p_a} = \frac{\partial\varphi}{\partial t}\frac{1}{\dot{p}_a}$, the explicit dependence on the variable t can be inserted. Furthermore, considering the Hamilton-Jacobi equation (6.31), the identification $\dot{S} = a$ and the identity (6.76), the Eq.(6.85) reduces to

$$\frac{d\rho_\varphi}{dt} = -\frac{l_p^2}{24\hbar^2\pi a^3(t)}\partial_i J^i_\varphi. \tag{6.86}$$

The continuity equation obtained in the polymer case is formally equivalent with respect to the standard case (6.86), whose differences are due to the time dependence of the isotropic vairable a (corresponding to the Eq.(6.70) in the polymer case) and to the definition of the quantum probability distribution given by the quantum wave function (6.82) with respect to the standard case (6.40). That said, performing again an integration over a $d\beta_+ d\beta_-$ volume for both sides of the continuity equation, a normalizable quantum probability distribution is obtained also in the polymer case:

$$\int\int d\beta_+ d\beta_- \rho_\varphi = 1 \tag{6.87}$$

In conclusion of this section we assert that it was not possible to build an entire conserved probability distribution as in the Eq.(2.206) but, as in the standard case, we were able to write a quantum normalizable probability distribution (6.87) together with a classical conserved quantity (6.72).

6.2.3 Expectation values of the anisotropies

We investigate the behavior of the anisotropies trough the evaluation of the quantum expectation values. As in the Section 6.1.4, the application of the Ehrenfest Theorem to $\widehat{\beta_\pm}$ brings to the same functional form

$$\frac{d < \widehat{\beta}_\pm >}{dt} = \frac{1}{i\hbar} < [\beta_\pm, \mathcal{H}_p] >= \frac{l_p^2 p_\pm}{12\pi\hbar a^3}, \tag{6.88}$$

where in this case the variable a behaves as in the Eq.(6.70). The previous differential equation can be solved by changing in the following way:

$$\frac{d < \widehat{\beta}_\pm >}{da} = \frac{l_p^2 p_\pm}{12\pi\hbar a^3 \dot{a}} = \frac{l_p p_\pm}{\sqrt{192\pi^3}\mu} \frac{1}{\sqrt{a^2 - a_{min}^2}}, \tag{6.89}$$

and the solution obtained is:

$$< \widehat{\beta}_\pm >_{a(t)} = \frac{l_p p_\pm}{\sqrt{192\pi^3}\mu} \ln\left[\frac{a(t)^2 + \sqrt{a(t)^2 - a_{min}^2}}{a(t^*)^2 + \sqrt{a(t^*)^2 - a_{min}^2}}\right]. \tag{6.90}$$

The integration constant has been chosen to reproduce, in the limit $\lambda \to 0$, the solutions of the standard case Eq.(6.53).

In Fig.6.4 is shown the behavior of the quantum expectation value $< \widehat{\beta_\pm} >$ in the polymer case (red trajectory) and in the standard case (black trajectory). First of all, for the two trajectories there is an overlapping in the limit $t \to \infty$, so for late times there are no polymer modification. Furthermore, the divergent character close to the initial singularity shown by the solution in the standard case disappears leaving the place to a minimum point (or a maximum depending on the relative sign between the parameters p and μ) corresponding to

$$< \widehat{\beta}_\pm >^* = \frac{l_p p_\pm}{\sqrt{192\pi^3}\mu} \ln\left[\frac{a_{min}^2}{a(t^*)^2 + \sqrt{a(t^*)^2 - a_{min}^2}}\right]. \tag{6.91}$$

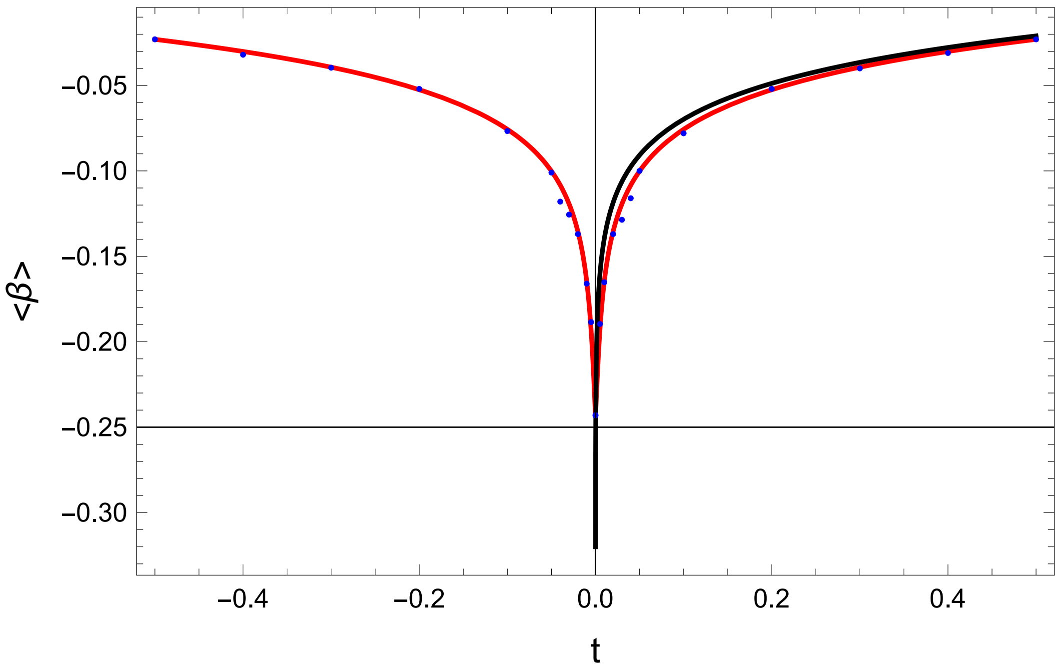

FIGURE 6.4: The black trajectory represents the standard divergent behavior of the anisotropies, as obtained through the Ehrenfest theorem in the Eq.(6.53). The red trajectories shows the finite value that the anisotropies assume in the turning point. Then, the blue points stands for the position of the maximum of the wave packets (6.99). The equivalence in the consideration of the Ehrenfest treatment and the wave packet dynamics is ensured in the total overlap between red trajectory and blue points.

The anisotropies cross over the singularity remaining finite assuming, in correspondence of $t = 0$, the value $< \widehat{\beta}_{\pm} >^*$ that depends on the choice of the parameters and the initial conditions t^*. As in the standard case, the evaluation of the standard deviation is a good tool to appreciate if the evolution (6.90) it is not so different from the classical trajectory.

The Ehrenfest Theorem for the operator $< \widehat{\beta}^2 >$ in the polymer case leads to:

$$\frac{d < \widehat{\beta}^2_{\pm} >}{dt} = \frac{1}{i\hbar} < [\beta^2_{\pm}, \mathcal{H}_p] >= \frac{l_p^2 < [\beta^2_{\pm}, p^2_{\pm}] >}{24 i\pi\hbar^2 a^3} = \frac{l_p^2}{12\pi\hbar a^3} < \beta_{\pm}p_{\pm} + p_{\pm}\beta_{\pm} >, \tag{6.92}$$

where, differently from the Eq.(6.54), the isotropic variable a concerns the Eq.(6.70). A new application of the Ehrenfest theorem on the quantity $< \beta_{\pm}p_{\pm} + p_{\pm}\beta_{\pm} >$ allow to obtain a differential equation for this term:

$$\frac{d < \beta_{\pm}p_{\pm} + p_{\pm}\beta_{\pm} >}{dt} = \frac{l_p^2 < [\beta_{\pm}p_{\pm} + p_{\pm}\beta_{\pm}, p^2_{\pm}] >}{24 i\pi\hbar^2 a^3} = \frac{l_p^2 p^2_{\pm}}{6\pi\hbar a^3}, \tag{6.93}$$

whose solution can be achieve with a change of variable such that:

$$\frac{d < \beta_{\pm}p_{\pm} + p_{\pm}\beta_{\pm} >}{da} = \frac{l_p^2 p^2_{\pm}}{6\pi\hbar a^3 \dot{a}} = \frac{l_p p^2_{\pm}}{4\pi\sqrt{3\pi}\mu} \frac{1}{\sqrt{a^2 - a^2_{min}}}, \tag{6.94}$$

and it corresponds to

$$< \beta_{\pm}p_{\pm} + p_{\pm}\beta_{\pm} >= \frac{l_p p^2_{\pm}}{4\pi\sqrt{3\pi}\mu} \left(\ln\left[a(t)^2 + \sqrt{a(t)^2 - a^2_{min}} \right] + C \right), \tag{6.95}$$

where C is an integration constant.

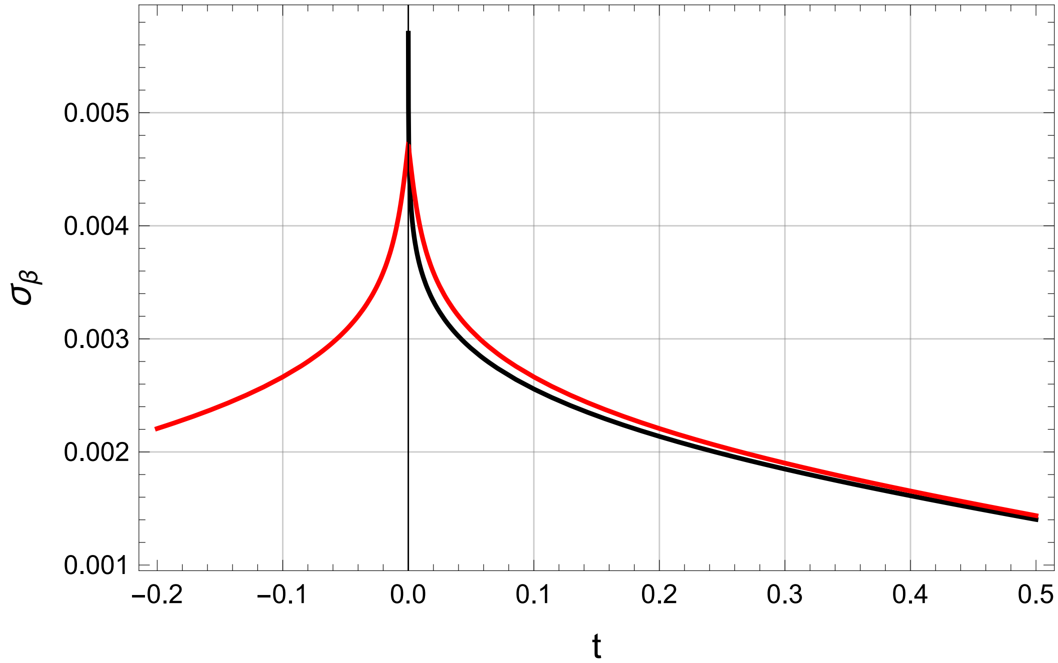

FIGURE 6.5: A comparison between the standard deviation in the canonical case (6.58)(black) and in the polymer case (6.98)(red). A regularization for the standard deviation in correspondence of the turning point emerges in the polymer scheme.

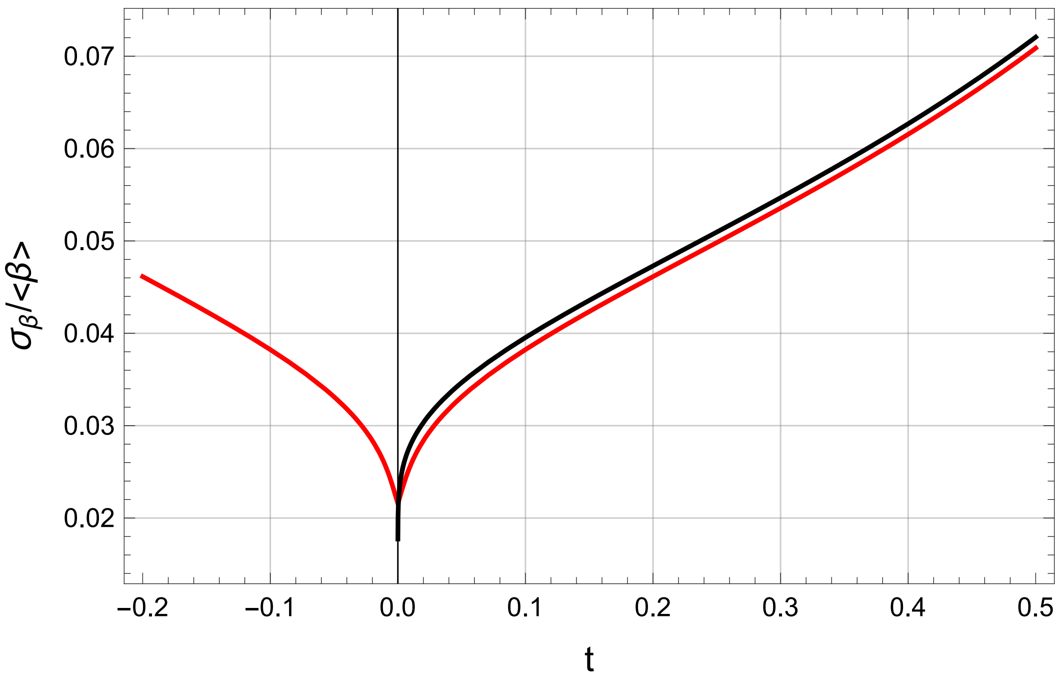

FIGURE 6.6: A comparison between the ratio $\frac{\sigma_\beta}{<\widehat{\beta}_\pm>}$ in the canonical case (6.59)(black) and in the polymer case (red). In the polymer scheme this ratio remains finite in correspondence of the turning point.

Using the same change of variable of the Eq.(6.92) we can arrive to a treatable form of the differential equation for the expectation value $<\widehat{\beta}^2_\pm>$ with the correspondent analytical solution:

$$\frac{d<\widehat{\beta}_{\pm}^{2}>}{da}=\frac{l_p^2p_{\pm}^2}{96\pi^3\mu^2}\frac{1}{\sqrt{a^2-a_{min}^2}}\left(\ln\left[a(t)^2+\sqrt{a(t)^2-a_{min}^2}\right]+C\right). \tag{6.96}$$

$$\begin{aligned}<\widehat{\beta}_{\pm}^{2}>_{a(t)}=\frac{l_p^2p_{\pm}^2}{192\pi^3\mu^2}&\left(2C\ln\left[\frac{a(t)^2+\sqrt{a(t)^2-a_{min}^2}}{a(t^*)^2+\sqrt{a(t^*)^2-a_{min}^2}}\right]+\right.\\ &\left.\ln^2\left[a(t)^2+\sqrt{a(t)^2-a_{min}^2}\right]-\ln^2\left[a(t^*)^2+\sqrt{a(t^*)^2-a_{min}^2}\right]\right)\end{aligned} \tag{6.97}$$

Then, the standard deviation for the operator $<\widehat{\beta}_{\pm}>$ in the polymer case can be written following the usual definition in order to obtain:

$$\sigma_\beta=\sqrt{<\widehat{\beta}_{\pm}^2>-<\widehat{\beta}_{\pm}>^2}=\frac{l_pp_{\pm}}{\sqrt{192\pi^3}\mu}\sqrt{2\left(-\ln^2\left[a(t^*)^2+\sqrt{a(t^*)^2-a_{min}^2}\right]+\right.}$$
$$\overline{\left.+C\ln\left[\frac{a(t)^2+\sqrt{a(t)^2-a_{min}^2}}{a(t^*)^2+\sqrt{a(t^*)^2-a_{min}^2}}\right]+\ln\left[a(t)^2+\sqrt{a(t)^2-a_{min}^2}\right]\ln\left[a(t^*)^2+\sqrt{a(t^*)^2-a_{min}^2}\right]\right)} \tag{6.98}$$

Here again, the presence of the square root in the definition of the standard deviation requires that,in order to have a real number associated to this quantity, the constant of integration C can assumes only particular values. The first difference respect to the standard case is glaring in the Fig.6.5, where the black line represents the standard deviation evaluated in the Eq.(6.58) while the red line is a representation of the modified equation (6.98). In presence of the polymer modification the standard deviation does not diverge in correspondence of the bounce but reaches a finite maximum value. Moreover, also the analysis of the ratio $\frac{\sigma_\beta}{<\widehat{\beta}_{\pm}>}$ confirms that the expectation values (6.88) is a genuine quantity. In fact, as it is shown in the Fig. 6.6, the condition $\frac{\sigma_\beta}{<\widehat{\beta}_{\pm}>}\ll 1$ remains valid throughout the time evolution of the anisotropies, including the crossing of the bounce.

In the polymer case too it is possible to obtain an additional confirm on the dynamics of the anisotropies by studying the behavior of the maximum of the wave packet built from the wave function (6.82), in this way:

$$\Psi_{k_{\pm}^*}(t,\beta_{\pm})=\int\int dk_{\pm}e^{-\frac{(k_+-k_+^*)^2}{2\sigma_+^2}}e^{-\frac{(k_--k_-^*)^2}{2\sigma_-^2}}\varphi(t,\beta_{\pm}), \tag{6.99}$$

where we choose Gaussian weights to peak the wave packets. A numerical integration has been realized to evaluate the evolution of the wave packets when the turning point is approached. As we can see in Fig. 6.4, the position of the maximum of the wave packet $|\Psi_{k_{\pm}^*}(t,\beta_{\pm})|$ as a function of t(correspondent to the collection of blue points) overlaps exactly the polymer trajectory founded by the Ehrenfest theorem in the Eq.(6.90).

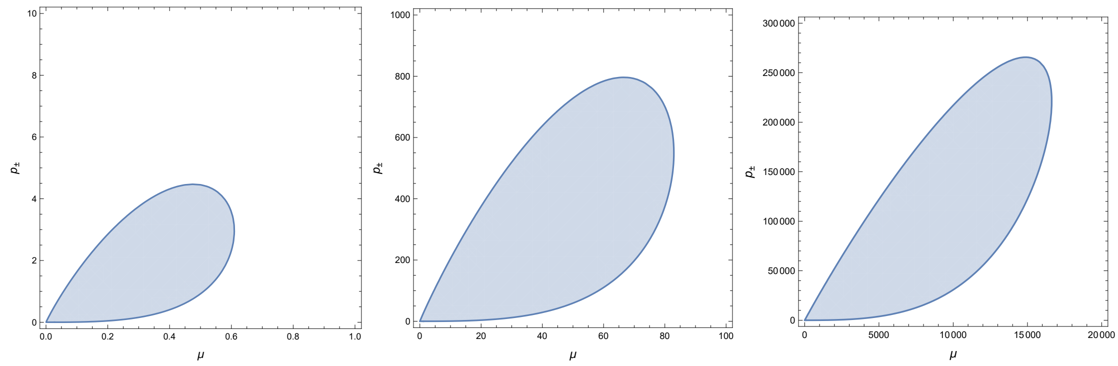

FIGURE 6.7: The blue region indicates the region of the configuration space $\{\mu, p_{\pm}\}$ in which the condition $\mathcal{V}^*_{IX}/\mathcal{K}^* < \frac{1}{100}$ is valid, sketched for the three values of the polymer scale $\lambda = 0.015, 0.0015, 0.00015$. The Bianchi IX potential term becomes more and more negligible with the decrease of the polymer scale.

6.3 Implication on the Bianchi IX Model

The purpose of this Section is to implement the proprieties founded before to a more general model. For this reason, we take into account a Bianchi IX model filled with a stiff matter considering the same polymer prescription in the Eq.(6.61) for the isotropic variable. The superHamiltonian constraint express through the configurational variables $\{a, \beta_+, \beta_-\}$ takes the form

$$\mathcal{H} = \frac{l_p^2}{24\pi\hbar}\left\{-\frac{2\hbar^2}{\lambda^2 a}\left[1 - \cos\left(\frac{\lambda p_a}{\hbar}\right)\right] + \frac{p_+^2 + p_-^2}{a^3} + \frac{12\pi^2\hbar^2}{l_p^4} a V_{IX}(\beta_\pm)\right\} + \frac{8\pi^2\mu^2}{\hbar a^3} = 0, \tag{6.100}$$

where the potential term, which accounts for the spatial curvature of the model, reads as

$$V_{IX}(\beta_\pm) = e^{-8\beta_+} - 4e^{-2\beta_+}\cosh(2\sqrt{3}\beta_-) + 2e^{4\beta_+}\left[\cosh(4\sqrt{3}\beta_-) - 1\right]. \tag{6.101}$$

This potential term can be obtained choosing the constants of structure $(\lambda_l, \lambda_m, \lambda_n) = (1, 1, 1)$. Looking at the Eq.(6.100) it is evident that the difference between the Bianchi I model and the Bianchi IX model is the presence of the potential term $\frac{12\pi^2\hbar^2}{l_p^4} a V_{IX}(\beta_\pm)$. Being the potential term associated to the anisotropies, it formally enters, performing a WKB expansion in $\hbar$ with a wave function of the Universe *a la* Vilenkin, in the first-order equation, *i.e.* the Schrodinger equation. Keeping this in mind, a possible way to estimate the importance of the potential term is to individuate the existence of a particular set of parameters for which the potential term of the Bianchi IX model is negligible with respect to $\frac{p_+^2 + p_-^2}{a^3}$, in other words the kinetic term of the anisotropies. Finding such a regime means that the results for the Bianchi I model obtained in Section 6.1.2 can be extended also to the Bianchi IX model and moreover, through the BKL conjecture, to a generic cosmological solution. To this aim, we consider the ratio between the potential term $\mathcal{V}^*_{IX} = \frac{12\pi^2\hbar^2}{l_p^4} a_{min} V_{IX}(\beta_\pm)$ and the kinetic term related to the anisotropies $\mathcal{K}^* = \frac{p_+^2 + p_-^2}{a_{min}^3}$, both evaluated at the bounce. In Fig. 6.7 are represented, for different values of the polymer scale λ, the regions in the space of the parameters $\{\mu, p_\pm\}$ where the ratio $\mathcal{V}^*_{IX}/\mathcal{K}^*$ become not relevant. In particular, the blue regions represent the values of $\{\mu, p_\pm\}$ for which the condition $\mathcal{V}^*_{IX}/\mathcal{K}^* < \frac{1}{100}$ is valid. Therefore, as it is clear from the figure, for any value of the parameter λ it is always possible to individuate a region where the Bianchi IX potential term is negligible respect to the kinetic term. Furthermore, the blue region becomes bigger as the parameter λ becomes smaller. This means that choosing smaller λ values implies that the condition for neglecting the potential term with respect to the kinetic term is verified for a large number of parameters couples $\{\mu, p_\pm\}$. The identification of such a regions bring us to conclude, providing proper parameters in order to neglect the potential term, that the Bianchi IX model in presence of a stiff matter contribution in the polymer approach possesses the same qualitatively features of the Bianchi I model previously analysed.

6.4 Concluding Remarks

In this Chapter, we analyzed in some detail how the anisotropies of a Bianchi type I model, represented by the Misner variables β_+ and β_-, behave when a Big-Bounce scenario is inferred via a polymer approach to the corresponding Misner variable α, describing the Universe volume. In order to be able to construct a proper dynamical Hilbert space for the anisotropy variables, we adopted a Vilenkin WKB representation of the Wheeler-DeWitt equation, in which the Universe volume is a quasi-classical configurational coordinate. In such a scheme, α recover its most genuine meaning of a time-like variable, since it does not correspond to a physical degree of freedom of the gravitational cosmological field. Since we adopted a polymer quantization procedure for such semi-classical component, we de facto deal with a modified classical Hamiltonian describing its evolution in the presence of stiff matter, *i.e.* a modified Friedmann equation for the presence of a typical length scale of cut-off.

In the analysis above, we obtained to main relevant achievements: i) the anisotropies of the Universe remain, in a Bianchi I model, finite across the Big-Bounce and they approach a localized quasi-classical behavior, according to the original idea of Misner [75];

ii) the same behavior remains valid for a Bianchi IX model, since for a non-zero set of initial conditions, the potential term, due to the spatial curvature (absent in the Bianchi I model) is dynamically negligible.

The first result suggests that the deviation of a primordial Universe from the isotropy can be controlled via the Cauchy problem, when the Bounce picture is recovered for the Universe volume. The second achievement allows to extend such an intriguing primordial feature, from a flat homogeneous Universe to a positive curved one. Furthermore, the Bianchi IX model has an high degree of generality and it mimics the generic cosmological solution near the initial singularity [15],[79]. By other words, we can infer that the proposed scenario remains valid even when we address the dynamics of a generic inhomogeneous model, near the Big-Bounce, as ensured by the polymer treatment of the α variable. Such a conjecture is based on the so-called *long wavelength approximation*, according to which, each space point, de facto each causal region of the Universe,dynamically decouples near enough to the initial singularity[15],[59],[78],[79], here replaced by a Big-Bounce .

From a cosmological point of view, the present study has the merit to demonstrate how, in the presence of a cut-off physics and a proper interpretation of the Universe wavefunction, the anisotropies do not explode asimptotically to the primordial turning point and the scenario of a Big-Bounce cosmology makes the quasi-isotropic Universe a more general solution with respect to a pure classical Einsteinian cosmology.

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