Classical and Quantum Features of the Mixmaster Singularity

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Abstract

This review article is devoted to analyze the main properties characterizing the cosmological singularity associated to the homogeneous and inhomogeneous Mixmaster model. After the introduction of the main tools required to treat the cosmological issue, we review in details the main results got along the last forty years on the Mixmaster topic. We firstly assess the classical picture of the homogeneous chaotic cosmologies and, after a presentation of the canonical method for the quantization, we develop the quantum Mixmaster behavior. Finally, we extend both the classical and quantum features to the fully inhomogeneous case. Our survey analyzes the fundamental framework of the Mixmaster picture and completes it by accounting for recent and peculiar outstanding results.

Keywords: Early cosmology; primordial chaos; quantum dynamics.
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1 Preface

The formulation by Belinski, Khalatnikov and Lifshitz (BKL) at the end of the Sixties about the general character of the cosmological singularity represents one of the most important contributions of the Landau school to the development of Theoretical Cosmology, after the work by Lifshitz on the isotropic Universe stability. The relevance of the BKL work relies on two main points: on one hand, this study provided a piecewise analytical solution of the Einstein equations, improving and implementing the topological issues of the Hawking-Penrose theorems; on the other hand, the dynamical features of the corresponding generic cosmological solution exhibit a chaotic profile.

Indeed the idea that the behavior of the actual Universe is somehow related to an inhomogeneous chaotic cosmology appears very far from what physical insight could suggest. In fact, the Standard Cosmological Model is based on the highly symmetric Friedman-Robertson-Walker (FRW) model, and observations agree with these assumptions, from the nucleosynthesis of light elements up to the age when structures formation takes place in the non-linear regime.

Furthermore a reliable (but to some extent, model-dependent) correspondence between theory and data exists even for an inflationary scenario and its implications. Several questions about the interpretation of surveys from which inferring the present status of the matter distribution and dynamics of the Universe remain open. However, in the light of an inflationary scenario, a puzzling plan appears unless the observation of early cosmological gravitational waves become viable, since such dynamics cancels out much of the pre-existent information thus realizing local homogeneity and isotropy.

The validity of the BKL regime must be settled down just in this pre-inflationary Universe evolution, although unaccessible to present observations. These considerations partly determined the persistent idea that this field of investigation could have a prevalent academic nature, according to the spirit of the original derivation of the BKL oscillatory regime.

In this paper, we review in details and under an updated point of view the main features of the Mixmaster model. Our aim is to provide a precise picture of this research line and how it developed over the last four decades in the framework of General Relativity and canonical quantization of the gravitational field.

We start with a pedagogical formulation of the fundamental tools required to understand the treated topics and then we pursue a consistent description which, passing through the classical achievements, touches the review of very recent understandings in this field. The main aim of this work is to attract interest, especially from researchers working on fundamental physics, to the fascinating features of the classical and quantum inhomogeneous Mixmaster model. Our goal would be to convince the reader that this dynamical regime is physically well motivated and is not only mathematical cosmology, effectively concerning the very early stages of the Universe evolution, which matches the Planckian era with the inflationary behavior.

The main reason underlying the relevance of the Mixmaster dynamics can be identified
as follows: the pre-inflationary evolution fixes the initial conditions for all the subsequent dynamical stages as they come out from the quantum era of the Universe, and hence the oscillatory regime concerns the mechanism of transition to a classical cosmology providing information on the origin of the actual notion of space-time.

Moreover, we emphasize three points strongly supporting that the very early Universe dynamics was described by more general paradigms than the isotropic model, indeed concerning the generic cosmological solution.

- The FRW model is backward unstable with respect to tensor perturbations, which increase as the inverse of the scale factor. Recent studies have shown how such instability holds for scalar perturbations too, as far as the presence of bulk viscosity is taken into account.

- The inflationary scenario offers an efficient isotropization mechanism, able to reconcile the primordial inhomogeneous Mixmaster with the local high isotropy of the sky sphere at the recombination age.

- In the Planckian era, the quantum fluctuations can be correlated at most on the causal scale, thus we should regard global symmetries as approximated toy models. In this respect, the assumption that the Universe was born in the homogeneous and isotropic configuration does not appear well grounded. On a more realistic point of view, the quantum dynamics has to be described in absence of any special symmetry, i.e. by the inhomogeneous Mixmaster Universe.

This article is organized as follows:

in Section 1 we review the fundamental tools for geometrodynamics, with particular relevance to the Hamiltonian formulation of General Relativity and to Singularity Theorems. In Section 2 we widely discuss the classifications of the homogeneous spaces and in particular the dynamics of the types I, II and VII of the Bianchi classification. In Section 3 the classical features of the Mixmaster model are analyzed in details, both in the field equations formalism and in the Hamiltonian one. Particular attention is paid to the chaotic properties and to the cosmological implications of the homogeneous dynamics, also pointing out the effects on chaos of matter fields and of the number of dimensions.

In Section 4 we face the quantization of the Mixmaster model in different framework: after reviewing the standard Wheeler-DeWitt approach, we derive the full energy spectrum in the Dirac quantization scheme, and finally we discuss the more recent Loop Quantum Gravity approach and the Generalized Uncertainty Principle.

In Section 5 we generalize the previous results to the inhomogeneous case, both on the classical and on the quantum level. We focus the attention also on several important topics of the Generic Cosmological Solution of the Einstein equations and its identification with the Mixmaster model.
2 Fundamental Tools

In this Section we will analyze and discuss some of the fundamental features of the classical theory of gravity, i.e. the Einstein theory of General Relativity (GR). In particular, after presenting the Einstein field equations, the way how the macroscopic matters fields are treated in such theory and a discussion about the tetradic formalism, we will analyze in some details the Hamiltonian formulation of the dynamics, which will be fundamental in the following. Then we will discuss the synchronous reference and finally review the fundamental singularity theorems although without entering in the rigorous proofs.

Let us fix our convention, following Landau and Lifschitz [319]: the space-time indices are given by the Latin letters in the middle of the alphabet, i.e. \( i, j, k \ldots \) and run from 0 to 3 (the Lorentzian indices are labeled as \( a, b, c \)). The spatial indices are the Greek letters \( \alpha, \beta, \gamma \ldots \) and run as 1, 2, 3. We adopt the signature \((+,−,−,−)\), unless differently specified.

2.1 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. Assigned a four-dimensional manifold \( M \), endowed with space-time coordinates \( x^i \) and a metric tensor \( g_{ij}(x^l) \), its line element reads as

\[
ds^2 = g_{ij}dx^idx^j.
\]

This quantity fixes the Lorentzian notion of distances. The motion of a free test particle on \( M \) corresponds to the geodesic equation

\[
\frac{du^i}{ds} + \Gamma_{jl}^i u^j u^l = 0,
\]

where \( u^i \equiv dx^i/ds \) is its four-velocity, defined as the vector tangent to the curve, and \( \Gamma_{jl}^i = g^{im}\Gamma_{jlm} \) are the Christoffel symbols given by

\[
\Gamma_{jl}^i = \Gamma_{jl}^{im} = \frac{1}{2} \left( \partial_j g_{lm} + \partial_l g_{jm} - \partial_m g_{jl} \right).
\]

The geodesic character of a curve requires to deal with a parallelly transported tangent vector \( u^i \). However, for a Riemannian manifold this curve extremizes the distance functional, i.e. it is provided by the variational principle

\[
\delta \int_M ds = \delta \int_M ds \sqrt{g_{ij}u^iu^j} = 0.
\]

If a test particle has zero rest mass, its motion is given by \( ds = 0 \) and therefore an affine parameter must be introduced to describe the corresponding trajectory.
The equivalence principle is here recognized as the possibility to have vanishing Christoffel symbols at a given point of \( M \) (or along a whole geodesic curve). The space-time curvature is ensured by a non-vanishing Riemann tensor

\[
R^i_{\ jkl} = \partial_k \Gamma^i_{jl} - \partial_j \Gamma^i_{kl} + \Gamma^m_{jk} \Gamma^i_{ml} - \Gamma^m_{jl} \Gamma^i_{mk},
\]

(2.1.5)

which has the physical meaning of tidal forces acting on two free-falling observers and their effect is expressed by the geodesic deviation equation

\[
u^l \nabla_l (u^k \nabla_k s^i) = R^i_{\ jlm} u^j u^l s^m,
\]

(2.1.6)

where \( s^i \) is the connecting vector between two nearby geodesics. The Riemann tensor obeys the algebraic cyclic sum

\[
R^i_{\ jkl} + R^i_{\ iljk} + R^i_{\ iklj} = 0
\]

(2.1.7)

and the first order equations

\[
\nabla_m R^i_{\ jkl} + \nabla_l R^i_{\ jmk} + \nabla_k R^i_{\ jlm} = 0.
\]

(2.1.8)

The constraint in Eq. (2.1.8) is called the Bianchi identity, being identically satisfied by the metric tensor, meanwhile it is an equation for the Riemann tensor where covariant derivatives are expressed in terms of the metric. Contracting the Bianchi identity with \( g^{ik} g^{jl} \), we get the equation

\[
\nabla_j G^i_j = 0,
\]

(2.1.9)

where the Einstein tensor \( G_{ij} \) reads as

\[
G_{ij} \equiv R_{ij} - \frac{1}{2} R g_{ij},
\]

(2.1.10)

in terms of the Ricci tensor \( R_{ij} \equiv R^l_{\ ilj} \) and of the scalar of curvature \( R \equiv g^{ij} R_{ij} \).

In order to get the Einstein equations in the presence of matter fields described by a Lagrangian density \( \Lambda_m \), we must fix a proper action for the gravitational field, i.e. for the metric tensor of the manifold \( M \). A gravity-matter action, satisfying the fundamental requirements of a covariant geometrical physical theory of the space-time, takes the Einstein-Hilbert matter form

\[
S = S_{E-H} + S_m = -\frac{1}{2\kappa} \int_M d^4x \sqrt{-g} (R - 2\kappa \Lambda_m) ,
\]

(2.1.11)

where \( g \) is the determinant of the metric tensor \( g_{ij} \) and \( \kappa \) is the Einstein constant. The variation of action (2.1.11) with respect to \( g^{ij} \) can be expressed in terms of the vector \( \delta W^i \) as

\[
\delta W^i = \delta^i_k \delta^{ij} \Gamma^j_{ik} - \delta^{ij} \delta^k_i \Gamma^k_{ij},
\]

(2.1.12)

for which the relation

\[
\sqrt{-g} g^{ij} \delta R_{ij} = \nabla_j \delta W^j
\]

(2.1.13)
2.2 Matter Fields

holds (for detailed calculation see [505, 242, 319, 349]), providing the field equations in presence of matter

\[ G_{ij} = \kappa T_{ij}. \] (2.1.14)

Here \( T_{ij} \) denotes the energy-momentum tensor of the matter field and reads as

\[ T_{ij} = \frac{2}{\sqrt{-g}} \left( \frac{\delta (\sqrt{-g} \Lambda_m)}{\delta g^{ij}} - \partial_i \frac{\delta (\sqrt{-g} \Lambda_m)}{\delta (\partial_j g^{ij})} \right). \] (2.1.15)

As a consequence of the Bianchi identity we find the conservation law \( \nabla_j T^j_i = 0 \), which describes the motion of matter and arises from the Einstein equations. The gravitational equations thus imply the equations of motion for the matter itself. Finally, by comparing the static weak field limit of the Einstein equations (2.1.14) with the Poisson equation of the Newton theory of gravity, we easily get the form of the Einstein constant in terms of the Newton constant as \( \kappa = 8\pi G \).

The whole analysis discussed so far regards the Einstein geometrodynamics formulation of gravity. In the gravity-matter action, the cosmological constant term is considered as vanishing, although it would be allowed by the paradigm of General Relativity. This choice is based on the idea that such term should come out from the matter contribution itself, eventually on a quantum level.

2.2 Matter Fields

In general relativity, continuous matter fields are described by the energy-momentum tensor \( T_{ij} \). We will focus our attention only on the tensor fields and will not discuss more general entities as the spinor fields for which we recommend the exhaustive discussion in [505] and for the related bi-spinor calculus [318]. In particular, we briefly review the cases of the perfect fluid, the scalar and the electromagnetic fields.

The definition of the symmetric tensor \( T_{ij} \) as in Eq. (2.1.15) differs from the energy-momentum tensor obtained from the Eulero-Lagrange equations. In fact, in the Minkowski space-time we have an alternative way to construct the energy-momentum tensor for a generic field Lagrangian. However, such tensor in general has not the symmetry requirement, thus we adopt the definition given as in Eq. (2.1.15). Let us stress that, from another point of view, the equations of motion of the matter field

\[ \nabla^i T_{ij} = 0 \] (2.2.1)

are obtained requiring the action for the matter \( S_m \) introduced in Eq. (2.1.11) to be invariant under diffeomorphisms. For the Einstein equations, the Bianchi identities \( \nabla^i G_{ij} = 0 \) may be viewed as a consequence of the invariance of the Hilbert action under diffeomorphisms. Let us now list the principal aspects of the three fields under consideration.

- The energy-momentum tensor of a perfect fluid is given by

\[ T_{ij} = (p + \rho) u_i u_j - p g_{ij}, \] (2.2.2)

where \( u_i \) is a unit time-like vector field representing the four-velocity of the fluid. The scalar functions \( p \) and \( \rho \) are the energy density and the pressure, respectively, as
measured by an observer in a locally inertial frame moving with the fluid, and are related by an equation of state \( p = p(\rho) \). Since no terms describing heat conduction or viscosity are introduced the fluid is considered as perfect. For the early Universe we have \( p = (\gamma - 1)\rho \), where \( \gamma \) is the polytropic index. In the particular case where \( p = 0 \) we deal with dust, whose fluid elements follow geodesic trajectories.

- The Lagrangian density for the linear, relativistic, scalar field theory reads as

\[
\Lambda_m = \frac{1}{2} \left( \partial^k \phi \partial_k \phi - m^2 \phi^2 \right) \tag{2.2.3}
\]

and in a curved space-time it is obtained by the minimal substitution rule \( \eta_{ij} \rightarrow g_{ij} \) and \( \partial_i \rightarrow \nabla_i \). The corresponding energy-momentum tensor is expressed as

\[
T_{ij} = \nabla_i \phi \nabla_j \phi - \frac{1}{2} g_{ij} \left( \nabla^k \phi \nabla_k \phi - m^2 \phi \right), \tag{2.2.4}
\]

and the Klein-Gordon equation becomes

\[
\left( \nabla^k \nabla_k + m^2 \right) \phi = 0. \tag{2.2.5}
\]

- The Maxwell field is described by the Lagrangian density

\[
\Lambda_m = -\frac{1}{16\pi} F_{ij} F^{ij} \tag{2.2.6}
\]

and the electromagnetic energy-momentum tensor reads as

\[
T_{ij} = \frac{1}{4\pi} \left( -F_{ik} F^{kj} + \frac{1}{4} g_{ij} F_{kl} F^{kl} \right), \tag{2.2.7}
\]

where \( F = dA \) is the curvature 2-form associated to the connection 1-form \( A = A_i dx^i \), i.e. \( F_{ij} = \nabla_i A_j - \nabla_j A_i \). We note that the trace of the energy-momentum tensor defined as in Eq. \( (2.2.7) \) is identically vanishing. Thus, the Maxwell equations in a curved space-time become

\[
\nabla^l F_{lk} = -4\pi j_k \tag{2.2.8a}
\]

\[
\nabla_{[i} F_{jk]} = 0, \tag{2.2.8b}
\]

where \( j_k \) is the current density four-vector of electric charge and \([\ ]\) denote the antisymmetric sum, or in the forms language equations \( (2.2.8) \) are written as

\[
d \star F = 4\pi \star j \tag{2.2.9a}
\]

\[
d F = 0 \tag{2.2.9b}
\]

where \( d \) is the exterior derivative and \( \star \) is the Hodge star operator \([505][370]\).
2.3 Tetradic Formalism

Let $M$ be a four-dimensional manifold and $e$ a one-to-one correspondence on it, $\hat{e} : M \to TM$, mapping tensor fields on $M$ to tensor fields in the Minkowski tangent space $TM$. The four linearly independent fields $e^a_i$ (tetrads or vierbein) ($a$ is the Lorentzian index) are an orthonormal basis for the local Minkowskian space-time and satisfy the condition

$$e^a_i e^b_j = \eta_{ab}$$  \hspace{1cm} (2.3.1)$$
only. In Eq. (2.3.1) $\eta_{ab}$ is a symmetric, constant matrix with signature $(+,-,-,-)$ and $\eta^{ab}$ is the inverse matrix of $\eta_{ab}$. Let us define the reciprocal (dual) vectors $e^i_a$, such that $e^a_i e^b_j = \delta^a_b$. By definition of $e^a_i$ and by (2.3.1), the condition $e^a_i e^b_j = \delta^a_b$ is also verified.

In this way, the Lorentzian index is lowered and raised with the matrix $\eta_{ab}$, and the metric tensor $g_{ij}$ assumes the form

$$g_{ij} = \eta_{ab} e^a_i e^b_j.$$  \hspace{1cm} (2.3.2)$$
We denote the projections of the vector $A^i$ along the four $e^a_i$ as “vierbein components”, $A^a = e^a_i A^i$, and $A^a_i = e^a_i A^i = \eta^{ab} A_b$. In particular, for the partial differential operator, we have $\partial_a = e^a_i \partial_i$, below denoted as a comma $(,)_a \equiv \partial_a$. The generalization to a tensor of any number of covariant or contravariant indices is straightforward.

Let us introduce a couple of quantities which will directly appear in the Einstein equations, the Ricci coefficients $\gamma_{abc}$, and their linear combinations $\lambda_{abc}$ by the following equations

$$\gamma_{abc} = \nabla_k e^a_i e^b_j e^c_k,$$  \hspace{1cm} (2.3.3)$$
$$\lambda_{abc} = \gamma_{abc} - \gamma_{acb}.$$  \hspace{1cm} (2.3.4)$$
With some algebra, the Riemann and the Ricci tensors can be expressed in terms of $\gamma_{abc}$ and of $\lambda_{abc}$ as

$$R_{abcd} = \gamma_{abc,d} - \gamma_{abd,c} + \gamma_{abf} \big( \gamma^f_{cd} - \gamma^f_{dc} \big) + \gamma_{afc} \gamma^f_{bd} - \gamma_{af} \gamma^f_{bd},$$  \hspace{1cm} (2.3.5)$$
$$R_{ab} = -\frac{1}{2} \left( \lambda^c_{ab} + \lambda^c_{ba} + \lambda^c_{ca,b} + \lambda^c_{cb,a} + \lambda^c_{ab} + \lambda^c_{ba} + \lambda^c_{cd} \lambda_{ab} d + \lambda^c_{cd} \lambda_{ba} d \right).$$  \hspace{1cm} (2.3.6)$$
With the use of the tetradic fields $e^a_i$, we are able to rewrite the Lagrangian formulation of the Einstein theory in a more elegant and compact form. Let us introduce the connection 1-forms $\omega^a_b$ and the curvature 2-forms associated to it by

$$R^a_b = d \omega^a_b + \omega^a_c \wedge \omega^c_b,$$  \hspace{1cm} (2.3.7)$$
which is the so-called I Cartan structure equation. In this formalism, the action for GR in absence of matter field reads as

$$S(e, \omega) = -\frac{1}{4\kappa} \int_M e_{abcd} e^a \wedge e^b \wedge R^{cd},$$  \hspace{1cm} (2.3.8)$$
where $\epsilon_{abcd}$ is the totally antisymmetric tensor on $T\mathcal{M}$ such that $\epsilon_{ijkl} = \epsilon_{abcd}e^ae^be^ce^d$. We stress that here we are working a la Palatini, i.e. in a first order formalism where the tetrads $e^a_i$ and the spin connections $\omega^a_b$ can be considered as independent variables. The variation of the action (2.3.8) with respect to the connections leads to the II Cartan structure equation, i.e. to the equations of motion for $\omega^a_b$

$$d\omega^a_b + \omega^a_be^b = 0 \Rightarrow \omega = \omega(e)$$ (2.3.9)

and to the identity $e^b \wedge R^g_b = 0$, while the variation with respect to the tetrad $e^a$ leads to the Einstein vacuum equations

$$\epsilon_{abcd}e^b \wedge R_{cd} = 0.$$ (2.3.10)

The solution to the II Cartan structure equation (2.3.9) can be written as $\omega^a_b = e^a_j \nabla^i e^b_j$, which corresponds to the relation $\omega^a_b = \gamma^a_b e^c_i$ for the Ricci coefficients. The two different notations are adopted accordingly as $\gamma$ in [319], and $\omega$ in [505].

### 2.4 Hamiltonian Formulation of the Dynamics

The aim of the first part of this paragraph is the Hamiltonian formulation of GR in the metric formalism [505, 280, 485, 310], and of the corresponding Hamilton-Jacoby theory in the following [259, 297]. For the theory of constrained Hamiltonian systems we refer to the standard textbooks [181, 251].

#### 2.4.1 Canonical General Relativity

The generally covariant system par excellence is the gravitational field, i.e. it is invariant under arbitrary changes of the space-time coordinates (four-dimensional diffeomorphisms). To perform a canonical formulation of General Relativity one has to assume that the topology of $M$ (the physical space-time) is $M = \mathbb{R} \times \Sigma$, where $\Sigma$ is a compact three-dimensional manifold (the three-space). As follows from standard theorems, all physically realistic space-times (globally hyperbolic) posses such topology; thus, $M$ can be foliated by a one-parameter family of embeddings $X_t : \Sigma \to M$, $t \in \mathbb{R}$, of $\Sigma$ in $M$. As a consequence, the mapping $X : \mathbb{R} \times \Sigma \to M$, defined by $(x, t) \to X_t$, is a diffeomorphism of $\mathbb{R} \times \Sigma$ to $M$. A useful parametrization of the embedding is given by the deformation vector field

$$T^i(X) \equiv \frac{\partial X^i(x,t)}{\partial t} = N(X)n^i(X) + N^i(X),$$ (2.4.1)

where $N^i(X) \equiv N^aX^i_a$. The vector field $T^i$, satisfying $T^i\nabla_i T = 1$, can be interpreted as the “flow of time” throughout the space-time. In Eq. (2.4.1), $n^i$ is the unit vector field normal to $\Sigma_t$, i.e. the relations

$$\begin{cases}
g_{ij}n^i n^j = 1 \\
g_{ij}n^i \partial_\alpha X^j = 0
\end{cases}$$ (2.4.2)

hold. The quantities $N$ and $N^a$ are the lapse function and the shift vector, respectively. This way the space-time metric $g_{ij}$ induces a spatial metric, i.e. a three-dimensional Riemannian metric $h_{\alpha\beta}$ on each $\Sigma_t$, by $-h_{\alpha\beta} = g_{ij} \partial_\alpha X^i \partial_\beta X^j$. The space-time line-element
2.4 Hamiltonian Formulation of the Dynamics

adapted to this foliation can be written as

\[ ds^2 = N^2 dt^2 - h_{\alpha\beta}(dx^\alpha + N^\alpha dt)(dx^\beta + N^\beta dt). \]  

(2.4.3)

This formalism was introduced by Arnowitt, Deser and Misner in 1962 [19] and is known as the ADM procedure.

The geometrical meaning of \( N \) and \( N^\alpha \) is now clear: the lapse function specifies the proper time separation between the hypersurfaces \( X_t(\Sigma) \) and \( X_{t+\delta t}(\Sigma) \) measured in the direction normal to the first hypersurface. On the other hand, the shift vector measures the displacement of the point \( X_{t+\delta t}(x) \) from the intersection of the hypersurface \( X_{t+\delta t}(\Sigma) \) with the normal geodesic drawn from the point \( X_t(x) \) (see Fig. 2.1). In order to have a future directed foliation of the space-time, we stress the requirement for the lapse function \( N \) to be positive everywhere in the domain of definition.

\[ \text{Figure 2.1: The geometric interpretation of the lapse function and of the shift vector (from [310]). In the figure latin indices denote spatial components, while greek ones space-time components.} \]

In the canonical analysis of General Relativity, the Riemannian metric \( h_{\alpha\beta} \) on \( \Sigma_t \) plays the role of the fundamental configuration variable. The rate of change of \( h_{\alpha\beta} \) with respect to the time label \( t \) is related to the extrinsic curvature \( K_{\alpha\beta} = -\frac{1}{2} \mathcal{L}_N h_{\alpha\beta} \) of the hypersurface \( \Sigma_t \) as

\[ K_{\alpha\beta}(x, t) = -\frac{1}{2N} (\partial_t h_{\alpha\beta} - (\mathcal{L}_N h)_{\alpha\beta}), \]  

(2.4.4)

where \( \mathcal{L}_a \) denotes the Lie derivative along the vector field \( a \).

Let us now pull-back the Einstein Lagrangian density by the adopted foliation \( X : \mathbb{R} \times \Sigma \rightarrow M \) and express the result \( X^* \) in terms of the extrinsic curvature, the three-metric \( h_{\alpha\beta} \), \( N \) and \( N^\alpha \). This gives

\[ X^* \left( \sqrt{-g} (4) R \right) = N \sqrt{h} \left( K_{\alpha\beta} K^{\alpha\beta} - (K^\alpha_{\alpha})^2 + (3) R \right) + \]

\[ -\frac{2}{dt} \left( \sqrt{h} K^\alpha_{\alpha} \right) - \partial_\beta \left( K^\alpha_{\beta} N^\alpha - h^{\alpha\beta} \partial_\alpha N \right) \]  

(2.4.5)

where \((n)R\) is the \( n \)-dimensional curvature scalar and \( \sqrt{-g} = N \sqrt{h} \), being \( h \) the determinant of the three-dimensional metric. We are able to re-cast the original Hilbert action into a \( 3 + 1 \) form by simply dropping the total differential in (2.4.5), i.e. the last two terms.
on the r.h.s. of (2.4.5)

\[ S(h, N, N^a) = -\frac{1}{2\kappa} \int dt \int d^3x N \sqrt{h} \left( K_{\beta\gamma} K^{\beta\gamma} - (K^\beta_\beta)^2 + (3)^R \right). \] (2.4.6)

Performing a Legendre transformation of the Lagrangian density appearing in equation (2.4.6) we obtain the corresponding Hamiltonian density. Let us note that the action (2.4.6) does not depend on the time derivatives of \( N \) and \( N^a \), and therefore using the definition (2.4.4) and the fact that \((3)^R\) does not contain time derivatives, we obtain for the conjugate momenta

\[ \frac{1}{\kappa} \Pi^{\alpha\beta}(x, t) \equiv \frac{\delta S}{\delta h_{\alpha\beta}(x, t)} = \frac{\sqrt{h}}{\kappa} (K^{\alpha\beta} - h^{\alpha\beta} K^\gamma_{\gamma}) \] (2.4.7a)

\[ \Pi(x, t) \equiv \frac{\delta S}{\delta N(x, t)} = 0 \] (2.4.7b)

\[ \Pi^\alpha(x, t) \equiv \frac{\delta S}{\delta N^\alpha(x, t)} = 0. \] (2.4.7c)

From equations (2.4.7) follows that not all conjugate momenta are independent, i.e. one cannot solve for all velocities as functions of coordinates and momenta: one can express \( \dot{h}_{\alpha\beta} \) in terms of \( h_{\alpha\beta}, N, N^a \) and \( \Pi^{\alpha\beta} \), but the same is not possible for \( \dot{N} \) and \( \dot{N}^a \). By other words, we have the so-called primary constraints

\[ C(x, t) \equiv \Pi(x, t) = 0, \quad C^a(x, t) \equiv \Pi^a(x, t) = 0, \] (2.4.8)

where “primary” emphasizes that the equations of motion are not used to obtain relations (2.4.8).

According to the theory of constrained Hamiltonian systems, let us introduce the new fields \( \lambda(x, t) \) and \( \lambda^a(x, t) \) as the Lagrange multipliers for the primary constraints, making the Legendre transformations invertible and the corresponding action reading as

\[ S = \int dt \int d^3x \left[ \dot{h}_{\alpha\beta} \Pi^{\alpha\beta} + \dot{N} \Pi + \dot{N}^a \Pi^a - (\lambda C + \lambda^a C^a + N^a H_a + NH) \right], \] (2.4.9)

where

\[ H_a \equiv -2h_{\alpha\gamma} \nabla_\beta \Pi^{\gamma\beta} \] (2.4.10a)

\[ H \equiv \mathcal{G}_{\alpha\beta\gamma\delta} \Pi^{\alpha\beta} \Pi^{\gamma\delta} - \sqrt{h} (3)^R \] (2.4.10b)

in which

\[ \mathcal{G}_{\alpha\beta\gamma\delta} \equiv \frac{1}{2\sqrt{h}} \left( h_{\alpha\gamma} h_{\beta\delta} + h_{\beta\gamma} h_{\alpha\delta} - h_{\alpha\beta} h_{\gamma\delta} \right) \] (2.4.10c)

is the so-called super-metric on the space of the three-metrics, and the functionals \( H_a \) and \( H \) are the super-momentum and super-Hamiltonian, respectively.

The classical canonical algebra of the system is expressed in terms of the standard Poisson brackets as
2.4 Hamiltonian Formulation of the Dynamics

\[ \{ h_{\alpha\beta}(x,t), h_{\gamma\delta}(x',t) \} = 0 \quad (2.4.11a) \]
\[ \{ \Pi^{\alpha\beta}(x,t), \Pi^{\gamma\delta}(x',t) \} = 0 \quad (2.4.11b) \]
\[ \{ h_{\gamma\delta}(x,t), \Pi^{\alpha\beta}(x',t) \} = \kappa \delta^\alpha_{(\gamma} \delta^\beta_{\delta)} \delta^3(x - x') \]  \quad (2.4.11c)

where the parentheses ( ) denote symmetrized indices. We can analyze the meaning of the Hamiltonian of the system, bracketed in equation (2.4.9)

\[ H \equiv \int_{\Sigma} d^3x \left( \lambda C + \lambda^a C_a + N^a H_a + NH \right) \equiv C(\lambda) + \tilde{C} \left( \tilde{\lambda} \right) + \tilde{H} \left( \tilde{N} \right) + H(N) \quad (2.4.12) \]

The variation of the action (2.4.9) with respect to the Lagrange multipliers \( \lambda \) and \( \lambda^a \) reproduces the primary constraints (2.4.8). The consistency of the dynamics is ensured by preserving them during the evolution of the system, i.e. requiring

\[ \dot{C}(x,t) \equiv \{ C(x,t), H \} = 0, \quad \dot{C}^a(x,t) \equiv \{ C^a(x,t), H \} = 0. \quad (2.4.13) \]

The Poisson brackets in equation (2.4.13) do not vanish, but equal to \( H(x,t) \) and \( H^a(x,t) \), respectively, and therefore the consistency of the motion leads to the secondary constraints

\[ H(x,t) = 0, \quad H^a(x,t) = 0, \quad (2.4.14) \]

by means of the equations of motion. Let us observe that the Hamiltonian in General Relativity is constrained as \( H \approx 0 \) being weakly zero, i.e. vanishing on the constraint surface. This is not surprising since we are dealing with a generally covariant system.

A problem that can arise is that the constraint surface, i.e. the surface where the constraints hold, could not be preserved under the motion generated by the constraints themselves, but this is not the case. In fact, the Poisson algebra of the super-momentum and super-Hamiltonian, computed using (2.4.11a)-(2.4.11c), is closed. In other words, the set of constraints is of first class, i.e. the Poisson brackets between the Hamiltonian \( H \) and any constraint weakly vanish, as arising from the relations

\[ \{ H, \tilde{H}(\tilde{f}) \} = \tilde{H}(\mathcal{L}_{\tilde{N}} \tilde{f}) - H(\mathcal{L}_f N) \]
\[ \{ H, H(f) \} = H(\mathcal{L}_{\tilde{N}} f) + \tilde{H}(\tilde{N}(N,f,h)) \]

where \( f \) is a smooth function and \( \tilde{N}^a(N,f,h) = h^{a\beta}(N\partial_{\beta}f - f\partial_{\beta}N) \). These equations are equivalent to the Dirac algebra [181].

Moreover, varying the action (2.4.9) with respect to the two conjugate momenta \( \Pi \) and \( \Pi^a \), we obtain

\[ \dot{N}(x,t) = \lambda(x,t), \quad \dot{N}^a(x,t) = \lambda^a(x,t) \]

ensuring that the trajectories of the lapse function and of the shift vector in the phase space are completely arbitrary.

The Hamiltonian of the theory is not a true one but a linear combination of constraints. From relations (2.4.15) and (2.4.16) it is possible to show that rather than generating time translations, the Hamiltonian generates space-time diffeomorphisms, whose parameters
are the completely arbitrary functions $N$ and $N^a$, and the corresponding motions on the phase space have to be regarded as gauge transformations. An observable is defined as a function on the constraint surface that is gauge invariant, and more precisely, in a system with first class constraints it can be described as a phase space function that has weakly vanishing Poisson brackets with the constraints. In our case, $A$ is an observable if and only if
\[
\{A, \mathcal{H}(\lambda, \lambda^a, N^a, N)\} \approx 0, \quad (2.4.18)
\]
for generic $\lambda$, $\lambda^a$, $N^a$ and $N$. By this definition, one treats on the same footing ordinary gauge invariant quantities and constants of motion with respect to evolution along the foliation associated to $N$ and $N^a$. The basic variables of the theory, $h_{\alpha\beta}$ and $\Pi_{\alpha\beta}$, are not observables as they are not gauge invariant. In fact, no observables for General Relativity are known, except for the particular situation with asymptotically flat boundary conditions.

Let us remark that the equations of motion
\[
\dot{h}_{\alpha\beta}(x, t) = \frac{\delta \mathcal{H}}{\delta \Pi_{\alpha\beta}(x, t)}; \quad \dot{\Pi}_{\alpha\beta}(x, t) = -\frac{\delta \mathcal{H}}{\delta h_{\alpha\beta}(x, t)} \quad (2.4.19)
\]
together with the eight constraints (2.4.8) and (2.4.14) are completely equivalent to the vacuum Einstein equations, $R_{ij} = 0$ [199].

### 2.4.2 Hamilton-Jacobi Equations for Gravitational Field

The formulation of the Hamilton-Jacobi theory for a covariant system is simpler than the conventional non-relativistic version. In fact, in such case the Hamilton-Jacoby equations are expressed as
\[
H \left( q_a, \frac{\partial S}{\partial q_a} \right) = 0, \quad (2.4.20)
\]
where $H$ and $S(q_a)$ denote the Hamiltonian and the Hamilton functions, respectively. For GR, the Hamilton-Jacobi equations arising from the super-Hamiltonian and super-momentum read as
\[
\hat{H} J S \equiv G_{\alpha\beta\gamma\delta} \frac{\delta S}{\delta h_{\alpha\beta}} \frac{\delta S}{\delta h_{\gamma\delta}} - \sqrt{h} (3) R = 0 \quad (2.4.21)
\]
\[
\hat{H} f S \equiv -2 h_{\alpha\gamma} \nabla_{\beta} \frac{\delta S}{\delta h_{\alpha\beta}} = 0. \quad (2.4.22)
\]
These four equations, together with the primary constraints (2.4.8), completely define the classical dynamics of the theory.

Let us point out how through a change of variable we can define a time coordinate. In fact, writing $h_{\alpha\beta} \equiv \eta^{4/3} u_{\alpha\beta}$ with $\eta \equiv h^{1/4}$ and $\det u_{\alpha\beta} = 1$, the super-Hamiltonian Hamilton-Jacobi equation (2.4.21) can be written as
\[
\hat{H} J S = -\frac{3}{16} \kappa \left( \frac{\delta S}{\delta \eta} \right)^2 + \frac{2\kappa}{\eta^2} u_{\alpha\gamma} u_{\beta\delta} \frac{\delta S}{\delta u_{\alpha\beta}} \frac{\delta S}{\delta u_{\gamma\delta}} - \frac{1}{2\kappa} \eta^{2/3} V(u_{\alpha\beta}, \nabla \eta, \nabla u_{\alpha\beta}), \quad (2.4.23)
\]
where the potential term $V$ comes out from the spatial Ricci scalar and $\nabla$ refers to spatial
gradients only. As we can see from Eq. (2.4.23), \(\eta\) has the correct signature for an internal time variable candidate. We will show later how this variable is nothing but a power of the isotropic volume of the Universe.

## 2.5 Synchronous Reference

In this paragraph we will focus our attention on one of the most interesting reference system, i.e. the synchronous one. For a detailed discussion see [319]. It is defined by the following choice for the metric tensor \(g_{ij}\)

\[
g_{00} = 1, \quad g_{0\alpha} = 0, \tag{2.5.1}
\]

thus in the 3 + 1 framework we have to require \(N = 1\) and \(N^\alpha = 0\) in (2.4.3). The first condition in (2.5.1) is allowed from the freedom to rescale the variable \(t\) with the transformation \(\sqrt{g_{00}}dt\), in order to reduce \(g_{00}\) to unity, and setting the time coordinate \(x^0 = t\) as the proper time at each point of space. The second one is allowed by the non-vanishing of \(|g_{\alpha\beta}|\) and allows the synchronization of clocks at different points of space. The elementary line interval is given by the expression

\[
ds^2 = dt^2 - dl^2, \tag{2.5.2}
\]

where

\[
dl^2 = h_{\alpha\beta}(t, x^\gamma) \, dx^\alpha dx^\beta, \tag{2.5.3}
\]

in which the three-dimensional tensor \(h_{\alpha\beta}\) defines the space metric.

In such a reference system, lines of equal times are geodesics in the four-space, as implied by the splitting definition. Indeed the four-vector \(u^i = dx^i/ds\) which is tangent to the world line \((x^\gamma = \text{const.})\), has components \(u^0 = 1, u^\alpha = 0\) and automatically satisfies the geodesic equations

\[
\frac{du^i}{ds} + \Gamma^i_{kl}u^k u^l = \Gamma^i_{00} = 0. \tag{2.5.4}
\]

The choice of such a reference is always possible and moreover it is not unique. In fact, considering a generic infinitesimal displacement

\[
t' = t + \zeta(t, x^\rho), \quad x'^\alpha = x^\alpha + \zeta^\alpha(t, x^\rho) \tag{2.5.5}
\]

and the associated four-metric change \(g'_{ij} = g_{ij} - 2\nabla_{(i}\zeta_{j)}\), the conditions of preserving the synchronous reference can be written as

\[
\partial_t \zeta = 0 \Rightarrow t' = t + \zeta(x^\rho) \tag{2.5.6a}
\]

\[
\partial_\alpha \zeta = 0 \Rightarrow x'^\alpha = x^\alpha + \partial_\beta \zeta \int h^{\alpha\beta} dt + \phi^\alpha(x^\rho), \tag{2.5.6b}
\]

\(\phi^\alpha\) being generic space functions.

In the reference defined by the metric (2.5.2), the Einstein equations are written in mixed
components as

\[ R^0_0 = -\frac{1}{2} \frac{\partial}{\partial t} \kappa_\alpha^\alpha - \frac{1}{4} \kappa_\alpha^\beta \kappa_\beta^\alpha = 8\pi G \left( T^0_0 - \frac{1}{2} T \right) \]  
\[ R^0_\alpha = \frac{1}{2} \left( \kappa_\beta^\alpha - \kappa_\beta^\beta \right) = 8\pi G T^0_\alpha \]  
\[ R^\beta_\alpha = -P^\beta_\alpha - \frac{1}{2\sqrt{h}} \frac{\partial}{\partial t} \left( \sqrt{h} \kappa_\beta^\alpha \right) = 8\pi G \left( T^\beta_\alpha - \frac{1}{2} \delta^\beta_\alpha T \right) \]  

where

\[ \kappa_\alpha^\beta = \frac{\partial h_\alpha^\beta}{\partial t}, \quad h \equiv |h_\alpha^\beta|, \]  

\( P_\alpha^\beta \) is the three-dimensional Ricci tensor obtained through the metric \( h_\alpha^\beta \) which is used to raise and lower indices within the spatial sections.

The metric \( h_\alpha^\beta \) allows to construct the three-dimensional Ricci tensor \( P^\beta_\alpha = h^{\beta\gamma} P_\alpha^\gamma \) as

\[ P_\alpha^\beta = \partial_\gamma \lambda^\gamma_\alpha^\beta - \partial_\alpha \lambda^\gamma_\beta^\gamma + \lambda^\gamma_\alpha^\beta \lambda_\gamma^\delta - \lambda^\gamma_\alpha^\delta \lambda_\beta^\gamma \]  

in which appear the pure spatial Christoffel symbols

\[ \lambda^\gamma_\alpha^\beta \equiv \frac{1}{2} h^{\gamma\delta} (\partial_\alpha h_{\delta\beta} + \partial_\beta h_{\alpha\delta} - \partial_\delta h_{\alpha\beta}) \].

From (2.5.7a) it is straightforward to derive, even in the isotropic case, the Landau-Raychaudhuri theorem, stating that the metric determinant \( h \) must monotonically vanish in a finite instant of time. However, we want to stress that the singularity in this reference system is not physical and of course can be removed passing to another one.

### 2.6 Singularity Theorems

In this Section we investigate space-time singularities. We will show how singularities are true, generic features of the Einstein theory of gravity and how they arise under certain, quite general, assumptions. We only enter in some details and we will not give the rigorous proofs, for which we refer to the standard literature \[247, 505\].

In particular, in this Section only we follow the signature of \[505\] \((-,-,+,+,+\).

We will treat here the classical aspects, referring to \[22, 217\] and references therein for a discussion on quantum cosmological singularities.

After defining what a space-time singularity means we will present some basic technology, and finally we will discuss the theorems.

#### 2.6.1 Definition of a Space-time Singularity

Let us clarify the meaning of a singularity of the space-time. In analogy with field theory, we can represent such a singularity as a "place" of the space-time where the curvature diverges, or where some similar pathological behavior of the geometric invariants takes place. Therefore, a first problem arises when characterizing the singularity as a "place". In fact, in General Relativity the space-time consists of a manifold \( M \) and a metric \( g_{ij} \)
2.6 Singularity Theorems

A singularity (as the Big-Bang singularity of the isotropic cosmological solution or the \( r = 0 \) singularity in the Schwarzschild space-time) can not be considered as a part of the manifold itself. We can speak of a physical event only when a manifold and a metric structure are defined around it. *A priori*, it is possible to add points to the manifold in order to describe the singularity as a real place (as a boundary of the manifold). But apart from very peculiar cases, no general notion or definition of a singularity boundary exists \[505, 208, 209, 285\]. Another problem is that singularities are not always accompanied by unbounded curvature as in the best known cases. There are several examples \[247\] of a singularity without diverging curvature. In fact, as we will see, this feature is not the basic mechanism behind singularity theorems.

The best way to clarify what a singularity means is the geodesic incompleteness, i.e. the existence of geodesics which are inextensible at least in one direction, but have only a finite range for the affine parameter. We can thus define a singular space-time as the one possessing one incomplete geodesic curve.

2.6.2 Preliminary notions

We initially define the notions of expansion and contraction of the congruence of time-like geodesics. The treatment of null geodesic congruences is conceptually similar and not reviewed here.

Let \( O \) be an open set of a manifold \( M \). A congruence in \( O \) is defined as a family of curves such that only one curve of this family passes through each point \( p \in O \). Let \( \xi^i \) be the vector field tangent to the geodesics such that \( \xi^i \xi_i = -1 \), and define the tensor \( B_{ij} = \nabla_j \xi_i \) to introduce the expansion \( \theta \) (as well as its trace part), the shear \( \sigma_{ij} \) (as its symmetric, trace-free part) and the twist \( \omega_{ij} \) (as its anti-symmetric part) of the congruence. Thus, \( B_{ij} \) can be written as

\[
B_{ij} = \frac{1}{3} \theta h_{ij} + \sigma_{ij} + \omega_{ij},
\]  

(2.6.1)

where the spatial metric is \( h_{ij} = g_{ij} + \xi_i \xi_j \). Given a deviation vector orthogonal to the vector field \( \xi^i \), the tensor \( B_{ij} \) measures its failure from being parallely transported along a geodesic in the congruence for this subfamily.

The rates of change of \( \theta, \sigma_{ij} \) and \( \omega_{ij} \) follow from the geodesic equation

\[
\zeta^k \nabla_k B_{ij} = \zeta^k \nabla_k \zeta^j (\nabla_j \zeta^i) = \zeta^k (\nabla_j \zeta^i + R_{kji} \zeta_l) =
\]

\[
= \nabla_j (\zeta^k \nabla_k \zeta^i) - (\nabla_j \zeta^k)(\nabla_k \zeta^i) + R_{kji} \zeta^k \zeta_l = -B_{kj} B_{ik} + R_{kji} \zeta^k \zeta_l. 
\]  

(2.6.2)

Taking the trace of Eq. (2.6.2), we obtain the Raychaudhuri equation

\[
\dot{\theta} = \zeta^k \nabla_k \theta = -\frac{1}{3} \theta^2 - \sigma_{ij} \sigma^{ij} + \omega_{ij} \omega^{ij} - R_{kli} \zeta^k \zeta^l. 
\]  

(2.6.3)

This result will be fundamental when proving the singularity theorems. Let us focus our attention on the right-hand side of it: using Einstein equations, the last term can be written as

\[
R_{kli} \zeta^k \zeta^l = \kappa \left( T_{ij} - \frac{1}{2} T g_{ij} \right) \zeta^i \zeta^j = \kappa \left( T_{ij} \xi^i \xi^j + \frac{1}{2} T \right). 
\]  

(2.6.4)
Let us state the physical criterion preventing the stresses of matter from becoming too large so that the right-hand side of (2.6.4) is not negative, obtaining

\[ T_{ij} \xi^i \xi^j \geq -\frac{1}{2} T, \]

which is known as the strong energy condition \[247\]. It is commonly accepted that every reasonable kind of matter would satisfy the condition (2.6.5). Therefore, from the Raychaudhuri equation (2.6.3) one can see that, if the congruence is non-rotating \[1\], which means \( \omega_{ij} = 0 \), and the strong energy condition holds, \( \theta \) always decreases along the geodesics. More precisely, we get

\[ \dot{\theta} + \frac{1}{3} \theta^2 \leq 0, \]

whose integral implies

\[ \theta^{-1}(\tau) \geq \theta_0^{-1} + \frac{1}{3} \tau, \]

(2.6.6)

where \( \theta_0 \) is the initial value of \( \theta \). For negative values of \( \theta_0 \) (i.e. the congruence is initially converging), \( \theta \) will diverge after a proper time no larger than \( \tau \leq 3/|\theta_0| \). By other words, the geodesics must intersect before such instant and form a caustic (a focal point). Of course, the singularity of \( \theta \) is nothing but a singularity in the congruence and not a space-time one, since the smooth manifold is well-defined on caustics.

Let us briefly discuss the meaning of the strong energy condition in the simple case of a perfect fluid, for which it reads as

\[ \rho + \sum_a p_a \geq 0, \quad \rho + p_\alpha \geq 0, \]

(2.6.7)

and is satisfied for \( \rho \geq 0 \) and for negative pressure components smaller in magnitude than \( \rho \).

We need to introduce some notions of differential geometry and topology to translate the occurrence of caustics into space-time singularities. Let \( \gamma \) be a geodesic with tangent \( \gamma \) defined on a manifold \( M \). A solution of the geodesic deviation equation is \( \eta^i \) satisfying \[2.1.6\] that constitutes a Jacobi field on \( \gamma \). If it is non-vanishing along \( \gamma \), but is zero at both \( p, q \in \gamma \), then \( p, q \) are said to be conjugate.

It is possible to show that a point \( q \in \gamma \) lying in the future of \( p \in \gamma \) is conjugate to \( p \) if and only if the expansion of all the time-like geodesics congruence passing through \( p \) approaches \( -\infty \) at \( q \) (i.e. a point is conjugate if and only if it is a caustic of such congruence). A necessary hypothesis in this statement is that the space-time manifold \( (M, g_{ij}) \) satisfy

\[ R_{ij} \xi^i \xi^j \geq 0, \]

for all time-like \( \xi^i \). Moreover, the necessary and sufficient condition for a timelike curve \( \gamma \), connecting \( p, q \in M \), that locally maximizes the proper time between \( p \) and \( q \), is that \( \gamma \) is a geodesic without any point conjugate to \( p \) between \( p \) and \( q \).

An analogous analysis can be made for time-like geodesics and a smooth space-like hypersurface \( \Sigma \). In particular, let \( \theta = K = h^{ij} K_{ij} \) be the expansion of the geodesic congruence orthogonal to \( \Sigma \), \( K_{ij} \) being the extrinsic curvature of \( \Sigma \). Then, for \( K < 0 \) at the point \( q \in \Sigma \), within a proper time \( \tau \leq 3/|K| \) a point \( p \) conjugate to \( \Sigma \) along the geodesic orthogonal to \( \Sigma \) exists, for a space-time \( (M, g_{ij}) \) satisfying \[2.1.6\]. As above, a time-like curve that locally maximizes the proper time between \( p \) and \( \Sigma \) has to be a geodesic orthogonal to \( \Sigma \).

---

\[1\] It is possible show that the congruence is orthogonal to the hypersurface if and only if \( \omega_{ij} = 0 \)

\[2\] In this case, a minus sign appears in the right-hand side of \[2.1.6\] due to the different signature of the metric.
2.6 Singularity Theorems

without conjugate point to \( \Sigma \).

The last step toward the singularity theorems is to prove the existence of maximum length curves in globally hyperbolic space-times. We recall that this is the case if they posses Cauchy surfaces in accordance with the determinism of classical Physics. Without entering in the details, in that case a curve \( \gamma \) for which \( \tau \) attains its maximum value exists, and a necessary condition is that \( \gamma \) be a geodesic without conjugate point.

2.6.3 Singularity Theorems

In the previous subsection we have summarized the necessary concepts to analyze the singularity theorems in some details, although we will discuss them without any proofs.

Let a space-time manifold be globally hyperbolic, with \( R_{ij} \xi^i \xi^j \geq 0 \) for all the time-like \( \xi^i \). Suppose that the trace \( K \) of the extrinsic curvature of a Cauchy surface everywhere satisfies \( K \leq C < 0 \), for a constant \( C \). Therefore, no past-directed time-like curves \( \lambda \) from \( \Sigma \) can have a length greater than \( 3/|C| \). In fact, if there were any, a maximum length curve would exist and would be a geodesic, thus contradicting the fact that no conjugate points exist between \( \Sigma \) and \( p \in \lambda \): therefore such curve cannot exist. In particular, all past-directed time-like geodesics are incomplete.

This theorem is valid in a cosmological context and expresses that, if the Universe is expanding everywhere at a certain instant of time, then it must have begun with a singular state at a finite time in the past.

It is also possible to show that the previous theorem remains valid also relaxing the hypothesis that the Universe is globally hyperbolic. The price to pay is the assumption that \( \Sigma \) be a compact manifold (dealing with a closed Universe) and especially that only one incomplete geodesic is predicted.

For the theorems proving null geodesic incompleteness in a gravitational collapse context, i.e. the existence of a singularity in a black hole space-time, we refer to the literature [407].

We conclude stating the most general theorem, which entirely eliminates the assumptions of a Universe expanding everywhere and the global hyperbolicity of the manifold \( (M, g_{ij}) \). On the other hand, we loose any information about the nature of one incomplete geodesic at least, since it does not distinguish between a time-like and a null geodesic.

The space-time is singular under the following hypotheses:

i) the condition \( R_{ij} v^i v^j \geq 0 \) holds for all time-like and null \( v^i \),

ii) no closed time-like curves exist and

iii) at least one of the following properties holds:

a) \( (M, g_{ij}) \) is a closed Universe,

b) \( (M, g_{ij}) \) possesses a trapped surface

\[ \text{c) there exists a point } p \in M \text{ such that the expansion } \theta \text{ of the future or past directed null geodesics emanating from it becomes negative along each geodesic in this congruence.} \]

\[ \text{\[3\]A trapped surface is a compact smooth space-like manifold } T, \text{ such that the expansion } \theta \text{ of either outgoing either ingoing future directed null geodesics is everywhere negative.} \]
In particular, our Universe must be singular. In fact, the conditions i)-ii) hold and $\theta$ for the past-directed null geodesics emanating from us at the present time becomes negative before the decoupling time, i.e. the time up to when the Universe is well described by the Friedmann-Robertson-Walker (FRW) model.

The occurrence of a space-time singularity undoubtedly represents a breakdown of the classical theory of gravity, i.e. the General Relativity. The removal of such singularities is a prerequisite for any fundamental theory, like the quantum theory of the gravitational field. Singularity theorems are very powerful instruments, although do not provide any information about the nature of the predicted singularity. Unfortunately, we do not have a general classification of singularities, i.e. many different types exist and the unbounded curvature is not the basic mechanism behind such theorems.

Let us conclude remarking how singularity theorems concern properties of differential geometry and topology. Einstein equations are used only with respect to the positive curvature case, being only used in the Raychaudhuri equation. Nevertheless, no general conditions for non-singular solutions are known, and therefore it is not possible to disregard the singularity in General Relativity.
3 Homogeneous Universes

In this Section we introduce the homogeneous cosmological models, in order to describe the dynamics of the Universe toward the cosmological singularity with a more realistic approach than the one offered by the homogeneous and isotropic Friedmann-Robertson-Walker one. We will summarize the derivation of the Bianchi classification, with particular attention to the dynamics of the Bianchi types II and VII, while we will dedicate the entire Section 4 to types VIII and IX, the so-called Mixmaster [54, 367, 368].

3.1 Homogeneous Spaces

The study of homogeneous models arises from breaking the hypothesis of space isotropy. We will focus in particular on space-times spatially homogeneous, without treating the non physical case of a space-time homogeneous manifold, i.e. where the metric is the same at all points of space and time, because it represents a Universe not expanding at all. We will follow in particular the description as in Refs. [505, 319, 446, 473].

When relaxing the space isotropy hypothesis we gain a significantly larger arbitrariness in the solution. In particular, the homogeneous and isotropic model possesses a single gravitational degree of freedom given by the scale factor leaving free only the curvature sign [310]. This larger class of solutions has still a finite number of degrees of freedom and very general properties characterize the dynamics during the evolution toward the initial singularity [54].

A spatially homogeneous space-time is defined as a manifold with a group of isometries, i.e. a group of transformations leaving invariant the metric $g$. The Killing vectors $\zeta$ are the corresponding infinitesimal generators, with vanishing Lie derivative $\mathcal{L}_\zeta g = 0$ and whose orbits are the space-like hypersurfaces which foliate the space-time. We will discuss in which sense the metric properties are the same in all space points under homogeneity.

3.1.1 Killing Vector Fields

The Lie algebras of Killing vector fields generate the groups of motions via infinitesimal displacements, yielding conserved quantities and allowing a classification of homogeneous spaces. Consider a group of transformations

$$x^\mu \to \tilde{x}^\mu = f^\mu (x, a) \quad (3.1.1)$$

on a space $M$ (eventually a manifold), where $\{a^\alpha\}_{\alpha = 1, \ldots, r}$ are $r$ independent variables which parametrize the group and let $a_0$ correspond to the identity

$$f^\mu (x, a_0) = x^\mu. \quad (3.1.2)$$
3 Homogeneous Universes

Take an infinitesimal transformation \(a_0 + \delta a\), i.e. one which is very close to the identity so that

\[ x^\mu \to \bar{x}^\mu = f^\mu (x, a_0 + \delta a) \approx f^\mu (x, a_0) + \left( \frac{\partial f^\mu}{\partial a^a} \right) (x, a_0) \delta a^a \]

\[ \equiv \xi_a^\mu (x) \]

i.e.

\[ x^\mu \to \bar{x}^\mu \approx x^\mu + \xi_a^\mu (x) \delta a^a = (1 + \delta a^a \xi_a^\mu ) x^\mu , \]

where the first-order differential operators \(\{ \xi_a \}\) are defined by \(\xi_a = \xi_a^\mu \frac{\partial}{\partial x^\mu}\) and correspond to the \(r\) vector fields with components \(\{ \xi_a^\mu \}\). These are the “generating vector fields” and when the group is a group of motions, they are called Killing vector fields, satisfying \(\mathcal{L}_{\xi^a} g = 0\), so that, under infinitesimal transformations (3.1.3) all points of the space \(M\) are translated by a distance \(\delta x^\mu = \delta a^a \xi_a^\mu \) in the coordinates \(\{ x^\mu \}\) and

\[ \bar{x}^\mu \approx (1 + \delta a^a \xi_a^\mu ) x^\mu \approx e^{\delta a^a \xi_a^\mu } x^\mu . \] (3.1.5)

In fact, the finite transformations of the group may be represented as

\[ \bar{x}^\mu \to \bar{x}^\mu = e^{\theta_a^a \xi^\mu_a} x^\mu \] (3.1.6)

where \(\{ \theta^a \}\) are \(r\) new parameters on the group.

These generators form a Lie algebra[146], i.e. a real \(r\)-dimensional vector space with basis \(\{ \xi_a \}\), which is closed under commutation, i.e. the commutators of the basis elements can be expressed as constant linear combinations of themselves

\[ [\xi_a, \xi_b] \equiv \xi_a \xi_b - \xi_b \xi_a = \pm C_{ab}^c \xi_c \] (3.1.7)

where \(C_{ab}^c\) are the structure constants of the Lie algebra ((+) refers to left-invariant groups, while (−) to right-invariant ones). Suppose \(\{ e_a \}\) is a basis of the Lie algebra \(g\) of a group \(G\)

\[ [e_a, e_b] = C_{ab}^c e_c \] (3.1.8)

and define

\[ \gamma_{ab} = C_{ad}^c C_{bc}^d = \gamma_{ba} \] (3.1.9)

which is symmetric by definition, providing a natural inner product on the Lie algebra

\[ \gamma_{ab} \equiv e_a \cdot e_b = \gamma (e_a, e_b) ; \]

(3.1.10)

when \(\det (\gamma_{ab}) \neq 0\), Eq. (3.1.10) is non-degenerate and the groups for which this is true are called semi-simple. The \(r\) vector fields \(\{ e_a \}\) may be used instead of the coordinate basis \(\{ \frac{\partial}{\partial x^a} \}\) as a basis in which to express an arbitrary vector field on \(G\). This basis is a frame.

3.1.2 Definition of Homogeneity

Suppose that the group acts on a manifold \(M\) as a group of transformations

\[ x^\mu \to f^\mu (x, a) \equiv f_a^\mu (x) \] (3.1.11)
and let us define the orbit of $x$

$$f_G(x) = \{ f_a(x) \mid a \in G \}$$  \hspace{1cm} (3.1.12)

as the set of all points that can be reached from $x$ under the group of transformations. Thus, the group of isotropy at $x$ is

$$G_x = \{ a \in G \mid f_a(x) = x \}$$  \hspace{1cm} (3.1.13)

i.e., it is the subgroup of $G$ which leaves $x$ fixed. Suppose $G_x = \{ a_0 \}$ and $f_G(x) = M$, i.e. every transformation of $G$ moves the point $x$, and every point in $M$ can be reached from $x$ by a unique transformation. Since $G|G_x = \{ aa_0 \mid a \in G \} = G$, $G$ is diffeomorphic to $M$ and one may identify the two spaces.

If $g$ is a metric on $M$ invariant under $G$, it corresponds to a left-invariant one on $G$, specified entirely by the inner products of the basis left-invariant vectors fields $e_a$. For three dimensions one obtains the family of spatially homogeneous space sections of the spatially homogeneous space-times.

Given a basis $\{e_a\}$ of the Lie algebra of a three dimensional Lie group $G$, with structure constants $C_{abc}^{\mu}$, the spatial metric at each moment of time is specified by the spatially constant inner products

$$e_a \cdot e_b = g_{ab}(t),$$  \hspace{1cm} (3.1.14)

which are six functions of time. The Einstein equations, as we will apply, become ordinary differential equations for these six functions, plus whatever functions of time are necessary to describe the matter of the Universe.

For both homogeneous and spatially homogeneous space-times, one needs only to consider a representative group from each equivalence class of isomorphic Lie groups of dimension four and three, respectively. In three dimensions the classification of inequivalent three-dimensional Lie groups is called the Bianchi classification [80] and determines the various symmetry types possible for homogeneous three spaces, just as $(k = +1, 0, -1)$ classify the possible symmetry types for homogeneous and isotropic three-spaces (FRW).

After obtaining all the three-dimensional Lie groups according to the Bianchi classification we will write down and discuss the corresponding Einstein equations.

### 3.1.3 Application to Cosmology

A homogeneous space-time is defined by space-like hypersurfaces $\Sigma$ such that for any points $p, q \in \Sigma$, there is a unique element $\tau \in G$ such that $\tau(p) = q$ (in this case the Lie group acts simply transitively on each $\Sigma$). Such uniqueness implies $\dim G = \dim \Sigma = 3$, and $G$ and $\Sigma$ can be identified (for example, in the simplest case of translations group we have $G = \mathbb{R}^3$); thus, the action of the isometries on $\Sigma$ is just the left multiplication on $G$ and tensor fields invariant under isometries are the left-invariant ones on $G$. In four dimensions one obtains the homogeneous space-times and the foliation of $M$ turns out to be $M = \mathbb{R} \times G$. In order to preserve metric properties at all points, let us consider the group of transformations of coordinates which transform the space into itself, leaving the
metric unchanged: if the line element before the transformation has the form

\[ dl^2 = h_{\alpha\beta} \left( x^1, x^2, x^3 \right) dx^\alpha dx^\beta , \]  

(3.1.15)

then it becomes

\[ dl^2 = h_{\alpha\beta} \left( x'^1, x'^2, x'^3 \right) dx'^\alpha dx'^\beta , \]  

(3.1.16)

where \( h_{\alpha\beta} \) has the same form in the new coordinates.

In the general case of a non Euclidean homogeneous three-dimensional space, there are three independent differential forms which are invariant under the transformations of the group of motions, however they do not represent the total differential of any function of the coordinates. We shall write them as \( \omega^a = e^a_\alpha dx^\alpha \). Hence the metric (3.1.16) is re-expressed as

\[ dl^2 = \eta_{ab} \left( e^a_\alpha dx^\alpha \right) \left( e^b_\beta dx^\beta \right) \]  

(3.1.17)

so that the metric tensor reads as

\[ h_{\alpha\beta} = \eta_{ab}(t)e^a_\alpha(x^\gamma)e^b_\beta(x^\gamma), \]  

(3.1.18)

where \( \eta_{ab} \) is a function of time only, symmetric in \( ab \) and in contravariant components we have

\[ h^{\alpha\beta} = \eta^{ab}(t)e^a_\alpha(x^\gamma)e^b_\beta(x^\gamma), \]  

(3.1.19)

where \( \eta^{ab} \) should be viewed as the components of the inverse matrix. All considerations developed in the previous Sections here apply straightforwardly.

The relationship between the covariant and contravariant expression for the three basis vectors is

\[ e_1 = \frac{1}{v} \left[ e^2 \wedge e^3 \right] , \quad e_2 = \frac{1}{v} \left[ e^3 \wedge e^1 \right] , \quad e_3 = \frac{1}{v} \left[ e^1 \wedge e^2 \right] , \]  

(3.1.20)

where \( e^a \) and \( e_\alpha \) are to be understood formally as Cartesian vectors with components \( e^a_\alpha \) and \( e^a_\alpha \), while \( v \) represents

\[ v = | e^a_\alpha | = e^1 \cdot [ e^2 \wedge e^3 ] . \]  

(3.1.21)

The determinant of the metric tensor (3.1.18) is given by \( \gamma = \eta v^2 \) where \( \eta \) is the determinant of the matrix \( \eta_{ab} \).

The invariance of the differential form (3.1.16) means that

\[ e^a_\alpha (x) dx^\alpha = e^a_\alpha (x') dx'^\alpha \]  

(3.1.22)

and \( e^a_\alpha \) on both sides of (3.1.22) are the same functions expressed in terms of the old and the new coordinates, respectively.

The algebra for the differential forms permits to rewrite (3.1.22) as

\[ \frac{\partial x'^\beta}{\partial x^\alpha} = e^a_\alpha (x') e^a_\alpha (x) . \]  

(3.1.23)

This is a system of differential equations which define the change of coordinates \( x'^\beta(x) \) in terms of given basis vectors.
Integrability over the system (3.1.23) is rewritten in terms of the Schwartz condition
\[
\frac{\partial^2 x'^\beta}{\partial x^a \partial x^\gamma} = \frac{\partial^2 x'^\beta}{\partial x^\gamma \partial x^a}
\]
which, explicitly, leads to
\[
\left[ \frac{\partial e^\beta_a (x')}{\partial x'^\alpha} e^\delta_b (x') - \frac{\partial e^\beta_b (x')}{\partial x'^\alpha} e^\delta_a (x') \right] e^\gamma_c (x) e^\delta_d (x) =
\]
\[
e^\beta_c (x') \left[ \frac{\partial e^\gamma_d (x)}{\partial x^\alpha} - \frac{\partial e^\gamma_d (x)}{\partial x^\gamma} \right].
\]
(3.1.25)

Multiplying both sides of (3.1.25) by \(e^\delta_a (x)e^\gamma_b (x)e^\beta_c (x')\) and differentiating, the left-hand side becomes
\[
e^\beta_c (x') \left[ \frac{\partial e^\gamma_d (x')}{\partial x'^\alpha} - \frac{\partial e^\gamma_d (x')}{\partial x'^\gamma} \right] =
\]
\[
= e^\gamma_c (x') \left[ \frac{\partial e^\beta_a (x)}{\partial x^\alpha} - \frac{\partial e^\beta_a (x)}{\partial x^\beta} \right]
\]
(3.1.26)

and the right-hand side gives the same expression but in terms of \(x\).

Since \(x\) and \(x'\) are arbitrary, both sides must be constant, and (3.1.26) reduces to
\[
\left( \frac{\partial e^\gamma_a}{\partial x^\beta} - \frac{\partial e^\beta_a}{\partial x^\gamma} \right) e^\delta_b e^\gamma_c = C^c_{ab},
\]
(3.1.27)

which gives the relations of the vectors with the group structure constants \(C^c_{ab}\). Multiplying (3.1.27) by \(e^\gamma_c\), we finally have
\[
e^\delta_a \frac{\partial e^\gamma_c}{\partial x^\beta} - e^\beta_b \frac{\partial e^\gamma_c}{\partial x^\beta} = C^c_{ab} e^\gamma_c.
\]
(3.1.28)

Similarly, such expression in the forms language is given by the left-invariant 1-form \(\omega^a\) satisfying the Maurer-Cartan equation
\[
d\omega^a = \frac{1}{2} C^c_{bc} \omega^b \wedge \omega^c.
\]
(3.1.29)

By construction, we have the antisymmetry property from (3.1.26) or (3.1.27)
\[
C^c_{ab} = -C^c_{ba}.
\]
(3.1.30)

Defining
\[
X_a = e^\alpha_a \frac{\partial}{\partial x^\alpha},
\]
(3.1.31)
equation (3.1.28) rewrites as
\[
[X_a, X_b] = C^c_{ab} X_c.
\]
(3.1.32)
3 Homogeneous Universes

Homogeneity is expressed as the Jacobi identity
\[
[[X_a, X_b], X_c] + [[X_b, X_c], X_a] + [[X_c, X_a], X_b] = 0 \tag{3.1.33}
\]
and explicitly
\[
C^f_{ab} C^d_{cf} + C^f_{bc} C^d_{af} + C^f_{ca} C^d_{bf} = 0. \tag{3.1.34}
\]
With this formalism, the Einstein equations for a homogeneous Universe can be written as a system of ordinary differential equations which involve only functions of time, provided all three-dimensional vectors and tensors are projected on the tetradic basis, while the explicit coordinate dependence of the basis vectors is not necessary for the equations ruling the dynamics. In fact, such choice is not unique as \( \epsilon_a = A_{bce} b \) yields again a set of basis vectors.

Introducing the two-index structure constants as \( C^c_{ab} = \epsilon^{cde} m^d_{ab} \), where \( \epsilon^{abc} = \epsilon^{abc} \) is the Levi-Civita tensor (\( \epsilon^{123} = +1 \)), the Jacobi identity \( \tag{3.1.34} \) becomes
\[
\epsilon_{bcd} C^c_{ab} C^d_{ba} = 0. \tag{3.1.35}
\]

The problem of classifying all homogeneous spaces reduces to finding all inequivalent sets of structure constants.

3.2 Bianchi Classification and Line Element

The list of all three-dimensional Lie algebras was first accomplished by Bianchi \([81]\) and each algebra uniquely determines the local proprieties of a three-dimensional group. If a space is homogeneous and its Lie group is the “Bianchi Type N” (N=I,...,IX), the subclassification of the Bianchi groups agrees with the one made by Ellis and MacCallum \([185, 446, 319]\).

Any structure constant can be written also as
\[
C^a_{bc} = \epsilon_{bcd} m^d_{ab} + \delta^c_{e} a^d_a - \delta^d_{e} a^c, \tag{3.2.1}
\]
where the matrix \( m^{ab} = m^{ba} \). The subclassification as class A and class B models refers to the cases \( a_c = 0 \) or \( a_c \neq 0 \), respectively.

The Jacobi identity \( \tag{3.1.34} \) written for the structure constants like in \( \tag{3.2.1} \) reduces to the condition
\[
m^{ab} a_b = 0. \tag{3.2.2}
\]
Without loss of generality, we can put \( a_c = (a, 0, 0) \) and the matrix \( m^{ab} \) can be described by its principal values \( n_1, n_2, n_3 \). The condition \( \tag{3.2.2} \) becomes nothing but \( an_1 = 0 \), i.e. either \( a \) or \( n_1 \) has to vanish. Condition \( \tag{3.1.35} \) rewrites explicitly as
\[
\begin{align*}
[X_1, X_2] &= -a X_2 + n_3 X_3 \\
[X_2, X_3] &= n_1 X_1 \\
[X_3, X_1] &= n_2 X_2 + a X_3
\end{align*}
\tag{3.2.3}
\]
where \( a \geq 0 \), \((n_1, n_2, n_3)\) can be rescaled to unity, and we finally get the Bianchi classification as in the Table \( \ref{table3.1} \).
Let us note that the Bianchi type I is isomorphic to the three-dimensional translation group $\mathbb{R}^3$, for which the flat FRW model is a particular case (once isotropy is restored) and analogously the Bianchi type V contains, as a particular case, the open FRW.

**Table 3.1:** Inequivalent structure constants corresponding to the Bianchi classification.

| 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  | $a$ | 0     | 1     | 1     |
| III ($a = 1$) | $a$ | 0     | 1     | -1 |
| VI ($a \neq 1$) | $a$ | 0     | 1     | -1 |

Not all anisotropic dynamics are compatible with a satisfactory Standard Cosmological Model but, as shown in the early Seventies, some can be represented, under suitable conditions, as a FRW model plus a gravitational waves packet [341, 225].

The interest in the Mixmaster [368, 367] relies on having invariant geometry under the $SO(3)$ group, shared with the closed FRW Universe. From a cosmological point of view, the relevance of this model arises also from the decomposition of the line element as

$$ds^2 = ds_0^2 - \delta_{(a)(b)} G^{(a)(b)}_{ik} dx^i dx^k$$  \hspace{1cm} (3.2.4)

where $ds_0$ denotes the line element of an isotropic Universe having positive constant curvature, $G^{(a)(b)}_{ik}$ is a set of spatial tensors and $\delta_{(a)(b)}(t)$ are amplitude functions, resulting small sufficiently far from the singularity. The tensors introduced in (3.2.4) satisfy the equations

$$G^{(a)(b);l}_{ik} = -(n^2 - 3) G^{(a)(b)}_{ik}, \quad G^{(a)(b)k}_{jk} = 0, \quad G^{(a)(b)i}_{i} = 0,$$  \hspace{1cm} (3.2.5)

in which the Laplacian is referred to the geometry of the sphere of unit radius.

Let us choose a basis of dual vector fields $\omega^a$, preserved under isometries. Therefore, recalling (3.1.19), the four-dimensional line element can be expressed as

$$ds^2 = N^2(t) dt^2 - \eta_{ab}(t) \omega^a \otimes \omega^b,$$  \hspace{1cm} (3.2.6)

parametrized by the proper time, where $\omega^a$ obey the Maurer-Cartan equations [31.29].

The explicit expression for the $\omega^a$ for Bianchi I, whose structure constants are $C^a_{bc} = 0$, is

$$\omega^1 = dx^1, \quad \omega^2 = dx^2, \quad \omega^3 = dx^3,$$  \hspace{1cm} (3.2.7)
while for Bianchi IX, being \( C_{bc}^d = \epsilon_{abc} \), will be specified in \((4.7.16b)\).

In order to distinguish between expansion (change of volume) and anisotropy (change of shape) it is useful to parametrize the metric on the spatial slices as

\[
\eta_{ab} = R_0^2 e^{2\alpha} \left( e^{2\beta} \right)_{ab}, \tag{3.2.8}
\]

where \( R_0 \) is the initial radius of the Universe and all the other parameters are functions of time only. The matrix \( \beta_{ab} \) satisfies the condition \( \text{Tr} \beta = 0 \), ensuring hypersurface three-volume dependance on the conformal factor \( \alpha \) only as \( V_{\text{Univ}} \sim R_0^3 e^{3\alpha} \).

For a review of works devoted to the study of the dynamics of Bianchi models in different cosmological paradigms see the collection of articles \[391, 421, 200, 441, 116, 348, 483, 445, 107, 313, 395, 396, 356, 137, 309, 207, 311, 192, 142, 260, 353, 184, 113, 488, 496, 454, 10, 13, 12\].

### 3.3 Field Equations

As we derived, the Einstein equations for a homogeneous Universe can be written in the form of a system of ordinary differential equations which involve functions of time only, once introduced the tetradic basis built as in the previous Section 2.3, whose projections in empty space take the form

\[
\begin{align*}
R_0^a &= -\frac{1}{2} \kappa_b^a - \frac{1}{4} \kappa_a^b \kappa_b^a, \tag{3.3.1a} \\
R_a^0 &= -\frac{1}{2} \kappa_b^c \left( C_{cb}^b - \delta_a^b C_{dc}^d \right), \tag{3.3.1b} \\
R_a^b &= -\frac{1}{2} \sqrt{\eta} \frac{\partial}{\partial t} \left( \sqrt{\eta} \kappa_b^b \right) - P_a^b, \tag{3.3.1c}
\end{align*}
\]

where the relations \( \kappa_{ab} = \dot{\eta}_{ab} \) and \( \kappa_a^b = \dot{\eta}_{ac} \eta^{cb} \) hold, the dot denotes differentiation with respect to \( t \), and the projection \( P_{ab} = \eta_{bc} P_a^c \) of the three-dimensional Ricci tensor becomes

\[
P_{ab} = -\frac{1}{2} \left( \epsilon^{cd} \epsilon_{da} C_{cd} + \epsilon^{cd} \epsilon_{da} C_{dc} - \frac{1}{2} \epsilon^{cd} \epsilon_{da} C_{cd} + \epsilon^{cd} \epsilon_{da} C_{db} + \epsilon^{cd} \epsilon_{da} C_{db} \right). \tag{3.3.2}
\]

The Einstein equations have reduced to a much simpler differential system, involving only ordinary derivatives with respect to the temporal variable \( t \).

In the following we will discuss the Kasner solution which will be generalized to the dynamics of Bianchi types VIII and IX.

### 3.4 Kasner Solution

The simplest and paradigmatic solution of the Einstein equations \(3.3.1a\)–\(3.3.1c\) in the framework of the Bianchi classification is the type I model, firstly obtained by Kasner\[289\] in 1921, which is appropriate to describe the gravitational field in empty space.

The simultaneous vanishing of the three structure constants and of the parameter \( a \) i-
plies the vanishing of the three-dimensional Ricci tensor as well
\[
e^{\alpha}_{\alpha} = \delta^{\alpha}_{\alpha}, \quad C^{\alpha}_{\alpha \beta} \equiv 0 \Rightarrow P_{ab} = 0. \tag{3.4.1}
\]
Furthermore, since the three-dimensional metric tensor does not depend on space coordinates, also \( R_{0\alpha} = 0 \), i.e. this model contains the standard Euclidean space as a particular case. Then the system \((3.3.1a)-(3.3.1c)\) describes a uniform space and reduces to
\[
\dot{\kappa}^{\alpha}_{\alpha} + \frac{1}{\sqrt{\eta}} \frac{\partial}{\partial t} \left( \sqrt{\eta} \kappa^{\beta}_{\alpha} \right) = 0. \tag{3.4.2b}
\]
From \((3.4.2b)\) we get the first integral
\[
\sqrt{\eta} \kappa^{\beta}_{\alpha} = 2 \lambda^{\beta}_{\alpha} = \text{const.}, \tag{3.4.3}
\]
and contraction of indices \( a \) and \( b \) leads to
\[
\kappa^{\alpha}_{\alpha} = \frac{\dot{\eta}}{\eta} = \frac{2}{\sqrt{\eta}} \lambda^{\alpha}_{\alpha}, \tag{3.4.4}
\]
and finally
\[
\eta = G t^2 \quad G = \text{const.}. \tag{3.4.5}
\]
Without loss of generality, a simple rescaling of the coordinates \( x^{\alpha} \) allows to put such a constant equal to unity, thus providing
\[
\lambda^{\alpha}_{\alpha} = 1. \tag{3.4.6}
\]
Substituting \((3.4.3)\) in \((3.4.2a)\) one obtains the relations among the constants \( \lambda^{\alpha}_{\alpha} \)
\[
\lambda^{\alpha}_{\alpha} \lambda^{\beta}_{\alpha} = 1, \tag{3.4.7}
\]
and lowering index \( b \) in \((3.4.3)\) one gets a system of ordinary differential equations with respect to \( \gamma_{ab} \)
\[
\dot{\gamma}_{ab} = \frac{2}{t} \lambda^{\alpha}_{\alpha} \eta_{cb}. \tag{3.4.8}
\]
The set of coefficients \( \lambda^{\alpha}_{\alpha} \) can be considered as the matrix of a certain linear transformation, reducible to its diagonal form. In such a case, denoting its eigenvalues as \( p_1, p_2, p_3 \) real and not equal to each other, and its eigenvectors as \( n^{(1)}, n^{(2)}, n^{(3)} \), the solution of \((3.4.8)\) writes as
\[
\eta_{ab} = t^{2p_1} n^{(1)}_{a} n^{(1)}_{b} + t^{2p_2} n^{(2)}_{a} n^{(2)}_{b} + t^{2p_3} n^{(3)}_{a} n^{(3)}_{b}. \tag{3.4.9}
\]
If we choose the frame of the eigenvectors (recall that \( e^{\alpha}_{\alpha} = \delta^{\alpha}_{\alpha} \)) and denote them with \( x^1, x^2, x^3 \), then the spatial line element reduces to
\[
dt^2 = t^{2p_1} (dx^1)^2 + t^{2p_2} (dx^2)^2 + t^{2p_3} (dx^3)^2. \tag{3.4.10}
\]
Here $p_1, p_2, p_3$ are the so-called Kasner indices, satisfying the relations

$$p_1 + p_2 + p_3 = p_1^2 + p_2^2 + p_3^2 = 1,$$  \(3.4.11\)

therefore only one of these numbers is independent. Except for the cases $(0,0,1)$ and $(-1/3,2/3,2/3)$, such indices are never equal, one of them being negative and two positive; in the peculiar case $p_1 = p_2 = 0, p_3 = 1$, the metric is reducible to a Galilean form by the transformation

$$t \sinh x^3 = \xi, \quad t \cosh x^3 = \tau,$$  \(3.4.12\)

i.e. with a fictitious singularity in a flat space-time.

Once that Kasner indices have been ordered according to

$$p_1 < p_2 < p_3,$$  \(3.4.13\)

their corresponding variation ranges are

$$-\frac{1}{3} \leq p_1 \leq 0, \quad 0 \leq p_2 \leq \frac{2}{3}, \quad \frac{2}{3} \leq p_3 \leq 1.$$  \(3.4.14\)

In parametric form we have the representation

$$p_1 (u) = \frac{-u}{1 + u + u^2}, \quad p_2 (u) = \frac{1 + u}{1 + u + u^2}, \quad p_3 (u) = \frac{u (1 + u)}{1 + u + u^2}$$  \(3.4.15\)

as the parameter $u$ varies in the range (see Fig.3.1)

$$1 \leq u < +\infty.$$  \(3.4.16\)

**Figure 3.1**: Evolution of Kasner indices in terms of the parameter $1/u$. The domain of $u$ is $[1, \infty)$; for lower values of $u$ the inversion property $3.4.17$ holds.

The values $u < 1$ lead to the same range following the inversion property

$$p_1 \left(\frac{1}{u}\right) = p_1 (u), \quad p_2 \left(\frac{1}{u}\right) = p_3 (u), \quad p_3 \left(\frac{1}{u}\right) = p_2 (u).$$  \(3.4.17\)
3.5 The role of matter

The line element from (3.4.9) describes an anisotropic space where all the volumes linearly grow with time, while linear distances grow along two directions and decrease along the third, differently from the Friedmann solution where all distances contract towards the singularity with the same behavior. This metric has only one non-eliminable singularity in $t = 0$ with the only exception of the case $p_1 = p_2 = 0, p_3 = 1$ mentioned above, corresponding to the standard Euclidean space.

For a discussion of the Bianchi I model in presence of several matter sources, see the following literature [390, 265, 451, 442, 121, 388, 2, 366, 210, 422, 127, 270, 30, 360, 364, 78, 232, 365, 388, 363, 463, 133, 423, 321, 126, 28, 490, 286, 123, 288, 352, 372, 193, 452, 414, 249, 136, 453, 119].

3.5 The role of matter

Here we discuss the time evolution of a uniform distribution of matter in the Bianchi type I space near the singularity; it will result that it behaves as a test fluid and thus it does not affect the properties of the solution.

Let us take a uniform distribution of matter and assume that we can neglect its influence on the gravitational field. The hydrodynamics equations describe the evolution [319] as

$$
\frac{1}{\sqrt{-g}} \frac{\partial}{\partial x^i} \left( \sqrt{-g} \sigma u^i \right) = 0 , \ (p + \epsilon) u^k \left( \frac{\partial u_i}{\partial x^k} - \frac{1}{2} u^l \frac{\partial g_{kl}}{\partial x^i} \right) = - \frac{\partial p}{\partial x^i} - u_i u^k \frac{\partial p}{\partial x^k} .
$$

(3.5.1)

Here $u^i$ is the four-velocity and $\sigma$ is the entropy density; in the neighbourhood of the singularity it is necessary to use the ultra-relativistic equation of state $p = \epsilon / 3$, and then we get $\sigma \sim \epsilon^{3/4}$.

As soon as all the quantities are functions of time, we have

$$
\frac{d}{dt} \left( abc u_0 \epsilon^{3/4} \right) = 0 , \quad 4 \epsilon \frac{du_a}{dt} + u_a \frac{d\epsilon}{dt} = 0 .
$$

(3.5.2)

From (3.5.2), we obtain the two integrals of motion

$$
abc u_0 \epsilon^{3/4} = \text{const.} , \quad u_a \epsilon^{1/4} = \text{const.} .
$$

(3.5.3)

From (3.5.3) we see that all the covariant components $u_a$ are of the same order. Among the contravariant ones, the greatest as $t \to 0$ is $u_3 = u_3$. Retaining only the dominant contribution in the identity $u_i u^i = 1$, we have $u_0^2 \approx u_3^2$ and, from (3.5.3),

$$
\epsilon \sim \frac{1}{ab^2} , \quad u_a \sim \sqrt{ab} ,
$$

(3.5.4)

or, equivalently, for the Kasner solution

$$
\epsilon \sim t^{-2(p_1 + p_2)} = t^{-2(1 - p_3)} , \quad u_a \sim t^{(1 - p_3)/2} .
$$

(3.5.5)

As expected, $\epsilon$ diverges as $t \to 0$ for all the values of $p_3$, except $p_3 = 1$ (this is due to the non-physical character of the singularity in this case).

The validity of the test fluid approximation is verified from a direct evaluation of the
components of the energy-momentum tensor $T^{k}_{l}$, whose dominant terms are

$$T^{0}_{0} \sim \epsilon u^{2}_{0} \sim t^{-(1+p_{3})}, \quad T^{1}_{1} \sim \epsilon \sim t^{-2(1-p_{3})},$$ (3.5.6a)

$$T^{2}_{2} \sim \epsilon u^{2} u^{2} \sim t^{-(1+2p_{2}-p_{3})}, \quad T^{3}_{3} \sim \epsilon u^{3} u^{3} \sim t^{-(1+p_{3})}.$$ (3.5.6b)

As $t \to 0$, all the components grow slower than $t^{-2}$, which is the behavior of the dominant terms in the Kasner analysis. Thus the fluid contribution can be disregarded in the Einstein equations.

This test character of a perfect fluid on a Kasner background remains valid even in the following Mixmaster scenario, both in the homogeneous as well as in the inhomogeneous case [54, 57]. The reason for the validity of such extension relies on the piece-wise Kasner behavior of the oscillatory regime. For a discussion on the effects of ultra-relativistic matter, of scalar and electromagnetic field on the quasi-isotropic solution, see [375, 378, 377].

### 3.6 The Dynamics of the Bianchi Models

The Kasner solution properly approximates those cases when the Ricci tensor appearing in the Einstein equations $P_{\alpha\beta}$ is of higher order in $1/t$ with respect to all other terms involved. However, since one of the Kasner exponents is negative, terms of order higher than $t^{-2}$ appear in the tensor $P_{\alpha\beta}$. In such a case the discussion of solutions has to be extended to the general anisotropic case, in the search of a general behaviour of the Universe towards the initial singularity. In fact, the outlined Kasner regime relies on a restriction over the phase space of the solution (not discussed here in the details, see [54], §3) which causes an instability with perturbations violating this condition.

A general solution, by definition,

- is completely stable, i.e. the effect of any perturbation is equivalent to a change of the initial conditions at some moment of time and
- must satisfy arbitrary initial conditions, i.e. the perturbation cannot change the form of the solution.

Nevertheless, the cited restriction over the Kasner solution makes it unstable with respect to perturbations destroying it: such perturbation promoting the transition to a new state cannot be considered small and lies outside the region of the infinitesimal ones.

Let us introduce three spatial vectors $e^{a} = l(x^{7}), m(x^{7}), n(x^{7})$ and take the matrix $h_{\alpha\beta}$ diagonal in the form

$$h_{\alpha\beta} = a^{2}(t)l_{\alpha} l_{\beta} + b^{2}(t)m_{\alpha} m_{\beta} + c^{2}(t)n_{\alpha} n_{\beta}.$$ (3.6.1)

Consequently, the Einstein equations in a synchronous reference system and for a generic
The dynamics of the Bianchi models

homogeneous cosmological model in empty space are given by the system

\[-R^l_i = \frac{(abc)'}{abc} + \frac{1}{2a^2b^2c^2} \left[ \lambda^2 a^4 - \left( \mu b^2 - \nu c^2 \right)^2 \right] = 0 \quad (3.6.2a)\]

\[-R^m_m = \frac{(abc)'}{abc} + \frac{1}{2a^2b^2c^2} \left[ \mu^2 b^4 - \left( \lambda a^2 - \nu c^2 \right)^2 \right] = 0 \quad (3.6.2b)\]

\[-R^n_or = \frac{(abc)'}{abc} + \frac{1}{2a^2b^2c^2} \left[ \nu^2 c^4 - \left( \lambda a^2 - \mu b^2 \right)^2 \right] = 0 \quad (3.6.2c)\]

and

\[-R^0_0 = \dddot{a} + \dddot{b} + \dddot{c} = 0 \quad (3.6.3)\]

where the other off-diagonal components of the four-dimensional Ricci tensor identically vanish as a consequence of the choice of the diagonal form as in (3.6.1). Eventually, the \(0\alpha\) components of the Einstein equations can be non-zero if some kind of matter is present, leading to an effect of rotation on the Kasner axes[54]. The constants \(\lambda, \mu, \nu\) correspond to the structure constants \(C_{11}, C_{22}, C_{33}\) respectively, introduced earlier in Section 3.1.3. In particular, we will study in details the cases of \((\lambda, \mu, \nu)\) for Bianchi type II (1, 0, 0), VII (1, 1, 0), VIII (1, 1, -1) and IX (1, 1, 1).

All these equations are exact and contain functions of time only, without any restriction regarding the vicinity to the singular point \(t = 0\). Through the notation

\[\alpha = \ln a, \quad \beta = \ln b, \quad \gamma = \ln c \quad (3.6.4)\]

and the new temporal variable \(\tau\) defined by

\[dt = abc \, d\tau, \quad (3.6.5)\]

Eqs. (3.6.2) and (3.6.3) simplify to

\[2\alpha_{\tau\tau} = \left( \mu b^2 - \nu c^2 \right)^2 - \lambda^2 a^4 \quad (3.6.6a)\]

\[2\beta_{\tau\tau} = \left( \lambda a^2 - \nu c^2 \right)^2 - \mu^2 b^4 \quad (3.6.6b)\]

\[2\gamma_{\tau\tau} = \left( \lambda a^2 - \mu b^2 \right)^2 - \nu^2 c^4, \quad (3.6.6c)\]

\[\frac{1}{2} \left( \alpha + \beta + \gamma \right)_{\tau\tau} = \alpha_{\tau} \beta_{\tau} + \alpha_{\tau} \gamma_{\tau} + \beta_{\tau} \gamma_{\tau}, \quad (3.6.7)\]

where subscript \(\tau\) denotes the derivative with respect to \(\tau\). Manipulating the system (3.6.6) and using (3.6.7), one obtains the first integral

\[\alpha_{\tau} \beta_{\tau} + \alpha_{\tau} \gamma_{\tau} + \beta_{\tau} \gamma_{\tau} = \frac{1}{4} \left( \lambda^2 a^4 + \mu^2 b^4 + \nu^2 c^4 - 2\lambda \mu a^2 b^2 - 2\lambda \nu a^2 c^2 - 2\mu \nu b^2 c^2 \right) \quad (3.6.8)\]

involving first derivatives only. The Kasner regime (3.4.10) discussed before is the solution of equations (3.6.6) corresponding to neglecting all terms on the right-hand side. However, such a situation cannot persist indefinitely as \(t \to 0\) since there are always some terms on the right-hand side of (3.6.6) which are increasing.
3.7 Application to Bianchi Types II and VII

In this paragraph, the dynamics of the types II and VII is discussed in some detail: these spaces, in fact, present some features in common with the Mixmaster model, as it will be clear in the Sections 4.1-4.2.

3.7.1 Bianchi type II

Introducing the structure constants for the type II model, the system (3.6.2) reduces to

\[ \frac{\dot{a}bc}{abc} = -\frac{a^2}{2b^2c^2}, \quad (3.7.1a) \]
\[ \frac{\dot{abc}}{abc} = \frac{a^2}{2b^2c^2}, \quad (3.7.1b) \]
\[ \frac{\dot{ab}c}{abc} = \frac{a^2}{2b^2c^2}, \quad (3.7.1c) \]
\[ \frac{\ddot{a}}{a} + \frac{\dot{b}}{b} + \frac{\dot{c}}{c} = 0. \quad (3.7.2) \]

In (3.7.1) the right-hand sides play the role of a perturbation to the Kasner regime; if at a certain instant of time \( t \) they could be neglected, then a Kasner dynamics would take place. This kind of evolution can be stable or not depending on the initial conditions; as shown earlier in Section 3.4, the Kasner dynamics has a time evolution which differs along the three directions, growing along two of them and decreasing along the other. For example, for a perturbation growing as \( a^4 \sim t^{p_a} \), toward the singularity, two scenarios are possible: if the perturbation is associated with one of the two positive indices, it will continue decreasing till the singularity and the Kasner epoch is stable; on the other hand, if \( p_a < 0 \), the perturbation grows and cannot be indefinitely neglected. In this case, the analysis of the full dynamical system is required, and this can be achieved with the logarithmic variables (3.6.4)-(3.6.5) and the system (3.6.6) becomes

\[ \alpha_{\tau\tau} = -\frac{1}{2} e^{4\alpha}, \quad (3.7.3a) \]
\[ \beta_{\tau\tau} = \gamma_{\tau\tau} = \frac{1}{2} e^{4\alpha}. \quad (3.7.3b) \]

The equation (3.7.3a) can be thought as the motion of a one-dimensional point-particle moving in an exponential potential: if the initial “velocity” \( da/d\tau \) is equal to \( p_a \), then the potential will slow down, stop and accelerate again the point up to a new “velocity” \( -p_a \). From there on, the potential will remain negligible forever. Furthermore, the second set of equations (3.7.3b) implies that the conditions

\[ \alpha_{\tau\tau} + \beta_{\tau\tau} = \alpha_{\tau\tau} + \gamma_{\tau\tau} = 0 \quad (3.7.4) \]
3.7 Application to Bianchi Types II and VII

hold. Considering the explicit solutions of (3.7.4)

\[ \alpha(\tau) = \frac{1}{2} \ln (c_1 \text{sech} (\tau c_1 + c_2)) \]  
\[ \beta(\tau) = c_3 + \tau c_4 - \frac{1}{2} \ln (c_1 \text{sech} (\tau c_1 + c_2)) \]  
\[ \gamma(\tau) = c_5 + \tau c_6 - \frac{1}{2} \ln (c_1 \text{sech} (\tau c_1 + c_2)) , \]

where \( c_1 \ldots , c_6 \) are integration constants and we see how this dynamical scheme describes two connected Kasner epochs, where the perturbation has the role of changing the values of the Kasner indices. Let us assume that the Universe is initially described by a Kasner epoch for \( \tau \to \infty \), with indices orderd as \( p_l < p_m < p_n \); the perturbation starts growing and the point bounces against the potential and a new Kasner epoch begins, where the old and the new indices (the primed ones) are related among them by the so-called BKL map [54]

\[ p'_l = \frac{|p_l|}{1 - 2|p_l|} , \quad p'_m = -\frac{1}{2} \frac{|p_l| - p_m}{1 - 2|p_l|} , \quad p'_n = \frac{p_n - 2|p_l|}{1 - 2|p_l|} . \]  

(3.7.6)

In this new era, the negative power is no longer related to the \( l \)-direction so that the previously increasing perturbation is damped and eventually vanishes toward the singularity. We will see how (3.7.6) will be valid in general.

For a detailed analysis on the main results concerning the Bianchi II model see the following literature [58, 48, 329, 338, 118, 437, 394, 322, 254, 138].

3.7.2 Bianchi type VII

The analysis of Bianchi type VII can be performed analogously, leading to the Einstein equations

\[ \frac{(\dot{a}bc)}{abc} = -\frac{a^4 + b^4}{2a^2b^2c^2} , \]  
\[ \frac{(\dot{a}bc)}{abc} = -\frac{a^4 - b^4}{2a^2b^2c^2} , \]  
\[ \frac{(\dot{a}bc)}{abc} = -\frac{(a^2 - b^2)^2}{2b^2c^2} , \]

and the constraint (3.7.2) holding unchanged. Comparison of (3.7.7a) with (3.7.1) allows a similar qualitative analysis: if the right-hand sides of (3.7.7a) are negligible at a certain instant of time, than the solution is Kasner-like and can be stable or unstable depending on initial conditions. If the negative index is associated with the \( n \) direction, than the perturbative terms \( a^4 \) and \( b^4 \), evolving as \( t^{4p_l} \) and \( t^{4p_m} \), decrease up to the singularity and the Kasner solution turns out to be stable; in all other cases, one and only one of the perturbation terms starts growing, blasting the initial Kasner evolution and ending as before in a new Kasner epoch.

The main difference between the types II and VII is that many other transitions can occur after the first one and this can happen, for example, if the new negative Kasner index is associated with the \( m \) direction, i.e. with \( b \). In this case, the \( b^4 \) term would start growing.
and a new transition would occur with the same law (3.7.6). The problem of understanding if, when and how this mechanism can break up is unraveled considering the BKL map written in terms of the parameter $u$, i.e.

$$
\begin{align*}
\{ p_l &= p_1(u), \\
\quad p_m &= p_2(u), \\
\quad p_n &= p_3(u) \} \Rightarrow \\
\{ p'_l &= p_2(u - 1), \\
\quad p'_m &= p_1(u - 1), \\
\quad p'_n &= p_3(u - 1) \}
\end{align*}
$$

(3.7.8)

In this representation and from the properties (3.4.15) and (3.4.17) we see how the exact number of exchanges among the $l$- and $m$-directions equates the integer part $K$ of the initial value $u_0$ describing the dynamics. In fact, for the first $K_0$ times, the negative index is exchanged among $l$ and $m$, then it passes to the $n$ direction, a new and final (toward the singularity) Kasner epoch begins, and no more oscillations take place. The collection of the total of $K$ epochs is called a Kasner era: in this sense we can say that in the general case the type VII dynamics is composed by one era and a final epoch.

For additional informations about the Bianchi VII model (as well as some interesting features regarding the Bianchi VI Universes) see the articles [427, 420, 440, 68, 504, 38, 282, 283, 359, 98, 11].
4 Chaotic Dynamics of the Bianchi Types VIII and IX Models

In this Section we provide the detailed construction of the oscillatory-like regime of the Mixmaster model while approaching the initial singularity both in the field equations formalism and in the ADM one. A relevant part is centered around the chaotic properties of its dynamics. The cosmological implementation is also discussed, and in the last three Sections the effects on chaos of matter fields and of the number of space dimensions is reviewed.

4.1 Construction of the solution

At this point we are going to address the solution of the system of equations (3.6.2) for the cases of Bianchi types VIII and IX cosmological models, following the standard approach of Belinsky, Khalatnikov and Lifshitz (BKL) \[54, 57\]. Although the detailed discussion is devoted to the Bianchi IX model, it can be straightforwardly extended to the type VIII. Explicitely, the Einstein equations (3.6.2) reduce to

\[
\begin{align*}
2\alpha_{\tau\tau} &= (b^2 - c^2)^2 - a^4 \\
2\beta_{\tau\tau} &= (a^2 - c^2)^2 - b^4 \\
2\gamma_{\tau\tau} &= (a^2 - b^2)^2 - c^4,
\end{align*}
\]

(4.1.1) together with the constraint (3.6.7) unchanged, leading to the consequent constant of motion

\[
\alpha_{\tau\tau} + \alpha_{\tau\gamma_{\tau\tau}} + \beta_{\tau\gamma_{\tau\tau}} = \frac{1}{4} \left( a^4 + b^4 + c^4 - 2a^2b^2 - 2a^2c^2 - 2b^2c^2 \right). \tag{4.1.2}
\]

Let us therefore consider again the case in which, for instance, the negative power of the \(p_i\)'s exponents corresponds to the function \(a(t)\) (that is to say \(p_1 = p_1\)): the perturbation of the Kasner regime results from the terms \(\lambda^2 a^4\) (remember that \(\lambda = 1\) for both models) while the other terms decrease with decreasing \(t\), in fact

\[
p_1 < 0 \rightarrow p_1 = -|p_1|, \quad \begin{cases} \alpha \sim -|p_1| \ln t \\ a \sim \frac{1}{t|p_1|} \end{cases} \quad \text{for } t \to 0 \tag{4.1.3}
\]
and along the other directions
\[ p_2 > 0 \rightarrow p_2 = |p_2|, \quad \beta \sim |p_2| \ln t \downarrow, \quad \text{for } t \to 0. \quad (4.1.4) \]

Preserving only the increasing terms on the right-hand side of equations (3.6.6), we obtain a system identical to (3.7.3a), whose solution describes the evolution of the metric from its initial state (3.4.10). Let us fix, for instance,
\[ p_l = p_1, \quad p_m = p_2, \quad p_n = p_3, \quad (4.1.5) \]

so that
\[ a \sim t^{p_1}, \quad b \sim t^{p_2}, \quad c \sim t^{p_3}, \quad (4.1.6) \]

and then
\[ abc = \Lambda t \]
\[ \tau = \frac{1}{\Lambda} \ln t + \text{const.} \quad (4.1.7) \]

where \( \Lambda \) is a constant, so that the initial conditions for (3.7.3a) can be formulated as
\[ \alpha_\tau = \Lambda p_1, \quad \beta_\tau = \Lambda p_2, \quad \gamma_\tau = \Lambda p_3, \quad (4.1.8) \]

for \( \tau \to \infty \).

The system (3.7.3a) with (4.1.8) is integrated to
\[ a^2 = \frac{2 | p_1 | \Lambda}{\cosh (2 | p_1 | \Lambda \tau)} \quad (4.1.9a) \]
\[ b^2 = b_0^2 \exp [2\Lambda (p_2 - |p_1|) \tau] \cosh (2 | p_1 | \Lambda \tau) \quad (4.1.9b) \]
\[ c^2 = c_0^2 \exp [2\Lambda (p_3 - |p_1|) \tau] \cosh (2 | p_1 | \Lambda \tau) \quad (4.1.9c) \]

where \( b_0 \) and \( c_0 \) are integration constants.

### 4.2 The BKL oscillatory approach

Let us consider the solutions (4.1.9) in the limit \( \tau \to \infty \): towards the singularity they simplify to
\[ a \sim \exp [-\Lambda p_1 \tau] \quad (4.2.1a) \]
\[ b \sim \exp [\Lambda (p_2 + 2p_1) \tau] \quad (4.2.1b) \]
\[ c \sim \exp [\Lambda (p_3 + 2p_1) \tau] \quad (4.2.1c) \]
\[ t \sim \exp [\Lambda (1 + 2p_1) \tau] \quad (4.2.1d) \]

that is to say, in terms of \( t \),
\[ a \sim t^{p_1}, \quad b \sim t^{p_2}, \quad c \sim t^{p_3}, \quad abc = \Lambda t, \quad (4.2.2) \]
where the primed exponents are related to the un-primed ones by

\[ p'_l = \frac{|p_1|}{1 - 2|p_1|}, \quad p'_m = -\frac{2|p_1|-|p_2|}{1 - 2|p_1|}, \quad (4.2.3a) \]

\[ p'_n = \frac{p_3 - 2|p_1|}{1 - 2|p_1|}, \quad \Lambda' = (1 - 2|p_1|)\Lambda, \quad (4.2.3b) \]

which, we note, is very similar to what found in the type II case with relations (3.7.6) plus the additional expression involving \( \Lambda \). Summarizing these results, we see the effect of the perturbation over the Kasner regime: a Kasner epoch is replaced by another one so that the negative power of \( t \) is transferred from the \( l \) to the \( m \) direction, i.e. if in the original solution \( p_l \) is negative, in the new solution \( p'_m < 0 \). The previously increasing perturbation \( \lambda^2 a^4 \) in (3.6.2) is damped and eventually vanishes. The other terms involving \( \mu^2 \) instead of \( \lambda^2 \) will grow, therefore permitting the replacement of a Kasner epoch by another. Such rules of rotation in the perturbing property can be summarized with the rules (3.7.8) of the BKL map, with the greater of the two positive powers remaining positive[55].

The following interchanges are characterized by a sequence of bounces, with a change of the negative power between the directions \( l \) and \( m \) continuing as long as the integral part of the initial value of \( u \) is not exhausted, i.e. until \( u \) becomes less than one. In terms of the parameter \( u \), the map (3.7.6) takes the form

\[ u' = u - 1 \quad \text{for} \quad u > 2, \quad u' = \frac{1}{u - 1} \quad \text{for} \quad u \leq 2. \quad (4.2.4) \]

At that point, according to (3.4.17), the value \( u < 1 \) is turned into \( u > 1 \), thus either the exponent \( p_l \) or \( p_m \) is negative and \( p_n \) becomes the smaller one of the two positive numbers, say \( p_n = p_2 \). The next sequence of changes will bounce the negative power between the directions \( n \) and \( l \) or \( n \) and \( m \).

The phenomenon of increasing and decreasing of the various terms with transition from a Kasner era to another is repeated infinitely many times up to the singularity. Let us analyze the implications of the BKL map (3.7.8) and of the property (3.4.17).

If we write \( u = k + x \) as the initial value of the parameter \( u \), with \( k \) and \( x \) being its integral and fractional part, respectively, the continuous exchange of shrinking and enlarging directions (3.7.8) proceeds until \( u < 1 \), i.e. it lasts for \( k^0 \) epochs, thus leading a Kasner era to an end. The new value of \( u \) is \( u' = 1/x > 1 \) (3.4.17) and the subsequent set of exchanges will be \( l-n \) or \( m-n \): for arbitrary initial values of \( u \), the process will last forever and an infinite sequence of Kasner eras takes place.

For an arbitrary, irrational initial value of \( u \) the changes (3.7.8) repeat indefinitely. In the case of an exact solution, the exponents \( p_l, p_m \) and \( p_n \) loose their literal meaning, thus in general, it has no sense to consider any well defined, for example rational, value of \( u \).

The evolution of the model towards the singularity consists of successive periods, the eras, in which distances along two axes oscillate and along the third axis decrease monotonically while the volume decreases following a law approximately \( \sim t \). The order in which the pairs of axes are interchanged and the order in which eras of different lengths (number of Kasner epochs contained in it) follow each other acquire a stochastic character. Successive eras ‘condense’ towards the singularity. Such general qualitative properties are not changed in the case of space filled in with matter, however the meaning of the solution would change: the model so far discussed would be considered as the principal
terms of the limiting form of the metric as $t \to 0$.

### 4.3 Stochastic properties and the Gaussian distribution

A decreasing sequence of values of the parameter $u$ corresponds to every $s$-th era there. This sequence, from the starting era has the form $u_{\text{max}}^{(s)}, u_{\text{max}}^{(s)} - 1, u_{\text{max}}^{(s)} - 2, \ldots, u_{\text{min}}^{(s)}$. We can introduce the notation

$$u^{(s)} = k^{(s)} + x^{(s)}$$  \hspace{1cm} (4.3.1)\]

then

$$u_{\text{min}}^{(s)} = x^{(s)} < 1, \quad u_{\text{max}}^{(s)} = k^{(s)} + x^{(s)}$$  \hspace{1cm} (4.3.2)\]

where $u_{\text{max}}^{(s)}$ is the greatest value of $u$ for an assigned era and $k^{(s)} = \left[u_{\text{max}}^{(s)}\right]$ (square brackets denote the greatest integer less or equal to $u_{\text{max}}^{(s)}$). The number $k^{(s)}$ denotes the era length, i.e. the number of Kasner epochs contained in it. For the next era we obtain

$$u_{\text{max}}^{(s+1)} = \frac{1}{x^{(s)}}, \quad k^{(s+1)} = \left[\frac{1}{x^{(s)}}\right].$$  \hspace{1cm} (4.3.3)\]

For large $u$, the Kasner exponents approach the values $(0, 0, 1)$ with the limiting form

$$p_1 \approx -\frac{1}{u}, \quad p_2 \approx \frac{1}{u}, \quad p_3 \approx 1 - \frac{1}{u^2},$$  \hspace{1cm} (4.3.4)\]

and the transition to the next era is governed by the fact that not all terms in the Einstein equations are negligible and some terms are comparable: in such a case, the transition is accompanied by a long regime of small oscillations[54] lasting until the next era, whose details will be discussed in Section 4.4 after which a new series of Kasner epochs begins.

The probability $\lambda$ of all possible values of $x^{(0)}$ which lead to a dynamical evolution towards this specific case is strongly converging to a number $\lambda \ll 1$[326]. If the initial value of $x^{(0)}$ is outside this special interval for $\lambda$, the special case cannot occur; if $x^{(0)}$ lies in this interval, a peculiar evolution in small oscillations take place, but after this period the model begins to regularly evolve with a new initial value $x^{(0)}$, which can only accidentally fall in this peculiar interval (with probability $\lambda$). The repetition of this situation can lead to these cases only with probabilities $\lambda, \lambda^2, \ldots$, which asymptotically approach zero.

If the sequence begins with $k^{(0)} + x^{(0)}$, the lengths $k^{(1)}, k^{(2)}, \ldots$ are the numbers appearing in the expansion for $x^{(0)}$ in terms of the continuous fraction

$$x^{(0)} = \frac{1}{k^{(1)} + \frac{1}{k^{(2)} + \frac{1}{k^{(3)} + \ldots}}},$$  \hspace{1cm} (4.3.5)\]

which is finite if related to a rational number, but in general it is an infinite one [287].

For the infinite sequence of positive numbers $u$ ordered as (4.3.3) and, admitting the expansion (4.3.5), it is possible to note that

i) a rational number would have a finite expansion;
ii) periodic expansion represents quadratic irrational numbers (i.e. numbers which are roots of quadratic equations with integral coefficients)

iii) irrational numbers have infinite expansion.

All terms $k^{(1)}, k^{(2)}, k^{(3)}, \ldots$ in the first two cases having the exceptional property to be bounded in magnitude are related to a set of numbers $x^{(0)} < 1$ of zero measure in the interval $(0, 1)$.

An alternative to the numerical approach in terms of continuous fractions is the statistic distribution of the eras’ sequence for the numbers $x^{(0)}$ over the interval $(0, 1)$, governed by some probability law. For the series $x^{(s)}$ with increasing $s$ these distributions tend to a stationary one $w(x)$, independent of $s$, in which the initial conditions are completely forgotten

$$w(x) = \frac{1}{(1 + x) \ln 2}.$$  \hspace{1cm} (4.3.6)

In fact, instead of a well defined initial value as in (4.3.1) with $s = 0$, let us consider a probability distribution for $x^{(0)}$ over the interval $(0, 1)$, $W_0(x)$ for $x^{(0)} = x$. Then also the numbers $x^{(s)}$ are distributed with some probability. Let $w_s(x)dx$ be the probability that the last term in the $s$-th series $x^{(s)} = x$ lies in the interval $dx$. The last term of the previous series must lie in the interval between $1/(k + 1)$ and $1/k$, in order for the length of the $s$-th series to be $k$.

The probability for the series to have length $k$ is given by

$$W_s(k) = \int_{1/(k + 1)}^{1/k} w_{s-1}(x)dx.$$  \hspace{1cm} (4.3.7)

For each pair of subsequent series, we get the recurrent formula relating the distribution $w_{s+1}(x)$ to $w_s(x)$

$$w_{s+1}(x)dx = \sum_{k=1}^{\infty} w_s \left( \frac{1}{k + x} \right) \left| \frac{d}{dx} \left( \frac{1}{k + x} \right) \right| dx,$$  \hspace{1cm} (4.3.8)

or, simplifying the differential interval,

$$w_{s+1}(x) = \sum_{k=1}^{\infty} \frac{1}{(k + x)^2} w_s \left( \frac{1}{k + x} \right).$$  \hspace{1cm} (4.3.9)

If for increasing $n$ the $w_{s+n}$ distribution (4.3.9) tends to a stationary one, independent of $s$, $w(x)$ has to satisfy

$$w(x) = \sum_{k=1}^{\infty} \frac{1}{(k + x)^2} w \left( \frac{1}{k + x} \right).$$  \hspace{1cm} (4.3.10)

A normalized solution to (4.3.10) is clearly given by (4.3.6) [54]; substituting it in (4.3.7) and evaluating the integral

$$W(k) = \int_{1/(k + 1)}^{1/k} w(x)dx = \frac{1}{\ln 2} \ln (k + 1)^2,$$  \hspace{1cm} (4.3.11)

we get the corresponding stationary distribution of the lengths of the series $k$. Finally, since $k$ and $x$ are not independent, they must admit a stationary joint probability distri-
4 Chaotic Dynamics of the Bianchi Types VIII and IX Models

Distribution

\[ w(k, x) = \frac{1}{(k + x)(k + x + 1) \ln 2} \]  

(4.3.12)

which, for \( u = k + x \), rewrites as

\[ w(u) = \frac{1}{u(u + 1) \ln 2}, \]  

(4.3.13)

i.e. a stationary distribution for the parameter \( u \).

The existence of the Gauss map was firstly demonstrated in the work of Belinskii, Khalatnikov and Lifshitz [54], showing how a statistical approach [295] describes the time evolution of the cosmological models near the singularity. These features opened the way to further investigations (see, for example [32]), in view also of the peculiar properties of the discrete map \( w \) leading to final form for a measure of the full degrees of freedom of the discrete Mixmaster dynamics expressed as a not separable function [31], and such map

- has positive metric- and topologic-entropy;
- has the weak Bernoulli properties (i.e., the map cannot be finitely approximated);
- is strongly mixing and ergodic [385].

Thus, we see that the approach to the initial singularity is characterized by an infinite series of Kasner epochs described by the stochastic properties of the associated map.

For a discussion of the chaotic behavior inherent the homogeneous early cosmologies, see [107, 236, 103, 443, 197, 65, 256, 477, 147, 171, 66, 429, 155, 134, 320, 159, 68, 475, 175, 120, 476, 157, 4, 350, 153, 356, 180, 125, 194, 284, 468].

4.4 Small Oscillations

Let us investigate a particular case of the general (homogeneous) solution constructed above. We analyze an era during which two of the three functions \( a, b, c \) (for example \( a \) and \( b \)) oscillate so that their absolute values remain close to each other and the third function (in such case \( c \)) monotonically decreases, so that \( c \) can be neglected with respect to \( a \) and \( b \). As before, we will discuss only the Bianchi IX model, since for the Bianchi VIII case the argumentations and results are qualitatively the same [54, 57]. Let us consider the equations we can obtain from (3.6.6) and (3.6.8)

\[ \alpha_{\tau\tau} + \beta_{\tau\tau} = 0, \]  

(4.4.1a)

\[ \alpha_{\tau\tau} - \beta_{\tau\tau} = e^{4\beta} - e^{4\alpha}, \]  

(4.4.1b)

\[ \gamma_{\tau}(\alpha_{\tau} + \beta_{\tau}) = -\alpha_{\tau}\beta_{\tau} + \frac{1}{4}(e^{2\alpha} - e^{2\beta})^2. \]  

(4.4.1c)

The solution of (4.4.1a) is

\[ \alpha + \beta = \frac{2n_{0}^{2}}{c_{0}}(\tau - \tau_{0}) + 2 \ln(a_{0}), \]  

(4.4.2)
where \( a_0 \) and \( \xi_0 \) are positive constants. For what follows we conveniently replace the time coordinate \( \tau \) with the new one \( \xi \) defined as

\[
\xi = \xi_0 \exp \left( \frac{2a_0^2}{\xi_0}(\tau - \tau_0) \right)
\]

in terms of which the equations (4.4.1b) and (4.4.1c) rewrite as

\[
\chi \xi \xi + \frac{1}{8} \xi \chi \xi + \frac{1}{2} \sinh(2\chi) = 0,
\]

\[
\gamma \xi = -\frac{1}{4\xi} + \frac{\xi}{8} \left( 2\chi^2 + \cosh(2\chi) - 1 \right),
\]

where we have introduced the notation \( \chi = \alpha - \beta \) and \( A_\xi \equiv dA/d\xi \). Since \( \tau \) is defined in the interval \([\tau_0, -\infty)\), from equation (4.4.3) we note that \( \xi \in [\xi_0, 0) \). Since a general analytic solution of the system (4.4.4) is not available, we shall consider the two limiting cases \( \xi \gg 1 \) and \( \xi \ll 1 \) only.

Let us start with the \( \xi \gg 1 \) region. In this approximation the solution of equation (4.4.4a) reads as

\[
\chi = \frac{2A}{\sqrt{\xi}} \sin(\xi - \xi_0),
\]

\( A \) being a constant and therefore obtaining \( \gamma \sim A^2(\xi - \xi_0) \). As we can see, the name “small oscillations” arises from the behavior of the function \( \chi \). The functions \( a \) and \( b \), i.e. the expressions for the scale factors, are straightforwardly obtained as

\[
a, b = a_0 \sqrt{\frac{\xi}{\xi_0}} \left( 1 \pm \frac{A}{\sqrt{\xi}} \sin(\xi - \xi_0) \right),
\]

\[
c = c_0 \exp \left[ -A^2(\xi_0 - \xi) \right].
\]

The synchronous time coordinate \( t \) can be re-obtained back from the relation \( dt = abc \, d\tau \) as

\[
t = t_0 \exp \left[ -A^2(\xi_0 - \xi) \right].
\]

Of course, these solutions only apply when the condition \( c_0 \ll a_0 \) is satisfied.

Let us discuss the region where \( \xi \ll 1 \). In such a limit, the function \( \chi \) reads as

\[
\chi = K \ln \xi + \theta, \quad \theta = \text{const.}
\]

where \( K \) is a constant which, for consistency, is constrained in the interval \( K \in (-1, 1) \). We can therefore derive all other related quantities, and in particular

\[
a \sim \xi^{(1+K)/2}, \quad b \sim \xi^{(1-K)/2}, \quad c \sim \xi^{-1-K^2}/4, \quad t \sim \xi^{(3+K^2)/2}.
\]

This is again a Kasner solution, with the negative power of \( t \) corresponding to \( c \) and the evolution is the same as the general one. Moreover, we can easily note how, for such a
Kasner epoch, the parameter \( u \) (introduced in (3.4.15)) becomes

\[
\begin{align*}
\text{for } K > 0 : & \quad u = \frac{1 + K}{1 - K}, \\
\text{for } K < 0 : & \quad u = \frac{1 - K}{1 + K}.
\end{align*}
\]

(4.4.10)

Summarizing, the system initially crosses a long time interval during which the functions \( a \) and \( b \) satisfy \((a - b)/a < 1/\xi\) and perform small oscillations of constant period \( \Delta \xi = 2\pi \), while the function \( c \) decreases with \( t \) as \( c = c_0 t/t_0 \). When \( \xi \sim O(1) \), equations (4.4.6a) and (4.4.6b) cease to be valid, thus after this period the \( c \) starts increasing and \( a \) and \( b \) decreasing. At the end, when condition \( c^2/(ab)^2 \sim t^{-2} \) is realized, a new period of oscillations is reached (Kasner epochs) and the natural evolution of the system is restored.

Let us stress how the matching of the constants of the above limit regions is possible. In particular we can express the constants \((K, \theta)\) in terms of \((A, \xi_0)\). Such procedure can be implemented also by replacing \( \sinh(2\chi) \) with \( 2\chi \) \((\chi \ll 1)\) in equation (4.4.4a), and finally the solution is expressed in terms of Bessel functions which can be asymptotically expanded and compared with the explicit mentioned solutions [15].

### 4.5 Hamiltonian Formulation of the Dynamics

So far we reviewed the formulation of General Relativity in terms of geometrodynamics, i.e. studying the equations governing the evolution of the metric tensor. In what follows we will consider a different interpretation of the terms involved, leading to a peculiar Hamiltonian formulation. This paragraph is devoted to specialize it to the Mixmaster dynamics, i.e. to the Bianchi VIII and IX models [368, 367, 370].

The space-time line element adapted to the 3+1 foliation can be written as in (2.4.3) [370] where, for a spatially homogeneous model, the three-metric tensor \( h_{\alpha\beta} \) is parametrized by three functions \( q^a = q^a(t) \), in particular

\[
h_{\alpha\beta} = e^{q_a} \delta_{ab} e^a(x) e^b(x),
\]

(4.5.1)

although such symmetry is valid in the case of absence of matter only. In fact, the Einstein equations in vacuum \( R_{0\alpha} = 0 \) allow the choice of a diagonal metric \( h_{\alpha\beta} \), thus leaving three degrees of freedom only. The presence of matter induces in general a non-diagonal metric (which will be analyzed later) while here we focus on the vacuum one.

Given the parametrization (4.5.1), considering that all the canonical variables, including the lapse function and the shift vector, are independent of the spatial coordinates and that this model identically satisfies the super-momentum constraint, we get the action as

\[
S = \int dt \left( p_a \partial_t q^a - NH \right),
\]

(4.5.2)

\( p_a = p_a(t) \) being the momenta canonically conjugate to \( q^a \). The super-Hamiltonian \( H \) reads explicitly as

\[
H = \frac{1}{\sqrt{\eta}} \left[ \sum_a (p_a)^2 - \frac{1}{2} \left( \sum_b p_b \right)^2 - \eta^{(3)} R \right],
\]

(4.5.3)

where $\eta \equiv \exp \sum_a q_a$ and the Ricci three-scalar $(^3R)$ plays the role of the potential in the dynamics.

Let us introduce the “anisotropy parameters”, which will be convenient in the following, as

$$Q_a \equiv \frac{q^a}{\sum_b q^b}, \quad \sum_a Q_a = 1.$$  \hspace{1cm} (4.5.4)

The functions defined as in (4.5.4) allow a clearer interpretation of the last term in the right-hand side of equation (4.5.3) as a potential form $U$ for the dynamics. In fact, it can be re-written in the more expressive form

$$U = \eta (^3R) = \sum_a \lambda_a^2 \eta^2Q_a - \sum_{b \neq c} \lambda_b \lambda_c \eta Q_b + Q_c,$$  \hspace{1cm} (4.5.5)

where the constants $\lambda_a$ specify the model under consideration, being $\lambda_a = (1, 1, -1)$ or $\lambda_a = (1, 1, 1)$ for Bianchi VIII and IX, respectively.

The main advantage of writing the potential as in (4.5.5), arises when investigating its proprieties in the asymptotical behavior toward the cosmological singularity ($\eta \to 0$). In fact, the second term in (4.5.5) becomes negligible, while the value of the first one results to be strongly sensitive to the sign of $Q_a$'s and the potential can be modeled by an infinite well as

$$U = \sum_a \Theta(Q_a)$$  \hspace{1cm} (4.5.6)

where

$$\Theta(x) = \begin{cases} +\infty, & \text{if } x < 0 \\ 0, & \text{if } x > 0. \end{cases}$$  \hspace{1cm} (4.5.7)

By (4.5.6) we see how the dynamics of the Universe resembles that of a particle moving in a dynamically-closed domain $\Pi_Q$, defined as the one where all the anisotropy parameters $Q_a$ are simultaneously positive.

### 4.6 The ADM Reduction of the Dynamics

The ADM reduction of the dynamics relies on the idea of identifying a temporal parameter as a functional of the geometric canonical variables, before applying any quantization procedure or, in other words, of solving the classical constraints before quantizing. For the moment, we will simply discuss the reduction of General Relativity to a pure canonical form focusing on the elimination of non-dynamical variables.

Let us count the degrees of freedom of the gravitational field. We have twenty phase-space variables, given in the 3+1 formalism by the set $(N, \Pi; N^a, \Pi_a; h_{\alpha\beta}, \Pi^{\alpha\beta})$ (see Section 2.4), subject to eight first-class constraints ($\Pi = 0, \Pi_a = 0, H = 0, H_\alpha = 0$). Since each constraint eliminates two phase-space variables, we remain with four of them, corresponding to 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.

After eliminating $N$ and $N^a$, we have $12 \times \infty^3$ variables $(h_{\alpha\beta}(x), \Pi^{\alpha\beta}(x))$. Then, we can remove $4 \times \infty^3$ variables thanks to the secondary constraints (2.4.14). The remaining $4 \times \infty^3$ non-physical degrees of freedom result from the lapse function and the shift vector.
In analogy with the Yang-Mills theory, also in this case it is necessary to impose some sort of gauge, fixing the lapse function and the shift vector.

In order to obtain a true canonical form for the canonical theory, we have to follow the key steps listed by Isham in [280]. With respect to this formulation, we refer to a canonical description of the physical degrees of freedom only and with the following procedure we are able to discard the non-physical variables.

i) Perform a canonical transformation

\[
(h_{\alpha\beta}(x), \Pi^{\alpha\beta}(x)) \rightarrow \left(\chi^A(x), P_A(x); \phi^r(x), \pi_r(x)\right), \quad A = 1, 2, 3, 4 \quad r = 1, 2
\]

where \(\chi^A(x)\) define a particular choice of the space and time coordinates, \(P_A(x)\) are the corresponding canonically conjugate momenta and the four phase space variables \((\phi^r(x), \pi_r(x))\) represent the physical degrees of freedom of the system. We emphasize that these “physical” fields are not Dirac observables, in the sense defined in Section 2.4.

Consequently, the symplectic structure is determined by

\[
\{\chi^A(x), P_B(x')\} = \delta^A_B \delta^3(x - x'), \quad (4.6.2a)
\]

\[
\{\phi^r(x), \pi_s(x')\} = \delta^r_s \delta^3(x - x'), \quad (4.6.2b)
\]

while all other Poisson brackets are vanishing.

ii) Express the super-momentum and super-Hamiltonian in terms of the new fields and then write the Lagrangian density as

\[
\mathcal{L}'(N, N^a, \chi^A, P_A, \phi^r, \pi_r) = P_A \dot{\chi}^A + \pi_r \dot{\phi}^r - NH' - N^a H'_a. \quad (4.6.3)
\]

iii) Remove \(4 \times \infty^3\) variables arising from the constraints \(H = 0\) and \(H_a = 0\) once solved with respect to \(P_A\) the equation

\[
P_A(x) + h_A(x, \chi, \phi, \pi) = 0 \quad (4.6.4)
\]

and re-inserting it in (4.6.3). Removing the remaining \(4 \times \infty^3\) non-dynamical variables we yield the so-called true Lagrangian density [280]

\[
\mathcal{L}_{\text{true}} = \pi_r \dot{\phi}^r - h_A \dot{\chi}^A, \quad (4.6.5)
\]

where the lapse function and the shift vector do not play any role, but specifying the form of the functions \(\dot{\chi}^A\). After solving the constraints, there is no longer information about the evolution of \(\chi^A\) in terms of the parametric time \(t\). Thus, in equation (4.6.5) we have chosen the conditions \(\chi^A(x, t) = \chi^A(t(x))\) and the true Hamiltonian is

\[
H_{\text{true}} = \int d^3x \chi^A(x) h_A(x, \chi(t), \phi(t), \pi(t)). \quad (4.6.6)
\]

\(^2\)These fields can be interpreted as defining an embedding of \(\Sigma\) in \(M\) via some parametric equations.
From (4.6.6) one can derive the equations of motion as

\[
\begin{align*}
\partial_t \phi^r &= \{ \phi^r, H_{\text{true}} \}_{\text{red}} \\
\partial_t \pi_s &= \{ \pi_s, H_{\text{true}} \}_{\text{red}},
\end{align*}
\]

where the notation \( \{ \ldots \}_{\text{red}} \) refers to the Poisson brackets evaluated in the reduced phase space with coordinates given by the physical modes \( \phi^r \) and \( \pi_s \).

This is an operative method to classically solve the constraints, i.e. pulling out all the gauges, and obtaining a canonical description for the physical degrees of freedom only.

We also note that such procedure violates the geometrical structure of General Relativity, since it removes parts of the metric tensor. Nevertheless, it avoids any obstacle at a classical level, but there are several problems when implemented in the quantum framework [280, 315, 26]. In particular, they are related to the one of the reduced-phase space quantization, for more details see [251].

### 4.7 Misner variables and the Mixmaster model

In order to implement the formalism to our purposes, we start introducing a new set of variables, as mentioned in expression (3.2.8). In fact, we parametrize the tetradic projection of the metric as

\[
\eta_{ab} = e^{2\alpha} \left( e^{2\beta} \right)_{ab} \leftrightarrow (\ln \eta)_{ab} = 2\alpha \delta_{ab} + 2\beta_{ab}
\]

where \( \beta_{ab} \) is a three-dimensional matrix with null trace of the kind \( \text{diag}(\beta_{11}, \beta_{22}, \beta_{33}) \) and the exponential matrix has to be intended as a power series of matrices, so that

\[
\det \left( e^{2\beta} \right) = e^{2 \text{tr} \beta} = 1
\]

and

\[
\eta = e^{6\alpha}.
\]

The BKL formalism used in Section 3.4 matches the present one (for the Bianchi I solution) once considering the expression

\[
p_{ab} = \frac{d (\ln \eta)_{ab}}{d \ln \eta}.
\]

From equations (4.7.1a) and (4.7.4) the relation

\[
p_{ab} = \frac{1}{3} \left[ \delta_{ab} + \left( \frac{d \beta_{ab}}{d \alpha} \right) \right]
\]

follows, so that the first Kasner condition (3.4.11) rewrites as

\[
1 = \sum_a p_a \equiv \text{tr} \ p_{ab} = 1 + \frac{1}{3} \text{tr} \left( \frac{d \beta}{d \alpha} \right)
\]
which is an identity since the trace \( \text{tr}\beta_{ab} = 0 \).

The second Kasner relation (3.4.11) rewrites as

\[
\text{tr} \left( p^2 \right) = 1 \quad (4.7.7)
\]

which, by virtue of (4.7.5) becomes

\[
\frac{1}{9} \text{tr} \left( 1 + 2 \frac{d\beta_{ab}}{d\alpha} + \left( \frac{d\beta_{ab}}{d\alpha} \right)^2 \right) = \frac{1}{3} + \frac{1}{9} \left( \frac{d\beta_{ab}}{d\alpha} \right)^2 = 1, \quad (4.7.8)
\]

and then

\[
\left( \frac{d\beta_{ab}}{d\alpha} \right)^2 = 6 \quad (4.7.9)
\]

which is no longer an identity but a consequence of the Einstein equations in empty space.

### 4.7.1 Misner Approach to the Mixmaster

Once seen how to perform the convenient change of variables for the diagonal case, we step further to approach the Mixmaster using this formalism.

The matrix \( \beta_{ab} \) has only two independent components defined as

\[
\beta_{11} = \beta_+ + \sqrt{3} \beta_- \quad (4.7.10a)
\]
\[
\beta_{22} = \beta_+ - \sqrt{3} \beta_- \quad (4.7.10b)
\]
\[
\beta_{33} = -2\beta_+ , \quad (4.7.10c)
\]

and then the Kasner relation for Bianchi I reads as

\[
\left( \frac{d\beta_+}{d\alpha} \right)^2 + \left( \frac{d\beta_-}{d\alpha} \right)^2 = 1. \quad (4.7.11)
\]

The variables \( \beta_\pm \) together with \( \alpha \) are the Misner coordinates. The relation (4.7.11) in terms of the Kasner exponents now is

\[
\frac{d\beta_+}{d\alpha} = \frac{1}{2} \left( 1 - 3p_3 \right) \quad (4.7.12a)
\]
\[
\frac{d\beta_-}{d\alpha} = \frac{1}{2} \sqrt{3} (p_1 - p_2) \quad (4.7.12b)
\]

or equivalently with the \( u \) parameter

\[
\frac{d\beta_+}{d\alpha} = -1 + \frac{3}{2} \frac{1}{1 + u + u^2} \quad (4.7.13a)
\]
\[
\frac{d\beta_-}{d\alpha} = -\frac{1}{2} \sqrt{3} \frac{1 + 2u}{1 + u + u^2}. \quad (4.7.13b)
\]

Such quantities represent the anisotropy velocity \( \beta' \)

\[
\beta' \equiv \left( \frac{d\beta_+}{d\alpha}, \frac{d\beta_-}{d\alpha} \right), \quad (4.7.14)
\]
4.7 Misner variables and the Mixmaster model

which measures the variation of the anisotropy amount with respect to the expansion as parametrized by the \( \alpha \) parameter. The volume of the Universe behaves as \( e^{3\alpha} \), tends to zero towards the singularity and is directly related to the temporal parameter.

Eventually, the presence of matter as well the effects of the spatial curvature can lead the norm \( ||\beta'|| \) to a deviation from the Kasnerian unity.

In order to develop a general metric for a homogeneous space-time we rewrite the line element in the general form

\[
d s^2 = N^2(t) d t^2 - e^{2\alpha(e^{2\beta})_{ab}} \omega^a \otimes \omega^b.
\]  

(4.7.15)

The cosmological problem reduces to the equations involving the functions \( \alpha, N, \beta_{ab} \) in terms of the independent temporal parameter \( t \), independently of the spatial coordinates.

Explicitly, the dual 1-forms associated to the Bianchi types VIII and IX are, respectively,

\[
\begin{align*}
\omega^1 &= - \sinh \psi \sin \theta d \phi + \cosh \psi d \theta \\
\omega^2 &= - \cosh \psi \sin \theta d \phi + \sinh \psi d \theta \\
\omega^3 &= \cosh \theta d \phi + d \psi \\
\end{align*}
\]  

(VIII) \quad (4.7.16a)

\[
\begin{align*}
\omega^1 &= \sin \psi \sin \theta d \phi + \cos \psi d \theta \\
\omega^2 &= - \cos \psi \sin \theta d \phi + \sin \psi d \theta \\
\omega^3 &= \cos \theta d \phi + d \psi \\
\end{align*}
\]  

(IX) \quad (4.7.16b)

For example, the \( 0-0 \) Einstein equation with \( N = 1 \) reads as

\[
3 \left( \dot{\alpha}^2 - \dot{\beta}_+^2 - \dot{\beta}_-^2 \right) + \frac{1}{2} \left( \frac{(3) R_B}{(3)} \right) = \kappa T^0_0,
\]  

(4.7.17)

where \( (3) R_B \) is the curvature scalar for the three-dimensional spatial surface corresponding to \( t = \text{const.} \) and the index \( B \) refers to the symmetry properties for the Bianchi cosmological models. Such term contains the peculiar difference between the nine types of the Bianchi classification, to be evaluated through expressions (3.3.2) in terms of the structure constants.

For the models referring to types VIII and IX such curvature scalar reads as

\[
\begin{align*}
(3) R_{\text{VIII}} &= \frac{1}{2} e^{-2\alpha} \left( 4 e^{4\beta_+} - 2 \text{tr} e^{-2\beta} - \text{tr} e^{4\beta} \right) \\
(3) R_{\text{IX}} &= \frac{1}{2} e^{-2\alpha} \text{tr} \left( 2 e^{-2\beta} - e^{4\beta} \right)
\end{align*}
\]  

(4.7.18a, b)

respectively, and the trace operation has to be intended over the exponential of diagonal matrices, without ambiguity.

Equation (4.7.17) with (4.7.18b) or (4.7.18a) can be interpreted as a contribution of the anisotropy energy, connected to the term \( T^0_0 \), to the volume expansion \( \dot{\alpha}^2 \), so that it appears as a potential term together with the kinetic ones \( \dot{\beta}_\pm^2 \). Close to the singularity, this term becomes negligible for small values of the anisotropy variables \( \beta_\pm \).

Finally, equation (4.7.17) has to be regarded as a constraint over the field equations.
4 Chaotic Dynamics of the Bianchi Types VIII and IX Models

4.7.2 Lagrangian Formulation in the Misner Variables

Despite the variables $q_a$ introduced in Section 4.5 are linked to the Misner ones by the linear transformations

\[ q_1 = 2\alpha + 2\beta_++ 2\sqrt{3}\beta_- \]  
(4.7.19a)

\[ q_2 = 2\alpha + 2\beta_+ - 2\sqrt{3}\beta_- \]  
(4.7.19b)

\[ q_3 = 2\alpha - 4\beta_- \]  
(4.7.19c)

nevertheless we conveniently restate *ab initio* the Lagrangian approach. From the general expression of the action (2.1.11) in vacuum, we get the variational principle

\[ \delta \int_{t_1}^{t_2} L \, dt = 0, \]  
(4.7.20)

in which $t_1$ and $t_2$ ($t_2 > t_1$) are two values of the temporal coordinate and integration is performed with respect to the spatial coordinates.

In particular, integration for the Bianchi type VIII is considered over a spatial volume $(4\pi)^2$, in order to have the same integration constant used for the type IX (and to keep a uniform formalism), having

\[ \int \omega^1 \wedge \omega^2 \wedge \omega^3 = \int \sin\theta d\phi \wedge d\theta \wedge d\psi = (4\pi)^2. \]  
(4.7.21)

This way, the Lagrangian $L$ is written as\(^3\)

\[ L = -\frac{6\pi}{N} e^{3\alpha} \left[ \alpha'^2 - \beta_+^2 - \beta_-^2 \right] + N\frac{\pi}{2} e^{\beta} U^{(B)} (\beta_+, \beta_-) \]  
(4.7.22)

where \( ()' = \frac{d}{dt} \) and $U^{(B)}$ is a function linear in $(3)R_B$ having a potential role. The variational principle rewrites explicitly as

\[ \delta S = \delta \int \left( p_\alpha \alpha' + p_\beta \beta_+ ' + p_\beta \beta_- ' - NH \right) dt = 0 \]  
(4.7.23)

in which $H$ is given by

\[ H = \frac{e^{-3\alpha}}{24\pi} \left( -p_\alpha^2 + p_\beta^2 + p_\beta^2 + V \right) \]  
(4.7.24)

and the potential $V$ as

\[ V = -12\pi^2 e^{4\alpha} U^{(B)} (\beta_+, \beta_-) \]  
(4.7.25)

where $U^{(B)}$ is specified for the two Bianchi models under study as

\[ U^{\text{VIII}} = e^{-8\beta_+} + 4e^{-2\beta_+} \cosh(2\sqrt{3}\beta_-) + 2e^{4\beta_+} \left( \cosh(4\sqrt{3}\beta_-) - 1 \right) \]  
(4.7.26a)

\[ U^{\text{IX}} = e^{-8\beta_+} - 4e^{-2\beta_+} \cosh(2\sqrt{3}\beta_-) + 2e^{4\beta_+} \left( \cosh(4\sqrt{3}\beta_-) - 1 \right). \]  
(4.7.26b)

\(^3\)Here we choose the Einstein constant $\kappa = 16\pi$, i.e. $G = 1$. 

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From Lagrangian (4.7.22) it is standard to derive the conjugate momenta

\[ p_\alpha = \frac{\partial L}{\partial \dot{\alpha}'} = -\frac{12\pi}{N} e^{3\alpha} \delta \alpha' \tag{4.7.27a} \]

\[ p_\pm = \frac{\partial L}{\partial \dot{\beta}_\pm} = \frac{12\pi}{N} e^{3\alpha} \beta_\pm' \tag{4.7.27b} \]

### 4.7.3 Reduced ADM Hamiltonian

In order to obtain Einstein equations, the variational principle requires \( \delta S \) to be null for arbitrary and independent variations of \( p_\pm, p_\alpha, \beta_\pm, N \). Variation with respect to \( N \) leads to the super-Hamiltonian constraint \( H = 0 \). As we have seen in Section 4.6, the procedure prescribes the choice of one of the field variables, or one of the momenta, as the temporal coordinate and subsequently one can solve the constraint (4.7.24) with respect to the corresponding conjugate quantity.

It is customary, as in this general approach, to set \( t = \alpha \) and solve \( H = 0 \) obtaining

\[ H_{ADM} = -p_\alpha = \sqrt{p_+^2 + p_-^2 + V}. \tag{4.7.28} \]

Within this equation a relation between the temporal gauge described by the function \( N \) and the dynamical quantity \( H_{ADM} \) is defined.

Through (4.7.28) we explicit \( p_\alpha \) in the action integral, so that the reduced variational principle in a canonical form reads as

\[ \delta S_{\text{red}} = 0 \tag{4.7.29} \]

\( S_{\text{red}} \) being written as

\[ S_{\text{red}} = \int (p_+ d\beta_+ + p_- d\beta_- - H_{ADM} d\alpha) \tag{4.7.30} \]

together with the equation defining the temporal gauge for \( \dot{\alpha} = 1 \)

\[ N_{ADM} = \frac{12\pi e^{3\alpha}}{H_{ADM}}. \tag{4.7.31} \]

### 4.7.4 Mixmaster Dynamics

In the present Section we will write in general the approach to the Mixmaster dynamics and later on it will be applied to prove specific properties, such as chaoticity in a covariant approach, with respect to the temporal gauge, and subsequent statistical effects.

The Hamiltonian introduced so far differs from the typical expression of classical mechanics for the non positive definiteness of the kinetic term, i.e. the sign in front of \( p_\alpha^2 \), and for the peculiar form of the potential as a function of \( \alpha \) (say time) and \( \beta_\pm \), reduced to the study of a function of the kind \( V(\beta_+, \beta_-) \).
A Hamiltonian approach permits to derive the equations of motion as

\begin{align}
\alpha' &= \frac{\partial H}{\partial p_\alpha}, \quad \alpha' = -\frac{\partial H}{\partial \alpha}, \\
\beta'_{\pm} &= \frac{\partial H}{\partial p_{\pm}}, \quad \beta'_{\pm} = -\frac{\partial H}{\partial \beta_{\pm}}.
\end{align}

(4.7.32a)  
(4.7.32b)

This set considered with the explicit form of the potential (see Figure 4.1 and 4.2), can be interpreted as the motion of a “point-particle” in a potential. The term $V$ is proportional to the curvature scalar and describes the anisotropy of the Universe, i.e. in the regions of the configuration space where it can be negligible the dynamics resembles the pure Kasner behaviour, corresponding to $|\beta'| = 1$. 

Figure 4.1: Equipotential lines of the Bianchi type VIII model in the $\beta_+, \beta_-$ plane.

Figure 4.2: Equipotential lines of the Bianchi type IX model in the $\beta_+, \beta_-$ plane.
In general, it is necessary a detailed study of the potential form which behaves as a potential well in the plane $\beta_+, \beta_-$. Asymptotically close to the origin, i.e. $\beta_\pm = 0$, equipotential lines for the Bianchi type IX are circles

$$U^\text{IX} (\beta_+, \beta_-) \simeq -3 + \left( \beta_+^2 + \beta_-^2 \right) + o(\beta^3),$$

(4.7.33)

while for Bianchi type VIII are ellipses

$$U^\text{VIII} (\beta_+, \beta_-) \simeq \left( 40\beta_+^2 + 24\beta_-^2 \right) - 8(\beta_+ + \beta_-) + 5 + o(\beta^3).$$

(4.7.34)

The expressions for large values of $\beta$ are the same for both types

$$U (\beta) \simeq e^{-8\beta_+}, \quad \beta_+ \longrightarrow -\infty$$

(4.7.35)

or

$$U (\beta) \simeq 48\beta_-^2 e^{4\beta_+}, \quad \beta_+ \longrightarrow +\infty$$

(4.7.36)

when

$$|\beta_-| \ll 1.$$  

(4.7.37)

In the figures 4.1 and 4.2 are represented some of the equipotential lines $U (\beta) = \text{const.}$, for which the potential value has an increment of a factor $e^8 \sim 3 \times 10^3$ for $\Delta\beta \sim 1$.

The Universe evolution is described as the motion of a point-like particle under the influence of such potentials and it corresponds to bounces on the potential walls when evolving towards the singularity. The behaviour of the anisotropy variables $\beta_\pm$ in this regime consists of a Kasner epoch followed by a bounce and then a new epoch with different Kasner parameters, in correspondence with the description given in Section 4.2 according to the BKL approach.

Let us describe in more detail the bounces performed by the billiard ball representing the Universe. From the asymptotic form (4.7.35) for the Bianchi IX potential, we get the equipotential line $\beta^\text{wall}$ cutting the region where the potential terms are significant. In particular we have

$$\beta^\text{wall} = \frac{\alpha}{2} - \frac{1}{8} \ln(3H^2),$$

(4.7.38)

where the super-Hamiltonian $H$ is defined as in (4.7.24). Since we have $H = \text{const.}$ inside the potential well, from (4.7.38) one gets $|\beta^\text{wall}'| = 1/2$, i.e. the $\beta$-point moves twice as fast as the receding potential wall, i.e. the particle will collide against the wall and will be reflected from one straight-line motion (Bianchi I) to another one.

A relation of reflection-type lays for the bounces [368]. In fact, considering the super-Hamiltonian (4.7.24) in the (4.7.35) case, if $\theta_i$ and $\theta_f$ are the angles of incidence and of reflection of the particle off the potential wall, respectively, the relation

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

(4.7.39)

holds and in terms of the parameter $u$ introduced in section 3.7.2 it is nothing but $u_f = u_i - 1.$
4.8 Misner-Chitre–like variables

A valuable framework of analysis of the Mixmaster evolution, able to join together the two points of view of the map approach and of the continuous dynamics evolution, relies on a Hamiltonian treatment of the equations in terms of Misner-Chitre variables [131]. This formulation allows to individualize the existence of an asymptotic (energy-like) constant of motion once performed an ADM reduction. By this result, the stochasticity of the Mixmaster can be treated either in terms of the statistical mechanics (by the micro-canonical ensemble) [276], either by its characterization as isomorphic to a billiard on a two-dimensional Lobachevsky space [17] and such scheme can be constructed independently of the choice of a time variable, simply providing very general Misner-Chitre–like (MCl) coordinates [273, 272].

To this purpose, let us here re-define the anisotropy parameters $Q_a$ (following [299, 302], [374, 303]) as the functions

\begin{align}
Q_1 &= \frac{1}{3} + \frac{\beta_+ + \sqrt{3} \beta_-}{3\alpha} \\
Q_2 &= \frac{1}{3} + \frac{\beta_+ - \sqrt{3} \beta_-}{3\alpha} \\
Q_3 &= \frac{1}{3} - \frac{2\beta_+}{3\alpha} ,
\end{align}

excluding the pathological cases when two or three of them coincide.

We then introduce the Misner-Chitre variables \{\tau, \zeta, \theta\} as

\begin{align}
\alpha &= -e^\tau \cosh \zeta \\
\beta_+ &= e^\tau \sinh \zeta \cos \theta \\
\beta_- &= e^\tau \sinh \zeta \sin \theta
\end{align}

where $0 \leq \zeta < \infty$, $0 \leq \theta < 2\pi$, and \(\tau\) plays the role of a “radial” coordinate coming out from the origin of the $\beta_\pm$ space [370]. In terms of (4.8.2), it is possible to study the first interesting approximation of the potential (4.7.26) as independent of $\tau$ towards the singularity, i.e. for $\alpha \to -\infty$.

To discuss the contrasting results concerning chaoticity and dynamical properties which arose from numerics [203, 443, 64, 257], it is necessary to introduce a slight modification to the set (4.8.2) via the MCI coordinates \{\Gamma(\tau), \xi, \theta\} through the transformations

\begin{align}
\alpha &= -e^{\Gamma(\tau)} \xi \\
\beta_+ &= e^{\Gamma(\tau)} \sqrt{\xi^2 - 1} \cos \theta \\
\beta_- &= e^{\Gamma(\tau)} \sqrt{\xi^2 - 1} \sin \theta
\end{align}

where $1 \leq \xi < \infty$, and $\Gamma(\tau)$ stands for a generic function of $\tau$: in the original work, Chitre took simply $\Gamma(\tau) \equiv \tau$ and set $\xi = \cosh \zeta$.

This modified set of variables permits to write the anisotropy parameters (4.8.1) $Q_a$ as
independent of the variable $\Gamma$ as

\begin{align*}
Q_1 &= \frac{1}{3} - \frac{\sqrt{\xi^2 - 1}}{3\xi} \left( \cos \theta + \sqrt{3} \sin \theta \right) \quad (4.8.4a) \\
Q_2 &= \frac{1}{3} - \frac{\sqrt{\xi^2 - 1}}{3\xi} \left( \cos \theta - \sqrt{3} \sin \theta \right) \quad (4.8.4b) \\
Q_3 &= \frac{1}{3} + \frac{2\sqrt{\xi^2 - 1}}{3\xi} \cos \theta. \quad (4.8.4c)
\end{align*}

All dynamical quantities, if expressed in terms of (4.8.4) will be independent of $\tau$ too.

**Figure 4.3:** The limited region $\Pi_Q(\xi, \theta)$ of the configuration space where the dynamics of the point Universe is restricted by means of the curvature term which corresponds to an infinite potential well. In this region the conditions $Q_a \geq 0$ are fulfilled.

### 4.8.1 The Hamilton Equations

The main advantage relying on the reformulation of the dynamics as a chaotic scattering process consists of replacing the discrete BKL map by a geodesic flow in a space of continuous variables \[124, 303-33, 377, 275].

In terms of (4.8.3), the Lagrangian (4.7.22) becomes

\begin{equation}
L = \frac{6D}{N} \left[ \left( e^{\Gamma'} \right)^2 \left( \xi^2 - 1 \right) + \left( e^{\Gamma} \right)^2 \left( \xi^2 - 1 \right) - \left( e^{\Gamma} \right)^2 \right] - \frac{N}{D} V(\Gamma, \xi, \theta), \quad (4.8.5)
\end{equation}

while $D$ expresses as

\begin{equation}
D = \exp \left\{ -3\xi e^{\Gamma(\tau)} \right\}, \quad (4.8.6)
\end{equation}

and since it vanishes towards the singularity independently of its particular form, the only property required for $\Gamma$ is to approach infinity in this limit.
The Lagrangian (4.7.22) leads to the conjugate momenta

\[ p_\tau = -\frac{12D}{N} \left( e^{r} \frac{d\Gamma}{d\tau} \right)^2 \tau' \]  
\[ p_\xi = \frac{12D}{N} e^{2r} (\xi^2 - 1) \xi' \]  
\[ p_\theta = \frac{12D}{N} e^{2r} (\xi^2 - 1) \theta' \]  

which by a Legendre transformation make the variational principle assume the form \[\delta \int \left( p_\xi \xi' + p_\theta \theta' + p_\tau \tau' - \frac{Ne^{-2r}}{24D} H \right) dt = 0,\]  

where 

\[ H = -\frac{p_\tau^2}{\left( \frac{d\Gamma}{d\tau} \right)^2} + p_\xi^2 (\xi^2 - 1) + \frac{p_\theta^2}{\xi^2 - 1} + 24Ve^{2r}. \]  

### 4.8.2 Dynamics in the Reduced Phase Space

Solving the super-Hamiltonian constraint we get the expression for \( \mathcal{H}_{ADM} \)

\[ \mathcal{H}_{ADM} = \frac{d\Gamma}{d\tau} \sqrt{\epsilon^2 + 24Ve^{2r}}, \]  

where 

\[ \epsilon^2 \equiv (\xi^2 - 1) p_\xi^2 + \frac{p_\theta^2}{\xi^2 - 1}. \]  

In terms of this constraint, the principle (4.8.8) reduces to the simpler form

\[ \delta \int \left( p_\xi \xi' + p_\theta \theta' - \Gamma' \mathcal{H}_{ADM} \right) dt = 0, \]  

whose variation provides the Hamilton equations for \( \xi' \) and \( \theta' \)

\[ \xi' = \frac{\Gamma'}{\mathcal{H}_{ADM}} (\xi^2 - 1) p_\xi \]  
\[ \theta' = \frac{\Gamma'}{\mathcal{H}_{ADM}} p_\theta. \]  

From (4.8.7a) we find the time-gauge relation

\[ N_{ADM}(t) = \frac{12D}{\mathcal{H}_{ADM}} e^{2r} \frac{d\Gamma}{d\tau'}, \]  

thus our analysis remains fully independent of the choice of the time variable until the form of \( \Gamma \) and \( \tau' \) is fixed.
By choosing $d\Gamma/d\tau = 1$, the principle (4.8.12) reduces to the two-dimensional one

$$
\delta \int \left( p_\xi \xi' + p_\theta \theta' - \mathcal{H}_{ADM} \right) dt = 0,
$$

where, remembering (4.5.5)

$$
\mathcal{H}_{ADM} = \sqrt{\varepsilon^2 + U}, \quad U \equiv 24Ve^{2\tau};
$$

moreover, the choice $\tau' = 1$ for the temporal gauge provides the lapse function as

$$
N_{ADM}(\tau) = \frac{12D}{\mathcal{H}_{ADM}} e^{2\tau}.
$$

The reduced principle (4.8.15) finally gives the Hamilton equations

$$
\xi' = \frac{(\xi^2 - 1)}{\mathcal{H}_{ADM}} p_\xi,
$$

$$
\theta' = \frac{1}{\mathcal{H}_{ADM} (\xi^2 - 1)} p_\theta,
$$

$$
p_\xi' = -\frac{\xi}{\mathcal{H}_{ADM}} \left[ p_\xi^2 - \frac{p_\theta^2}{(\xi^2 - 1)^2} \right] - \frac{1}{2\mathcal{H}_{ADM}} \frac{\partial U}{\partial \xi} \xi',
$$

$$
p_\theta' = -\frac{1}{2\mathcal{H}_{ADM}} \frac{\partial U}{\partial \theta},
$$

where, because of the choice of the time gauge, $(\quad)' = \frac{d}{d\tau}$.

### 4.8.3 Billiard Induced from the Asymptotic Potential

The Hamilton equations are equivalently viewed through the two time variables $\Gamma$ and $\tau$ and then, for this Section only, we choose the natural time gauge $\tau' = 1$, in order to write the variational principle (4.8.12) in terms of the time variable $\Gamma$ as

$$
\delta \int \left( p_\xi \frac{d\xi}{d\Gamma} + p_\theta \frac{d\theta}{d\Gamma} - \mathcal{H}_{ADM} \right) d\Gamma = 0.
$$

Nevertheless, for any choice of time variable $\tau$ (i.e. $\tau = t$), there exists a corresponding function $\Gamma (\tau)$ (i.e. a set of MC variables leading to the scheme (4.8.19)) defined by the (invertible) relation

$$
\frac{d\Gamma}{d\tau} = \frac{\mathcal{H}_{ADM}}{12D} N(\tau) e^{-2\tau}.
$$

The asymptotically vanishing of $D$ is ensured by the Landau-Raichaudhury theorem near the initial singularity (which occurs by convention at $T = 0$, where $T$ now denotes the synchronous time, i.e. $dT = -N(\tau) d\tau$, for $T \to 0$ we have $d\ln D/dT > 0$. In terms of the adopted variable $\tau$ we have

$$
D \to 0 \quad \Rightarrow \quad \Gamma (\tau) \to \infty,
$$

(4.8.21)
consequently, by (4.8.6) and (4.8.20), also
\[
\frac{d \ln D}{d \tau} = \frac{d \ln D}{dT} \frac{dT}{d \tau} = -\frac{d \ln D}{dT} N(\tau)
\] (4.8.22)
and therefore \(D\) monotonically vanishes even in the generic time gauge as soon as \(d\Gamma/d\tau > 0\) for increasing \(\tau\), according to (4.8.20).

Approaching the initial singularity, the limit \(D \to 0\) for the Mixmaster potential (4.5.5) implies an infinite potential well behavior, as discussed in Section 4.5.

Furthermore, by (4.8.10) the important relation
\[
\frac{d}{dt} (\mathcal{H}_{ADM}\Gamma') = \frac{\partial (\mathcal{H}_{ADM}\Gamma')}{\partial \Gamma} \implies \frac{d (\mathcal{H}_{ADM}\Gamma')}{d\Gamma} = \frac{\partial (\mathcal{H}_{ADM}\Gamma')}{\partial \Gamma},
\] (4.8.23)
holds, i.e. explicitly
\[
\frac{\partial \mathcal{H}_{ADM}}{\partial \Gamma} = \frac{e^{2\Gamma}}{2\mathcal{H}_{ADM}} 24 \left(2U + \frac{\partial U}{\partial \Gamma}\right).
\] (4.8.24)

In this reduced Hamiltonian formulation, the functional \(\Gamma(t)\) simply plays the role of a parametric function of time and we recall how actually the anisotropy parameters \(Q_a\) are functions of the variables \(\xi, \theta\) only (see (4.8.4)).

Therefore in the dynamically allowed domain \(\Pi_Q\) (see Fig.4.3) the ADM Hamiltonian becomes (asymptotically) an integral of motion
\[
\forall \{\xi, \theta\} \in \Pi_Q\quad \left\{ \begin{array}{l}
\frac{\partial \mathcal{H}_{ADM}}{\partial \Gamma} = 0 = \frac{\partial E}{\partial \Gamma} \\
\mathcal{H}_{ADM} = \sqrt{\epsilon^2 + 24U} \cong \epsilon = E = \text{const.}
\end{array} \right.,
\] (4.8.25)

### 4.8.4 The Jacobi Metric and the Billiard Representation

Since above we have shown that asymptotically to the singularity (\(\Gamma \to \infty\), i.e. \(a \to -\infty\)) \(d\mathcal{H}_{ADM}/d\Gamma = 0\), i.e. \(\mathcal{H}_{ADM} = \epsilon = \bar{E} = \text{const.}\), the variational principle (4.8.19) reduces to
\[
\delta \int (p_\xi d\xi + p_\theta d\theta - Ed\Gamma) = 0, \quad (4.8.26)
\]
where we dropped the third term on the left-hand side since it behaves as an exact differential.

By following the standard Jacobi procedure [17] to reduce our variational principle to a geodesic one in terms of the configuration variables \(x^a\), we set \(x'^a = g^{ab} p_b\), and by the Hamilton equation (4.8.13) we obtain the metric [273, 276]
\[
g^{\xi \xi} = \frac{\Gamma'}{E} (\xi^2 - 1), \quad g^{\theta \theta} = \frac{\Gamma'}{E} \frac{1}{\xi^2 - 1}.
\] (4.8.27)

By (4.8.27) and by the fundamental constraint relation obtained rewriting (4.8.11) as
\[
(\xi^2 - 1) p_\xi^2 + \frac{p_\theta^2}{\xi^2 - 1} = E^2,
\] (4.8.28)
we get
\[ g_{ab}x^a x^b = \frac{\Gamma'}{E} \left( \xi^2 - 1 \right) p_{\xi}^2 + \frac{p_{\theta}^2}{\xi^2 - 1} = \Gamma' E. \]  
(4.8.29)

Using the definition
\[ x^a' = \frac{dx^a}{ds} \frac{ds}{dt} \equiv u^a \frac{ds}{dt}, \]  
(4.8.30)
equation (4.8.29) is rewritten as
\[ g_{ab}u^a u^b \left( \frac{ds}{dt} \right)^2 = \Gamma' E, \]  
(4.8.31)
which leads to the key relation
\[ dt = \sqrt{\frac{g_{ab}u^a u^b}{\Gamma' E}} ds. \]  
(4.8.32)

Indeed the expression (4.8.32) together with \( p_{\xi} \xi' + p_{\theta} \theta' = \Gamma' E \) allows us to put the variational principle (4.8.26) in the geodesic form
\[ \delta \int \Gamma' E dt = \delta \int \sqrt{G_{ab}u^a u^b} \Gamma' E ds = \delta \int \sqrt{G_{ab}u^a u^b} ds = 0, \]  
(4.8.33)
where the metric \( G_{ab} \equiv \Gamma' E g_{ab} \) satisfies the normalization condition \( G_{ab}u^a u^b = 1 \) and therefore
\[ \frac{ds}{dt} = \frac{E \Gamma'}{E} \Rightarrow \frac{ds}{d\Gamma} = E, \]  
(4.8.34)
where we take the positive root since we require that the curvilinear coordinate \( s \) increases monotonically with increasing values of \( \Gamma \), i.e. approaching the initial cosmological singularity.

Summarizing, the dynamical problem in the region \( \Pi_Q \) reduces to a geodesic flow on a two-dimensional Riemannian manifold described by the line element \[ ds^2 = E^2 \left[ \frac{d\xi^2}{\xi^2 - 1} + (\xi^2 - 1) d\theta^2 \right]. \]  
(4.8.35)
The above metric has negative curvature, since the associated curvature scalar is \( R = -2/\xi^2 \); therefore the point-Universe moves over a negatively curved bidimensional space on which the potential wall (4.5.6) cuts the region \( \Pi_Q \), depicted in Figure 4.3.

By a way completely independent of the temporal gauge we provided a satisfactory representation of the system as isomorphic to a billiard on a Lobachevsky plane [17].

From a geometrical point of view, the domain defined by the potential walls is not strictly closed, since there are three directions corresponding to the three corners in the traditional Misner picture [368, 367] from which the point universe could in principle escape (see Fig 4.3).

However, as discussed in Section 4.2 for the Bianchi models, the only case in which an asymptotic solution of the field equations has this behaviour corresponds to having two scale factors equal to each other (i.e. \( \theta = 0 \)); but, as shown by [50], these cases are dynamically unstable and correspond to sets of zero measure in the space of the initial
conditions. Thus, it has no sense to speak of a probability to reach certain configurations and the domain is de facto dynamically closed.

The bounces (billiard configuration) against the potential walls together with the geodesic flow instability on a closed domain of the Lobachevsky plane imply the point-Universe to have stochastic features, with a formalism true for any Bianchi type model. Indeed the types VIII and IX are the only Bianchi models having a compact configuration space, hence the claimed compactness of the domain bounded by the potential walls guarantees that the geodesic instability is upgraded to a real stochastic behaviour [18, 150, 384]. On the other hand, the possibility to deal with a stochastic scattering is justified by the constant negative curvature of the Lobachevsky plane and therefore these two notions (compactness and curvature) are both necessary for our considerations [509, 60].

4.9 The Invariant Liouville Measure

Here we show how the derivation of an invariant measure for the Mixmaster model (performed by [124, 303, 379] within the framework of the statistical mechanics) can be extended to a generic time gauge [272] (more directly than in previous approaches relying on fractal methods as in [152, 151]) provided the Misner-Chitre-like variables used so far. We have seen how the (ADM) reduction of the variational problem asymptotically close to the cosmological singularity permits to modelize the Mixmaster dynamics by a two-dimensional point-Universe randomizing in a closed domain with fixed “energy” (just the ADM kinetic energy) (4.8.25); the key point addressed here is that we consider an approximation dynamically induced by the asymptotic vanishing of the metric determinant.

From the statistical mechanics point of view [278], such a stochastic motion within the closed domain \( \Pi_Q \) of the phase-space, induces a suitable ensemble representation which, in view of the existence of the “energy-like” constant of motion, has to have the natural features of a microcanonical one. Therefore, the stochasticity of this system can be described in terms of the Liouville invariant measure

\[
dQ = \text{const} \times \delta(E - \epsilon) \, d\xi d\theta dp_{\xi} dp_{\theta} \tag{4.9.1}
\]

characterizing the microcanonical ensemble, having denoted by \( \delta(x) \) the Dirac function. The particular value taken by the constant \( \epsilon \) (\( \epsilon = E \)) cannot influence the stochasticity property of the system and must be fixed by the initial conditions. This useless information from the statistical dynamics is removable by integrating over all admissible values of \( \epsilon \). Introducing the natural variables \((\epsilon, \phi)\) in place of \((p_{\xi}, p_{\theta})\) by

\[
p_{\xi} = \frac{\epsilon}{\sqrt{\epsilon^2 - 1}} \cos \phi, \quad p_{\theta} = \epsilon \sqrt{\xi^2 - 1} \sin \phi, \quad 0 \leq \phi < 2\pi \tag{4.9.2}
\]

the integration removes the Dirac function, leading to the uniform and normalized invariant measure [272]

\[
d\mu = d\xi d\theta d\phi \frac{1}{8\pi^2} \tag{4.9.3}
\]

The approximation on which our analysis is based (i.e. the potential wall model) is reliable since it is dynamically induced, no matter what time variable \( \tau \) is adopted. Further-
more, such invariant measure turns out to be independent on the choice of the temporal
gauge, as shown in [272].

The use of the invariant measure and of the Artins theorem [20] provides the complete
equivalence between the BKL piece-wise description and the Misner-Chitre continuous one [303].

According to the analysis presented in [379], by virtue of (4.8.13) and (4.8.34), the a-
symptotic functions $\xi(\Gamma), \theta(\Gamma), \phi(\Gamma)$ during the free geodesic motion are governed by the equations

\[
\begin{align*}
\frac{d\xi}{d\Gamma} &= \sqrt{\xi^2 - 1} \cos \phi \quad (4.9.4a) \\
\frac{d\theta}{d\Gamma} &= \frac{\sin \phi}{\sqrt{\xi^2 - 1}} \quad (4.9.4b) \\
\frac{d\phi}{d\Gamma} &= -\frac{\xi \sin \phi}{\sqrt{\xi^2 - 1}} \quad (4.9.4c)
\end{align*}
\]

whose parametric solution $\xi(\Gamma)$ has the form

\[
\begin{align*}
\xi(\phi) &= \frac{\rho}{\sin^2 \phi} \quad (4.9.5a) \\
\Gamma(\phi) &= \frac{1}{2} \arctanh \left( \frac{1}{2} \frac{\rho^2 + a^2 \cos^2 \phi}{a \rho \cos \phi} \right) + b \quad (4.9.5b) \\
\rho &= \sqrt{a^2 + \sin^2 \phi} \quad a, b = \text{const.} \in \mathbb{R}.
\end{align*}
\]

However, the global behaviour of $\xi$ along the whole geodesic flow is described by the
invariant measure (4.9.3) and therefore the temporal behavior of $\Gamma(\tau)$ acquires a stochas-
tic character: if we assign one of the two functions $\Gamma(\tau)$ or $N(\tau)$ with an arbitrary analytic
functional form, then the other one will exhibit a stochastic behaviour. Finally, by retaining
the same dynamical scheme adopted in the construction of the invariant measure, we
see how the one-to-one correspondence between any lapse function $N(\tau)$ and the associ-
ated set of MCI variables (4.8.3) guarantees the covariance with respect to the time-gauge.

### 4.10 Chaos covariance

We have discussed the oscillatory regime whose properties characterize the behavior of
the Bianchi types VIII and IX cosmological models in the BKL formalism [54, 57, 367] near
a physical singularity, in which it is outlined the appearance of chaotic properties [402]:
firstly, the dynamics evolution of the Kasner exponents characterized the sequence of the
Kasner epochs, each one described by its own line element, with the epochs sequence
nested in multiple eras. Secondly, the use of the parameter $u$ and its relation to dynamical
functions offered the statistical treatment connected to each Kasner era, finding an appro-
priate expression for the distribution over the space of variation: the entire evolution has
been decomposed in a discrete mapping in terms of the rational/irrational initial values
attributed to $u$.

The limits of this approach essentially reside in the non-continuous evolution toward the
initial singularity and the lack of an assessment of chaoticity in accordance with the indi-
cators commonly used in the theory of dynamical systems, say in terms of the estimate of Lyapunov exponents.

A wide literature faced over the years this subject in order to provide the best possible understanding of the resulting chaotic dynamics [49, 64].

The research activity developed overall in two different, but related, directions:

(i) on one hand, the dynamical analysis was devoted to remove the limits of the BKL approach due to its discrete nature (by analytical treatments [33, 124, 105, 82, 152, 151, 393, 376] and by numerical simulations [443, 64, 67, 74, 74].

(ii) on the other one, to get a better characterization of the Mixmaster chaos (especially in view of its properties of covariance [198, 196, 480, 258].

The first line of investigation provided satisfactory representations of the Mixmaster dynamics in terms of continuous variables [87], mainly studying the properties of the BKL map and its reformulation as a Poincaré one [32].

In parallel to these studies, detailed numerical descriptions have been performed with the aim to test the precise validity of the analytical results [443, 64, 75, 71, 156].

The efforts [82, 148, 443] to develop a precise characterization of the chaoticity observed in the Mixmaster dynamics found non-trivial difficulties due to the impossibility, or in the best cases the ambiguity, to apply the standard chaos indicators to relativistic systems. However, the chaotic properties summarized so far were questioned when numerical evolution of the Mixmaster equations yielded zero Lyapunov exponents [104] [258, 203]. Nevertheless, exponential divergence of initially nearby trajectories was found by other numerical studies yielding positive Lyapunov numbers. This issue was understood when in [64] and [198] numerically and analytically was shown how such calculations depend on the choice of the time variable and parallely to the failure of the conservation of the Hamiltonian constraint in the numerical simulations by [54], although was still debated by [258].

In particular, the first clear distinction between the direct numerical study of the dynamics and the map approximation, stating the appearance of chaos and its relation with the increase of entropy, has been introduced by [105]. The puzzle consisted of simulations providing even in the following years zero (see for example [196]) Lyapunov numbers, claiming that the Mixmaster Universe is non-chaotic with respect to the intrinsic time (associated with the function $\alpha$ introduced for the Hamiltonian formalism) but chaotic with respect to the synchronous time (i.e. the temporal parameter $t$). The non-zero claims [480] about Lyapunov exponents, using different time variables, have been obtained reducing the Universe dynamics to a geodesic flow on a pseudo-Riemannian manifold: on average, local instability has been discussed for the BKL approximations. Moreover, a geometrized model of dynamics defining an average rate of separation of nearby trajectories in terms of a geodesic deviation equation in a Fermi basis has been interpreted for detection of chaotic behavior as a principal Lyapunov exponent. A non-definitive result was given: the principal Lyapunov exponents result always positive in the BKL approximations but, if the period of oscillations in the long phase (the evolution of long oscillations, i.e. when the particle enters the corners of the potential) is infinite, the principal Lyapunov exponent tends to zero.

For example, the author of [64] reports the dependence of the Lyapunov exponent on the choice of the time variable. Through numerical simulations, the Lyapunov exponents
were evaluated along some trajectories in the \((\beta_+, \beta_-)\) plane for different choices of the time variable, more precisely \(\tau\) (BKL), \(\Omega\) (Misner) and \(\lambda\), the “mini-superspace” one, i.e. 
\[
d\lambda = | - p_0^2 + p_+^2 + p_-^2 |^{1/2} d\tau.
\]
It is shown that the same trajectory giving zero Lyapunov exponent for \(\tau\) or \(\Omega\)-time, fails for \(\lambda\).

Such contrasting results can find a clear explanation realizing the non-covariant nature of these indicators and their inapplicability to hyperbolic manifolds. The existence of such difficulties prevented, up to now, to say a definitive word about the general picture concerning the covariance of the Mixmaster chaos, with particular reference to the possibility of removing the observed chaotic features by a suitable choice of the time variable, apart from the indications provided by [152, 151].

Interest in these covariance aspects has increased in recent years in view of the contradictory and often dubious results that emerged. The confusion which arises regarding the effect of a change of the time variable in this problem depends on some special properties of the Mixmaster model when represented as a dynamical system, in particular the vanishing of the Hamiltonian and its non-positive definite kinetic term (typical of a gravitational system). These peculiar features prevent the direct application of the most common criteria provided by the theory of dynamical systems for characterizing chaotic behavior (for a review, see [258]).

Although a whole line of research opened up [418, 482], the first widely accepted indications in favor of covariance were derived with a fractal formalism by [152, 151] (see also [387]). Indeed, the requirement of a complete covariant description of the Mixmaster chaoticity when viewed in terms of continuous dynamical variables, due to the discrete nature of the fractal approach, leaves this subtle question open and prevents a general consensus in this sense from being reached.

### 4.10.1 Invariant Lyapunov Exponent

In order to characterize the dynamical instability of the billiard in terms of an invariant treatment (with respect to the choice of the coordinates \(\xi, \theta\)), let us introduce the following (orthonormal) tetradic basis [273]

\[
v^i = \left( \frac{1}{E} \sqrt{\xi^2 - 1} \cos \phi, \frac{1}{E} \frac{\sin \phi}{\sqrt{\xi^2 - 1}} \right), \quad (4.10.1a)
\]
\[
w^i = \left( \frac{1}{E} \sqrt{\xi^2 - 1} \sin \phi, \frac{1}{E} \frac{\cos \phi}{\sqrt{\xi^2 - 1}} \right). \quad (4.10.1b)
\]

Indeed, the vector \(v^i\) is nothing else than the geodesic field, i.e. it satisfies

\[
\frac{Dv^i}{ds} = \frac{dv^i}{ds} + \Gamma^i_{kl}v^k v^l = 0, \quad (4.10.2)
\]

while the vector \(w^i\) is parallely transported along the geodesic, according to the equation

\[
\frac{Dw^i}{ds} = \frac{dw^i}{ds} + \Gamma^i_{kl}v^k w^l = 0, \quad (4.10.3)
\]
where \( \Gamma^i_{kl} \) are the Christoffel symbols constructed by the reduced metric (4.8.35). Projecting the geodesic deviation equation along the vector \( w^i \) (its component along the geodesic field \( v^i \) does not provide any physical information about the system instability), the corresponding connecting vector (tetradic) component \( Z \) satisfies the following equivalent equation

\[
\frac{d^2 Z}{ds^2} = \frac{Z}{E^2}.
\]

This expression, as a projection on the tetradic basis, is a scalar one and therefore completely independent of the choice of the variables. Its general solution reads as

\[
Z(s) = c_1 e^{sE} + c_2 e^{-sE}, \quad c_{1,2} = \text{const.}
\]

and the corresponding invariant Lyapunov exponent [343] is defined as [409]

\[
\lambda_v = \sup \lim_{s \to \infty} \frac{\ln \left( Z^2 + \left( \frac{dZ}{ds} \right)^2 \right)}{2s},
\]

which, in terms of (4.10.5), takes the value [273]

\[
\lambda_v = \frac{1}{E} > 0.
\]

The limit (4.10.6) is well defined as soon as the curvilinear coordinate \( s \) approaches \( \infty \). In fact, from (4.8.34) we see that the singularity corresponds to the limit \( \Gamma \to \infty \), and this implies \( s \to \infty \).

When the point-Universe bounces against the potential walls, it is reflected from a geodesic to another one, thus making each of them unstable. Though with the limit of our potential wall approximation, this result shows that, independently of the choice of the temporal gauge, the Mixmaster dynamics is isomorphic to a well described chaotic system. Equivalently, in terms of the BKL representation, the free geodesic motion corresponds to the evolution during a Kasner epoch and the bounces against the potential walls to the transition between two of them. By itself, the positive Lyapunov number (4.10.7) is not enough to ensure the system chaoticity, since its derivation remains valid for any Bianchi type model; the crucial point is that for the Mixmaster (types VIII and IX) the potential walls reduce the configuration space to a compact region \( \Pi_Q \), ensuring that the positivity of \( \lambda_v \) implies a real chaotic behaviour (i.e. the geodesic motion fills the entire configuration space).

Furthermore, it can be shown that the Mixmaster asymptotic dynamics and the structure of the potential walls fulfill the hypotheses at the basis of the Wojtkowsky theorem [509, 60]; this result ensures that the largest Lyapunov exponent has a positive sign almost everywhere.

Generalizing, for any choice of the time variable, we are able to give a stochastic representation of the Mixmaster model, provided the factorized coordinate transformation in [386] it is shown that, given a dynamical system of the form \( \frac{dx}{dt} = F(x) \), the positiveness of the associated Lyapunov exponents are invariant under the following diffeomorphism: \( y = \phi(x, t), dt = \lambda(x, t)dt \), as soon as several requirements hold, fulfilled by the Mixmaster [60].

\[70\]
the configuration space

\[
\begin{align*}
\alpha &= -e^{\Gamma(\tau)} a (\theta, \xi) \\
\beta_+ &= e^{\Gamma(\tau)} b_+ (\theta, \xi) \\
\beta_- &= e^{\Gamma(\tau)} b_- (\theta, \xi),
\end{align*}
\]

(4.10.8a,b,c)

where \(\Gamma, a, b_\pm\) denote generic functional forms of the variables \(\tau, \theta, \xi\).

It is worth noting that this analysis relies on the use of a standard ADM reduction of the variational principle (which reduces the system by one degree of freedom) and overall because, adopting MCI variables, the asymptotic potential walls are fixed in time. This effectively is the difference between the above approach and the one presented in [481, 474] (see also for a critical analysis [102]), though in those works the problem of the Mixmaster chaos covariance is faced even with respect to the choice of generic configuration variables.

### 4.10.2 On the Occurrence of Fractal Boundaries

In order to give an invariant characterization of the dynamics chaoticity, many methods along the years have been proposed, but not all approaches have reached an undoubtable consensus. A very interesting one, relying on techniques considering fractality of the basin of initial conditions evolution has been proposed in 1997 in [152] and opened a whole line of debate. The conflict among different approaches has been tackled by using an observer-independent fractal method, though leaving some questions open about the conjectures lying at the basis of it.

The asymptotic behaviour towards the initial singularity of a Bianchi type IX trajectory depends on whether or not we have a rational or irrational initial condition for the parameter \(u\) in the BKL map. In such a scheme, the effect of the Gauss map has been considered together with the evolution of the equations of motion, in order to “uncover” dynamical properties about the possible outcoming configurations with the varying of the corresponding initial conditions.

Nevertheless, such approach led to some doubts regarding the reliability of the method itself. In fact, let us observe that rational numbers initial conditions are dense and yet constitute a set of zero measure and moreover correspond to fictitious singularities [54, 367, 368]. The nature of this initial set needs to be compared with the one regarding the complete set of initial conditions, with finite measure over a finite interval: the conclusions obtained after the dynamical evolution are not necessarily complementary between the two initial assumptions.

In [151, 152], Cornish and Levin used a coordinate-independent fractal method to show that the Mixmaster Universe is indeed chaotic. By exploiting techniques originally developed to study chaotic scattering, they gained a new perspective on the evolution of the Mixmaster cosmology, finding a fractal structure, namely the strange repellor (see Fig.4.4), that well describes chaos. A strange repellor is the collection of all Universes periodic in \((u, v)\), and an aperiodic one will typically experience a transient age of chaos if it brushes against the repellor. The fractal pattern was exposed in both the exact Einstein equations and in the discrete map used to approximate the solution. The most important feature gained is a fractal approach independent of the adopted time coordinate and the chaos reflected in the fractal weave of Mixmaster Universes is unambiguous.
The approach used in [152, 151] is based on the method firstly stated in [84] where it is shown how fractal boundaries can occur for some solutions involving chaotic systems. The space of initial conditions is spanned giving rise to different exit behaviours whose borders have fractal properties: this constitutes a conjecture as a typical property of chaotic Hamiltonian dynamics with multiple exit modes.

For the case of the Bianchi IX model potential (see Figure 4.2) the openings are obtained widening the three corners, on the basis that the point representing the evolution spends much of the time there nearby.

This method has three essential fallacies:

i) the case-points chosen as representatives within this framework are the ones whose dynamics proceeds never reaching the singularity;

ii) the “most frequent” dynamical evolution is the one in which the point enters the corner with the velocity not parallelly oriented towards the corner’s bisecting line and, after some oscillations, it is sent back in the middle of the potential. This effect is altered when opening the potential corners;

iii) the artificial opening up of the potential corners adopted in the basin boundary approach could be creating the fractal nature of it.

In particular, the third observation is supported by the existence of strange attractors that are not chaotic, as counter-exampled by [224] and discussed by [248]. The choice of the method adopted to characterize the property of chaos or its absence is very relevant, especially when based on the presence of fractal boundaries in the dynamics underlying Bianchi IX models. This is important to be checked, first of all, because the result of
4.10 Chaos covariance

[152] [151] relies on the conjecture as in [84] that opening gates in a chaotic Hamiltonian system can result in the presence of fractal basin boundaries (which needs in principle to be checked in the case of Bianchi IX), not satisfying the necessity of a general statement concerning chaos: even the opening of the corners does not solve the question about what happens when taking the limit of closing them and if there is an universal behaviour (for general systems).

Secondly, it is needed to integrate the Bianchi IX flow and this operation is not necessarily commuting with the statement regarding the remaining (and equally relevant) part of the set of initial conditions constituted by the irrational numbers, which needs to be checked.

Motter and Letelier, in [387] in the criticism to the paper of [152] [151], claim the same results with more accurate comprehension of the global chaotic transient and afford calculations involving a more stable constraint check and a higher order integrator. Again the same criteria used by [152] [151] is followed to get the same results. The informations obtained following the Farey map approach are not relevant (only rational values of $u$ are led to the three peculiar outcomes) because the corresponding invariant set contains almost every point of phase space. But they claim it is possible to get strict indications of chaos with the Hamiltonian exit method [84] [461] [168] [167] [85].

Firstly one has to fix the width ($\rightarrow u_{\text{exit}}$) of the open corners, then let the system evolve. The future invariant set leads to a box-counting dimension $D_0$ (estimated from the uncertainty exponent method [402]) coherent with previous results, which is, by construction, a function of the width itself. The value of $D_0$ found, equal numerically to 1.87, is dependent on the change done to the original potential, and converges to the value of 2, which is an indicator of non-chaoticity [169]. Any of such fundamental properties, if outlined in a specific case, must be jointed through a limit procedure to the general one.

Pianigiani and Yorke in [410] study the evolution of a ball on a billiard table with smooth obstacles so that all trajectories are unstable with respect to initial data. This is a system energy conserving and then they open a small hole on such table in order to allow the ball to go through. Such two differences have not been taken account of in the Bianchi IX analysis.

In the work by [461] Schneider et al. it is supposed to show the existence of a chaotic saddle, whose signature is the chaotic basin.

The paper by [169] declares the absence of such points, in a model with $\Lambda = 0$, hence we infer the inapplicability of that method to discover a supposed unknown feature of a dynamical system.

They stress too that the limit (not unnatural) for $\Lambda \to 0$ doesn’t matches: it doesn’t permit to characterize the chaos in mixmaster vacuum model: a continuous change in a parameter of the theory heavily affects the method’s applicability, mainly while the study of Bianchi IX dynamics is of interest towards the initial singularity, where the BKL approach applies: in such approximation, the domain walls close to a circle.

Hence there are objections which are subject for interesting further investigation

(i ) has the opening of a polygonal domain the same effect as the opening a circle (which has curvature)?

(ii ) Is the system truly independent from temporal reparameterization?

(iii ) Is the opening independent of temporal (either spatial) reparameterization?
Could exist a temporal reparameterization whose effect is to close the artificial openings?

How to interpret this eventuality?

Even if this is not relevant for dynamical system in classical mechanics, in General Relativity it would; for example, Cornish and Levin claim that they open a non compact domain, differently from Misner.

For all the criticism here outlined we consider an analytical approach crucial to distinguish among chaos indicators relying on numerical properties not well-manageable via numerical simulations.

4.11 Isotropization Mechanisms

The isotropic FRW model can accurately describe the evolution of the Universe until the decoupling time, i.e. $10^{-3} - 10^{-2}$ seconds after the Big-Bang\[310]. On the other hand, the description of its very early stages requires more general models, like at least the homogeneous ones. Therefore we are interested to investigate some mechanisms allowing a transition between these two cosmological epochs. When the anisotropy of the Universe is sufficiently suppressed, we can speak of a quasi-isotropization of the model \[472, 139, 140, 146\] (for a detailed discussion of the isotropization mechanism see \[183, 182, 460, 366, 191, 232, 47, 271, 233, 126, 504, 114, 192, 282, 113, 359, 413\]) and such mechanism can be regarded as a “bridge” between the two stages.

In this paragraph we will discuss the origin of a background space when a real self-interacting scalar field $\phi$ is taken into account, following the work \[305\]. Let us extend the Misner-like variables \[302\] (see (4.5.1))

$$q^a = A^a_j \beta^j + \alpha, \quad \beta^3 = \frac{\phi}{\sqrt{3}},$$

(4.11.1)

where $j = 1, 2$, $a = 1, 2, 3$ and $A^a_j$ satisfy

$$\sum_a A^a_j = 0, \quad \sum_a A^a_j A^a_k = 6 \delta_{jk}. \quad (4.11.2)$$

As usual, $\alpha$ parametrizes the isotropic change of the metric with the singularity appearing as $\alpha \to -\infty$ and the $\beta^j$ the anisotropies of the model. When these variables approach some constants as a limit we can speak of a quasi-isotropization of the model (for a discussion on the quasi-isotropic solution see \[325, 293, 292, 277\]).

The action expressed in terms of them writes as

$$S = \int dt \left[ P_r \partial_t \beta^r + P_a \partial_t \alpha - \frac{N}{6 \sqrt{h}} \left( \sum_r P_r^2 + 6U - P_a^2 \right) \right], \quad (4.11.3)$$

The chaotic nature of the evolution toward the singularity implies that the geometry, and therefore all the geometric quantities, should be described in an average sense only. With this respect, the Universe does not possess a stable background near the singularity \[299, 304\].
4.11 Isotropization Mechanisms

where $r = 1, 2, 3$, $h = \exp(3\alpha)$ and the potential term (4.8.16) is now defined as $U = h(W - (3)R)$ with $W(\phi) = \frac{1}{2}[h^i\partial_i\phi^2] + V(\phi)$. From the action (4.11.3) an inflationary solution comes out imposing the constraint

$$\frac{1}{h} U \simeq V(\phi) \simeq \text{const.} \gg (3)R$$

which can be realized by an appropriate process of spontaneous symmetry breaking, exhaustively studied in [305, 377]. Let us consider the situation where $U = h\Lambda$, where $\Lambda = \text{const.}$ The Hamilton-Jacobi equation is

$$\sum_r \left( \frac{\delta S}{\delta \beta r} \right)^2 - \left( \frac{\delta S}{\delta \alpha} \right)^2 + 6\exp(3\alpha)\Lambda = 0,$$

whose solution can be expressed as

$$S(\beta^r, \alpha) \sim K_r\beta^r + 2K_a + \frac{K}{3} \ln \left| \frac{K_a - K}{K_a + K} \right|,$$

where $K_a(K_r, \alpha) = \pm \sqrt{\sum_r K_r^2 + 6\Lambda\exp(3\alpha)}$, with some generic constants $K = \sqrt{\sum_r K_r^2}$ and $K_r$. The equation of motion for $\alpha$ is readily obtained as from (4.11.3)

$$\frac{\partial \alpha}{\partial t} = -\frac{NP_a}{3\exp(3\alpha/2)}.$$

Choosing $\alpha$ as the time coordinate, i.e. $\partial_t \alpha = 1$, the time gauge condition becomes $N = -3\exp(3\alpha/2)/P_a$. Since the lapse function is positive defined we must also have $P_a < 0$.

Accordingly to the Hamilton-Jacobi method, one has firstly to differentiate with respect to $K_r$ and then, equating the results to arbitrary constants, one finds the solutions describing the trajectories of the system as

$$\frac{\delta S}{\delta K_r} = \beta'_0 \Rightarrow \beta'(\alpha) = \beta'_0 + \frac{K_r}{3K} \ln \left| \frac{K_a - K}{K_a + K} \right|,$$

where $\beta'_0$ are new arbitrary constants. Let us investigate the two limits of interest. First of all, let us note that for $h \to \infty$ (i.e. $\alpha \to \infty$, $K \to \infty$) the solution (4.11.8) transforms into the inflationary one obtained in [472], corresponding to the quasi-isotropization of the model as the functions $\beta^r$ approach the constants $\beta'_0$. On the opposite limit, i.e. for $h \to 0$ ($\alpha \to -\infty$, $K_a \to K$), the solution (4.11.8) provides the generalized Kasner one as expected, simply modified by the presence of the scalar field [53]

$$\beta'(\alpha) = \beta'_0 - \frac{K_r}{K}(\alpha - \alpha_0),$$

$\alpha_0$ being the remaining constants.

The existence of the solution (4.11.8) shows how the inflationary scenario [230, 231, 327, 462] can provide the necessary dynamical “bridge” between the fully anisotropic and the quasi-isotropic epochs of the Universe evolution. In fact, during that time the anisotropies $\beta_{\pm}$ are dumped and the only effective dynamical variable is $\alpha$, i.e. the one related to the
isotropic volume of the Universe. This shows how the dominant term during the inflation is \( \Lambda e^{3a} \) and any term in the spatial curvature becomes more and more negligible although increasing like (at most) \( e^{2a} \).

For a sample of works dealing with the Bianchi models dynamics involving a cosmological term, see [464, 507, 118, 135, 415, 414, 453, 119, 411].

### 4.12 Cosmological Implementation of the Bianchi Models

In this paragraph we shall examine the cosmological issues of the Bianchi models. In particular, we will focus attention on the question about the corresponding theoretical predictions regarding the relic Cosmological Background Radiation (CMB) anisotropy [166, 323]. Confirmed observations [239, 417, 469, 342, 392] show that the large-scale relic radiation anisotropy \( \Delta T/T \) is about

\[
\Delta T/T \leq 2 \cdot 10^{-5},
\]

in terms of the equivalent black body radiation temperature \( T \). Therefore the Universe becomes transparent to the relic radiation at an epoch when the expansion anisotropy is “small”. A comparison between the theory and the experimental observations requires the analysis of a quasi-isotropic stage of the Bianchi models.

The discussion which follows is mainly based on the textbook [516] and references therein (see also [471]). Initially we approach the Bianchi I model and then we focus attention on the more general Bianchi IX model.

#### 4.12.1 Expected Anisotropy of CMB for Bianchi I

Let us analyze the Bianchi I model, characterized by a flat, comoving three-dimensional space.

We will include in the dynamics an ordered magnetic field having oriented fluxes of relativistic particles since they inevitably develop as a consequence of the processes during the early stages of anisotropic expansion. Let the magnetic field be oriented along the \( z \)-axis, \( W \) be its energy density and \( p_x, p_y, p_z \) components of the pressure of the free particles along the corresponding axes. Let us also assume \( \epsilon \gg W \) and \( \epsilon \gg p_x, p_y, p_z \) and moreover \( a^{-1}da/dt \sim b^{-1}db/dt \sim c^{-1}dc/dt \), \( \epsilon \) being the energy density of ordinary matter. Such relations ensure that, to first approximation, the expansion isotropically takes place and thus the equations of motion read as

\[
\begin{align*}
\frac{1}{abc} \frac{d}{dt} \left[(a^{-1}da/dt - b^{-1}db/dt) \ abc\right] = \kappa(p_x - p_y) \quad (4.12.2a) \\
\frac{1}{abc} \frac{d}{dt} \left[(a^{-1}da/dt - c^{-1}dc/dt) \ abc\right] = \kappa[(p_x - p_z) + 2W]. \quad (4.12.2b)
\end{align*}
\]

Suppose that \( P \) is the pressure associated to \( \epsilon \) and consider the particular case of ultra-relativistic matter \( P = \epsilon/3 \) (corresponding to \( a \sim b \sim c \sim t^{1/2} \)). In this case, we can derive the behavior of the deformation anisotropies (defined as the left-hand sides of the following equations (4.12.3)) when the expansion is almost periodic and (4.12.2) rewrite
as

\[ \frac{a^{-1}da/dt - b^{-1}db/dt}{a^{-1}da/dt} = \frac{3(p_x - p_y)}{e} + 2 \left( \frac{t^*}{t} \right)^{1/2} \]  
\( (4.12.3a) \)

\[ \frac{a^{-1}da/dt - c^{-1}dc/dt}{a^{-1}da/dt} = \frac{3(p_x - p_z)}{e} + 6 \frac{W}{e} + 2 \left( \frac{t^*}{t} \right)^{1/2}, \]  
\( (4.12.3b) \)

\( t^* \) being a constant. In absence of matter the anisotropy decays as \( t^{-1/2} \). On the other hand, when the expansion is almost periodic, the ratios \( (p_x - p_y)/e \) as well as \( W/e \) remain constant. Therefore, in presence of a magnetic field or of a flux of relativistic particles, the deformation anisotropy is conserved during the era when \( P = e/3 \). In conclusion, the anisotropy of the stress-energy tensor slows down the isotropization of solution. This statement can be generalized for all (reasonable) kinds of matter and in particular for the case \( P = 0 \).

Let us discuss the equation for the anisotropy of the relic radiation temperature and how it is related to the expansion anisotropy, and consider an observer receiving the radiation from the direction of the two axes with scale factors \( a \) and \( b \). The observed difference of temperature in those two directions is

\[ \Delta T \bigg|_{t \to \infty} = \frac{a - b}{a} \bigg|_{z_1} \]  
\( (4.12.4) \)

where \( z_1 \) is the redshift associated to the time when the Universe is transparent to the radiation and the radiation field is isotropic.

If the sharply anisotropic stage ends before the time when the radiation density \( \rho_r \) equates the baryon one \( \rho_m \), then the deformation anisotropy \( (4.12.3a) \) is conserved. After this stage, in the \( P = 0 \) epoch the anisotropy decreases according to

\[ \frac{a - b}{a} = 6 \frac{\rho_{anis}}{\rho_m} \sim t^{-2/3}, \]  
\( (4.12.5) \)

\( \rho_{anis} \) being the density of the anisotropic neutrino flux \( (\rho_{anis}/\rho_r \sim 0.1 - 1) \). Assuming the transparency redshift as \( z_1 = 8 \), one obtains

\[ \Delta T \bigg|_{t \to \infty} = \frac{a - b}{a} \bigg|_{z_1=8} = 6 \frac{\rho_{anis}}{\rho_m} \bigg|_{z_1=8} \simeq 10^{-4} - 10^{-3}. \]  
\( (4.12.6) \)

Hence, expression \( (4.12.6) \) gives the expected value for the relic radiation anisotropy although it is valid only in the case \( \rho_m = \rho_{crit} \) (flat space).

### 4.12.2 Expected Anisotropy of CMB for Bianchi IX

In the homogeneous cosmological models with curved comoving space, as Bianchi IX is, the deformation anisotropy behaves in a way similar to the one described above. In fact, it is constant during the radiation dominated era up to the time when \( \rho_r = \rho_m \). Nevertheless, the difference relies in the role played by the non-interacting particles in Bianchi I, which actually is taken by the spatial curvature. Then, after this epoch, the

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\[ ^6 \text{After this time the radiation freely propagates.} \]
anisotropy decreases as $t^{-2/3}$, while during the time when $\rho_r = \rho_m$ the matter becomes transparent to the background radiation and the photons freely propagate.

Therefore, let us underline two main aspects of the relic radiation anisotropy in the anisotropic models. The first feature is related to the conservation of the deformation anisotropy during the radiation dominated era, and it is responsible for the amplitude of $\Delta T / T$. The second characteristic is connected to the curvature of the comoving space and the consequent motion of the photons which gives rise to the different angular distributions on the sky of the background anisotropy.

The anisotropy of the relic radiation temperature can now be calculated with the same arguments given above for Bianchi I and it depends on three characteristic temporal steps:

i) $t_\phi$, the time of the beginning of the isotropic stage, when $a \simeq b$;

ii) $t_c$, when the equation of the state changes, i.e. when it effectively becomes $P = 0$ and after this time all the deviations from exact isotropy decay as a power law;

iii) $t_e$, when matter becomes transparent.

Explicitly, the anisotropy of the temperature background reads as \[ \frac{\Delta T}{T} \simeq \frac{8}{\ln[(t_c/t_\phi)^{e^8}]} \left(\frac{t_c}{t_e}\right)^{2/3}. \] (4.12.7)

It is worth noting that the above formula (4.12.7) is alarmingly unstable to small numerical changes in underlying parameters. This feature is widely discussed in [36] where an analysis of the cosmological evolution of matter sources with small anisotropic pressures is performed (see also [37] for applications to the magnetic case and [35] in which a more general analysis is shown). Furthermore the dependence of (4.12.7) on the isotropization time $t_\phi$ is extremely weak. In fact, taking $t_c \simeq t_e$ and assuming $\Delta T / T \sim \mathcal{O}(10^{-3})$, one has $t_\phi \sim \mathcal{O}(t_P)$, where $t_P \sim \mathcal{O}(10^{-44}\text{s})$ is the Planck time. Therefore isotropization would take place in the region when the applicability of classical General Relativity is expected to fail. On the other hand, $\Delta T / T$ is of order of the values experimentally observed only if the factor $(t_c/t_e)^{2/3}$ is small, i.e. if the matter becomes transparent much later than the end of the radiation dominated epoch ($t_e \gg t_c$) and this is possible only if the amount of ionized intergalactic gas is so relevant that the critical parameter is $\Omega \sim \mathcal{O}(1)$.

With respect to the angular distribution, we stress that the light propagates along the principal direction of the deformation tensor and therefore the anisotropy has a quadrupole character.

As last point, we have to stress that in above analysis no mention to inflation is made. Indeed it would a major damping effect on any primordial anisotropy, massively reducing it below (4.12.7) though. About this point we refer to [36, 37, 35].

### 4.13 The Role of a Scalar Field

In this Section we face the influence of a scalar field when approaching the cosmological singularity. As shown in the initial studies [52, 53], such field can suppress the Mixmaster oscillations during the evolution toward the singularity.
4.13 The Role of a Scalar Field

Following the approach given in [69], let us consider the Mixmaster Universe in the presence of a self-interacting scalar field $\phi$. As we have seen previously, the Einstein equations are obtained from the variation of the Hamiltonian constraint $H = 0$, where ($N \propto e^{3\alpha}$)

$$H = H_K + H_V,$$

where $H_K$ and $H_V$ being the kinematic and potential part of the Hamiltonian, respectively. In particular we have

$$H_K = -p_+^2 + p_-^2 + p_\phi^2,$$  (4.13.2)

and

$$H_V = e^{4\alpha} \left[ e^{-8\beta_+} + e^4 \beta_+ \left( + e^4 \beta_- - 4\sqrt{3} \beta_- \right) \right] + e^{6\alpha} V(\phi),$$  (4.13.3)

where with $V(\phi)$ we denote a generic potential of the scalar field. Working with such Misner variables the cosmological singularity appears as $\alpha \to -\infty$. Therefore, unless $V(\phi)$ contains terms exponentially growing with $\alpha$, the very last term in (4.13.3) can be neglected at early times, i.e. $e^{6\alpha} V(\phi) \to 0$ as $\alpha \to -\infty$.

Let us consider the kinematic part $H_K$. Its variation yields equations whose solution reads as

$$\begin{align*}
\beta_\pm &= \beta_\pm^0 + v_\pm |\alpha| \\
\phi &= \phi^0 + v_\phi |\alpha|,
\end{align*}$$  (4.13.4)

where $v_\pm = p_\pm / |p_\alpha|$ and $v_\phi = p_\phi / |p_\alpha|$. Therefore the constraint $H_K = 0$ becomes

$$v_+^2 + v_-^2 + v_\phi^2 = 1.$$  (4.13.5)

Let us firstly analyze the case without the scalar field, i.e. $\phi \equiv 0$. Introducing polar coordinates in the anisotropy planes as $v_+ = \cos \theta$ and $v_- = \sin \theta$, through equations (4.13.4) the potential (4.13.3) rewrite as

$$H_V \sim e^{-4 |\alpha| (1 + 2 \cos \theta)} + e^{-4 |\alpha| (1 - \cos \theta - \sqrt{3} \sin \theta)} + e^{-4 |\alpha| (1 - \cos \theta + \sqrt{3} \sin \theta)},$$  (4.13.6)

where we maintained the dominant terms only, i.e. the first three terms in (4.13.3). Except for the set of zero measure of values $\theta = (0, 2\pi / 3, 4\pi / 3)$, any generic value of $\theta$ will cause the growth of one of the terms on the r.h.s. of (4.13.6).

Let us consider the case $\phi \neq 0$ and hence $v_\phi^2 > 0$. Equation (4.13.5) is replaced by

$$v_+^2 + v_-^2 = 1 - v_\phi^2 < 1,$$  (4.13.7)

thus none of the terms in (4.13.6) will grow if the following conditions are satisfied

$$\begin{align*}
1 + 2v_+ &> 0 \\
1 - v_+ - \sqrt{3} v_- &> 0 \\
1 - v_+ + \sqrt{3} v_- &> 0,
\end{align*}$$  (4.13.8)
situation which is realized if $v_{\pm}^2 < 1/2$ and $v_0^2 < 1/12$, which occur if $2/3 < v_{\phi}^2 < 1$. In [74] it is described how $p_0$ decreases at each bounce, and therefore for any initial value of $p_{\phi}$ it is always $v_{\phi}^2 > 2/3$.

As we have seen, the approach to the singularity of the Bianchi IX model is described by a particle moving in a potential with exponentially closed walls bounding a triangular domain. During the evolution, the particle bounces against the walls providing an infinite number of oscillations toward the singularity. The scalar field influences such dynamics so that for values of $v_{\pm}$ satisfying (4.13.8), there are not further bounces and the solution approaches (4.13.4). In other words there will be an instant of time after which the point-Universe does not ever reach the potential walls and no more oscillations appears. In this sense the scalar field can suppress the chaotic Mixmaster dynamics toward the classical cosmological singularity.

### 4.14 Multidimensional Homogeneous Universes

When the number of spatial dimensions is greater than three, homogeneous models can loose their chaotic dynamics, as already arises in the four-dimensional case. The question of chaos in higher dimensional cosmologies has been widely investigated, and many authors [42, 206, 238, 237] showed that none of higher-dimensional extensions of the Bianchi IX model possesses proper chaotic features and the crucial difference is given by the finite number of oscillations characterizing the dynamics near the singularity. Without loss of generality we will follow the analysis proposed by Halpern [238, 237] and limit our discussion to the case of a homogeneous model with four spatial dimensions.

The work of Fee [195] classifies the four-dimensional homogeneous spaces in 15 types, named $G_0 – G_{14}$, and it is based on the analysis of the corresponding Lie groups. The line element can be written using the Cartan basis of left-invariant forms and explicitly reads as ($N = 1$)

$$ds^2 = dt^2 - 4 \eta_{rs}(t) \omega^r \otimes \omega^s. \quad (4.14.1)$$

The 1-forms $\omega^r$ obey the relation $d\omega^r = \frac{1}{2} C^r_{pq} \omega^p \wedge \omega^q$, where the $C^r_{pq}$ are the four-dimensional structure constants. The discussion remains quite general even limiting it to the case of a diagonal matrix $4 \eta_{rs}$

$$4 \eta_{rs} = \text{diag}(a^2, b^2, c^2, d^2). \quad (4.14.2)$$
The Einstein equations are obtained with the standard procedure as

\[
\begin{align*}
R^0_0 &= \frac{\ddot{a} + \dot{b} + \dot{c} + \dot{d}}{a} = 0, \\
R^1_1 &= \frac{(\dot{a} \dot{b} \dot{c} \dot{d})}{abcd} + S^1_1 = 0, \\
R^2_2 &= \frac{(\dot{a} \dot{b} \dot{c} \dot{d})}{abcd} + S^2_2 = 0, \\
R^3_3 &= \frac{(\dot{a} \dot{b} \dot{c} \dot{d})}{abcd} + S^3_3 = 0, \\
R^4_4 &= \frac{(\dot{a} \dot{b} \dot{c} \dot{d})}{abcd} + S^4_4 = 0, \\
R^n_n &= \left(\frac{x_n}{x_n} - \frac{\dot{x}_n}{x_n}\right) C^m_{mn} = 0;
\end{align*}
\]

where \(x_n\) \((n = 1, 2, 3, 4)\) denote the scale factors \(a, b, c, d\), respectively, and the \(S^n_n\) are functions of them and of the structure constants.

The analysis developed for the standard Bianchi type IX can be straightforwardly generalized to the five-dimensional case, obtaining the system

\[
\begin{align*}
\alpha_{\tau\tau} &= -\Lambda^2 S^1_1, \quad \beta_{\tau\tau} = -\Lambda^2 S^2_2, \\
\gamma_{\tau\tau} &= -\Lambda^2 S^3_3, \quad \delta_{\tau\tau} = -\Lambda^2 S^4_4, \\
\alpha_{\tau\tau} + \beta_{\tau\tau} + \gamma_{\tau\tau} + \delta_{\tau\tau} &= \\
&= 2\alpha_{\tau}\beta_{\tau} + 2\alpha_{\tau}\gamma_{\tau} + 2\alpha_{\tau}\delta_{\tau} + 2\beta_{\tau}\gamma_{\tau} + 2\beta_{\tau}\delta_{\tau} + 2\gamma_{\tau}\delta_{\tau}, \\
\end{align*}
\]

and

\[
R^n_n = 0.
\]

The dynamical scheme \(4.14.4\) is valid for any of the 15 models using the corresponding \(S^n_n\).

Among the five-dimensional homogeneous space-times, \(G_{13}\) is the analogous of the Bianchi type IX, having the same set of structure constants.

The Einstein equations can be written as

\[
\begin{align*}
2\alpha_{\tau\tau} &= \left[ (b^2 - c^2)^2 - a^4 \right] d^2, \\
2\beta_{\tau\tau} &= \left[ (a^2 - c^2)^2 - b^4 \right] d^2, \\
2\gamma_{\tau\tau} &= \left[ (b^2 - a^2)^2 - c^4 \right] d^2, \\
\delta_{\tau\tau} &= 0,
\end{align*}
\]

toggether with \(4.14.4b\). If we assume that the BKL approximation is valid, i.e. that the right-hand sides of equations \(4.14.5\) are negligible, then the asymptotic solution for
$\tau \to -\infty$ is the five-dimensional and Kasner-like line element

$$ds^2 = dt^2 - \sum_{r=1}^{4} t^2 p_r (dx^r)^2,$$  \hspace{1cm} (4.14.6)

with the Kasner exponents $p_r$ satisfying the generalized Kasner relations

$$\sum_{r=1}^{4} p_r = \sum_{r=1}^{4} p_r^2 = 1.$$  \hspace{1cm} (4.14.7)

This regime can only hold until the BKL approximation works; however, as $\tau$ approaches the singularity, one or more of the terms may increase. Let us assume $p_1$ as the smallest index; then $a = \exp(\alpha)$ is the largest contribution and we can neglect all other terms, obtaining

$$\alpha_{\tau\tau} = -\frac{1}{2} \exp(4\alpha + 2\delta),$$
$$\beta_{\tau\tau} = \gamma_{\tau\tau} = \frac{1}{2} \exp(4\alpha + 2\delta),$$
$$\delta_{\tau\tau} = 0.$$  \hspace{1cm} (4.14.8)

As soon as the asymptotic limits for $\tau \to \pm \infty$ are considered, from the solution to (4.14.8) we obtain the map

$$p'_1 = -\frac{p_1 + p_4}{1 + 2p_1 + p_4}, \quad p'_2 = \frac{p_2 + 2p_1 + p_4}{1 + 2p_1 + p_4},$$
$$p'_3 = \frac{p_3 + 2p_1 + p_4}{1 + 2p_1 + p_4}, \quad p'_4 = \frac{p_4}{1 + 2p_1 + p_4};$$  \hspace{1cm} (4.14.9)

$$abcd = \Lambda' t, \quad \Lambda' = (1 + 2p_1 + p_4) \Lambda.$$  \hspace{1cm} (4.14.10)

The difference of this dynamical scheme with the four-dimensional case relies in the conditions needed to undergo a transition: analysing the behavior of the potential terms in (4.14.5) we see how two of the four parameters must satisfy the inequality

$$1 - 3p_1^2 - 3p_2^2 - 2p_1p_2 + 2p_1 + 2p_2 \geq 0,$$  \hspace{1cm} (4.14.11)

and one of the following ones

$$3p_1^2 + p_2^2 + p_1 - p_2 - p_1p_2 < 0,$$
$$3p_2^2 + p_1^2 + p_2 - p_1 - p_1p_2 < 0,$$
$$3p_1^2 + p_2^2 - 5p_1 - 5p_2 + 5p_1p_2 + 2 < 0.$$  \hspace{1cm} (4.14.12)

Figure 4.5 shows the existence of a region where condition (4.14.11) is satisfied but none of (4.14.12) is, thus the Universe undergoes a certain number of transitions and Kasner epochs and eras; as soon as the Kasner indices $p_1, p_2$ assume values in the shaded region, then no more transitions can take place and the evolution remains Kasner-like until the singular point is reached.
4.15 The Role of a Vector Field

Figure 4.5: The shaded region corresponds to all of the couples \((p_1, p_2)\) not satisfying (4.14.12): as soon as a ey \((p_1, p_2)\) takes values in that portion, the BKL mechanism breaks down and the Universe experiences the last Kasner epoch till the singular point.

Type G14 case is quite similar to G13: for this model, the structure constants are the same as Bianchi type VIII and, under the same hypotheses, only a finite sequence of epochs occurs.

The results of this analysis for the five-dimensional homogeneous space-times can be extended to higher dimensions and reveal how chaos is a dimensional phenomenon, for the homogeneous case, limited to the four-dimensional space-time.

4.15 The Role of a Vector Field

In this section we investigate the effects of an Abelian vector field on the dynamics of a generic \((n + 1)\)-dimensional homogeneous model in the BKL scheme: the chaos is restored for any number of dimensions, and a BKL-like map, exhibiting a peculiar dependence on the dimension number, is worked out\[59\]. These results have also been inserted in more general treatment by Damour and Hennaux\[164\].

A generic \((n + 1)\)-dimensional space-time coupled to an Abelian vector field \(A_{\mu} = (\phi, A_\alpha)\), with \(\alpha = (1, 2, \ldots, n)\) in the ADM framework is described by the action

\[
S = \int d^n x dt \left( \Pi^\alpha_{\beta} \frac{\partial}{\partial t} h_{\alpha\beta} + \Pi^\alpha \frac{\partial}{\partial t} A_\alpha + \phi D_\alpha \Pi^\alpha - NH - N^\alpha H_\alpha \right),
\]

where

\[
H = \frac{1}{\sqrt{n}} \left[ \Pi^\alpha_{\beta} \Pi^\beta_{\alpha} - \frac{1}{n - 1} (\Pi^\alpha)^2 \frac{1}{2} h_{\alpha\beta} \Pi^\alpha \Pi^\beta + h \left( \frac{1}{4} F_{\alpha\beta} F^{\alpha\beta} - \frac{1}{2} (n) R \right) \right],
\]

\[
H_\alpha = -\nabla_\beta \Pi^\beta_{\alpha} + \Pi^\beta F_{\alpha\beta},
\]

denote the super-Hamiltonian and the super-momentum respectively, while \(F_{\alpha\beta}\) is the
spatial electromagnetic tensor, and the relation $D_\alpha \equiv \partial_\alpha + A_\alpha$ holds. Moreover, $\Pi^a$ and $\Pi^{a\beta}$ are the conjugate momenta to the electromagnetic field and to the $n$-metric, respectively, which result to be a vector and a tensorial density of weight 1/2, since their explicit expressions contain the square root of the spatial metric determinant. The variation with respect to the lapse function $N$ yields the super-Hamiltonian constraint $H = 0$, while with respect to $\varphi$ it provides the constraint $\partial_\alpha \Pi^a = 0$.

We will deal with a source-less Abelian vector field and in this case one can consider the transverse (or Lorentz) components for $A_\alpha$ and $\Pi^\alpha$ only. Therefore, we choose the gauge conditions $\varphi = 0$ and $\partial_\alpha \Pi^\alpha = 0$, enough to prevent the longitudinal parts of the vector field from taking part to the action.

It is worth noting how, in the general case, i.e. either in presence of the sources, or in the case of non-Abelian vector fields, this simplification can no longer take place in such explicit form and the terms $\varphi (\partial_\alpha + A_\alpha) \Pi^\alpha$ must be considered in the action principle.

A BKL-like analysis can be developed as well as done previously, following some steps: after introducing a set of Kasner vectors $\vec{l}_a$ and the Kasner-like expanding factors $\exp(q^a)$, the dynamics is dominated by a potential of the form $\sum e^{q^a} \vec{\lambda}_a^2$, where $\vec{\lambda}_a$ are the projection of the momenta of the Abelian field along the Kasner vectors. With the same spirit of the Mixmaster analysis, an unstable $n$-dimensional Kasner-like evolution arises, nevertheless the potential term inhibits the solution to last up to the singularity and, as usual, induces the BKL-like transition to another epoch. Given the relation $\exp(q^a) = t^{p_a}$, the map that links two consecutive epochs is

$$p'_1 = \frac{-p_1}{1 + \frac{2}{n-2} p_1}, \quad p'_a = \frac{p_a + \frac{2}{n-2} p_1}{1 + \frac{2}{n-2} p_1}, \quad (4.15.3a)$$

$$\vec{\lambda}_1' = \vec{\lambda}_1, \quad \vec{\lambda}_a' = \vec{\lambda}_a \left(1 - 2 \frac{(n-1) p_1}{(n-2) p_a + np_1}\right). \quad (4.15.3b)$$

An interesting new feature, resembling that of the inhomogeneous Mixmaster (as we will discuss later), is the rotation of the Kasner vectors,

$$\vec{l}_a' = \vec{l}_a + \sigma_a \vec{l}_1, \quad (4.15.4a)$$

$$\sigma_a = \frac{\vec{\lambda}_a' - \vec{\lambda}_a}{\vec{\lambda}_1} = -2 \frac{(n-1) p_1}{(n-2) p_a + np_1} \frac{\vec{\lambda}_a}{\vec{\lambda}_1}. \quad (4.15.4b)$$

which completes our dynamical scheme.

The homogeneous Universe in this case approaches the initial singularity described by a metric tensor with oscillating scale factors and rotating Kasner vectors. Passing from one Kasner epoch to another, the negative Kasner index $p_1$ is exchanged between different directions (for instance $\vec{l}_1$ and $\vec{l}_2$) and, at the same time, these directions rotate in the space according to the rule (4.15.4b). The presence of a vector field is crucial because, independently of the considered model, it induces a dynamically closed domain on the configuration space.

In correspondence to these oscillations of the scale factors, the Kasner vectors $\vec{l}_a$ rotate and the quantities $\sigma_a$ remain constant during a Kasner epoch to lowest order in $q^a$; thus, the vanishing of the determinant $h$ approaching the singularity does not significantly affect the rotation law (4.15.4b).
There are two most interesting features of the resulting dynamics: the map exhibits a \textit{dimensional-dependence}, and it reduces to the standard BKL one for the four-dimensional case.
5 Quantum dynamics of the Mixmaster

This Section faces the question of the quantum evolution of the Mixmaster model. In particular, after a discussion on the Wheeler-DeWitt approach and the so-called problem of time, the first quantization of the model is achieved in both Misner variables and MCl ones. Furthermore, the model is also analyzed in the Loop Quantum Gravity framework (with particular attention to the disappearance of chaos) and in the Generalized Uncertainty Principle one. A brief discussion of the so-called Quantum Chaos closes the Section.

In the rest of the paper, we set $\hbar = 1$.

5.1 The Wheeler-DeWitt Equation

In this Section we will briefly review the Wheeler-DeWitt approach to the quantum gravity formulation, in the metric formalism. For the detailed literature about this topic we refer to [280, 315, 26, 190, 244].

This scheme relies on the Dirac approach to a first-class constrained system [251, 181], i.e. the quantum theory is constructed without solving the constraints. Of course this method carries some un-physical information that will be removed imposing some conditions to select the physical states. In particular, if $G_a$ is a first class constraint, a physical state must remain unchanged when performing a transformation generated by $G_a$. Thus, the physical states are the ones annihilated by the quantum operator constraints, i.e. $\hat{G}_a|\Psi\rangle = 0$.

The quantization of General Relativity in a canonical formalism prescribes to implement the Poisson algebra (2.4.11a-2.4.11c) in the form of the canonical commutation relations

\[
\begin{align*}
[\hat{h}_{\alpha\beta}(x,t),\hat{h}_{\gamma\delta}(x',t)] &= 0 \quad (5.1.1a) \\
[\hat{\Pi}^{\alpha\beta}(x,t),\hat{\Pi}\delta^\beta_\delta(x',t)] &= 0 \quad (5.1.1b) \\
[\hat{h}_{\gamma\delta}(x,t),\hat{\Pi}\delta^\beta_\delta(x',t)] &= i\kappa\delta^\gamma_\gamma\delta^{\beta\delta}(x-x') \quad (5.1.1c)
\end{align*}
\]

We note that equation (5.1.1a) is a kind of microcausality condition for the three-metric field, though the functional form of the constraint is independent of any foliation of spacetime: thus this confirms that the points of the three-manifold $\Sigma$ are space-like separated.

In the next step, we impose the constraint equations (2.4.14) as operators to select the physically allowed states

\[
\begin{align*}
\hat{H} \left( x; \hat{h}, \hat{\Pi} \right) \Psi &= 0 \quad (5.1.2a) \\
\hat{H}^a \left( x; \hat{h}, \hat{\Pi} \right) \Psi &= 0 \quad (5.1.2b)
\end{align*}
\]
Since the dynamics of General Relativity is fully contained in the classical constraints, we do not have to analyze the dynamical equations, whose meaning is readily obtained. As we have seen, the Hamiltonian for GR (2.4.12) reads as
\[ \mathcal{H} \equiv \int_{\Sigma} d^3x \left( N H + N^a H_a \right), \] (5.1.3)
and therefore, considering (5.1.2a) and (5.1.2b), in a putative Schrödinger-like equation
\[ i \frac{d}{dt} \Psi(t) = \hat{\mathcal{H}} \Psi(t) = 0 \] (5.1.4)
the wave functional \( \Psi \) (also known as “the wave function of the Universe” [245]) turns out to be independent of “time”. This is the so-called “frozen formalism”, because it apparently implies that nothing evolves in a quantum theory of gravity. By other words, we have an identification of the quantum Hamiltonian constraint as the zero-energy Schrödinger equation \( \hat{\mathcal{H}} \Psi = 0 \). This is known as the problem of time and has deep consequences on the interpretation of the wave function of the Universe and deserves to be treated in some details in Section 5.2.

When writing the expression (5.1.3), we assumed the primary constraints
\[ C(x,t) \equiv \Pi(x,t) = 0, \quad C^a(x,t) \equiv \Pi^a(x,t) = 0, \] (5.1.5)
implemented at a quantum level and therefore the wave functional \( \Psi = \Psi(h_{\alpha\beta}, N, N^a) \) becomes function of the three-metric only, i.e. \( \Psi = \Psi(h_{\alpha\beta}) \).

Let us now explicitly discuss the meaning of constraints (5.1.2a) and (5.1.2b). First of all, a representation of the canonical algebra can be chosen to be
\[ \hat{h}_{\alpha\beta} \Psi = h_{\alpha\beta} \Psi, \quad \hat{\Pi}^\alpha{}^\beta \Psi = -i \kappa \frac{\delta \Psi}{\delta h_{\alpha\beta}}. \] (5.1.6)
This is the widely used representation of the canonical approach to quantum gravity in the metric formalism. However, the above equations do not define proper self-adjoint operators because of the absence of any Lebesgue measure on \( \Sigma \) [280].

Let us firstly address the constraint (5.1.2b), which is the so-called diffeomorphisms one, because the wave functional \( \Psi(h_{\alpha\beta}) \) depends on a whole class of three-geometries \( \{h_{\alpha\beta}\} \) (invariant under three-diffeomorphisms) and not only on the three-metric, i.e. \( \Psi = \Psi(\{h_{\alpha\beta}\}) \). Therefore the configuration space for quantum gravity will be the Wheeler superspace [370]. In literature this is referred to as the “kinematical constraint”. The dynamics is generated via the scalar constraint (5.1.2a), providing the famous Wheeler-DeWitt equation [177, 178, 179], which explicitly reads as
\[ \hat{H}(x) \Psi = -G^{\alpha\beta\gamma\delta}(x) \frac{\delta^2 \Psi}{\delta h_{\alpha\beta}(x) \delta h_{\gamma\delta}(x)} - \sqrt{h} \, (3) R \Psi = 0, \] (5.1.7)
where \( G^{\alpha\beta\gamma\delta} \) is the supermetric (2.4.10c). This equation is at the heart of the Dirac constraint quantization approach and the key aspects of the canonical quantum gravity are all connected to it.

There are several problems in the WDW approach to quantum gravity, both mathemat-
5.2 The Problem of Time

A major conceptual problem in quantum gravity is the issue of what time is and how it has to be treated once a formalism is adopted (for a detailed discussion see [280], while for the role of conformal three-geometries we refer to [513]). This task is deeply connected with the special role assigned to temporal concepts in all theories of physics different from GR. For example, in Newtonian physics, as well as in non relativistic quantum mechanics, time is an external parameter to the system itself and is treated as a background degree of freedom. In ordinary quantum field theory the situation is similar since the Minkowski background is fixed and the Newtonian time is replaced by the time measured in a set of relativistic inertial frames. Such notion of “time” plays a crucial role in the conceptual foundations of the quantum theory. In fact, in the conventional Copenhagen interpretation of quantum mechanics, an observable is a quantity whose value can be measured at fixed time. Moreover, the scalar product is conserved under the time evolution and the quantum fields have to satisfy the microcausality conditions. Finally, it can be shown [495] how a perfect clock, in the sense of a quantum observable $T$ whose values monotonically grow with abstract time $t$, is not compatible with the physical requirement of a positive spectrum of the energy, and this is a peculiar feature of the quantum theory.

The problem of time arises also in the canonical formulation of the quantum theory of gravity, as happens in any diffeomorphism-invariant quantum field theory, and the Schrödinger equation is replaced by a Wheeler-DeWitt one, where the time coordinate is not present in the formalism.

The proposals to address this fundamental problem are often related with the introduction of a reference system. In fact, this can be achieved in two different ways: the first one consists in adding a dynamical fluid or fields to the vacuum gravitational picture (see [99, 433, 432, 44]), while the other in fixing the frame in a geometrical way ([316, 99, 380, 362]). However, both of them lead to an equivalent evolutionary quantum dynamics [433, 432, 99, 361]. Below we will discuss the Brown and Kuchař mechanism, the so-called evolutionary quantum gravity and, finally, the multi-time approach.

5.2.1 The Brown and Kuchař mechanism

This approach [99] is devoted to find a medium leading to a Schrödinger equation when applying the Dirac quantization to a constrained system. In particular, an incoherent dust, i.e. one with the gravitational interaction only, is included in the dynamics. This
Quantum dynamics of the Mixmaster procedure leads to the new constraints $H^\uparrow(X)$ and $H^\uparrow_\alpha(X)$ in which the dust plays the role of time and the true Hamiltonian does not depend on the dust variables.

Let us introduce the variables $T, Z^\alpha$ and the corresponding conjugate momenta $M, W^\alpha$, so that the values of $Z^\alpha$ be the comoving coordinates of the dust particles and $T$ be the proper time along their worldlines. In this scheme the new constraints read as

$$H^\uparrow = P(X) + h(X, h_{(\alpha\beta)}, \Pi_{\alpha\beta}) = 0 \quad (5.2.1a)$$
$$H^\uparrow_\alpha = P_\alpha(X) + h_\alpha(X, T, z^\alpha, h_{\alpha\beta}, \Pi_{\alpha\beta}) = 0 \quad (5.2.1b)$$

where

$$h = -\sqrt{G(X)}, \quad G(X) = H^2_{(\text{grav})} - h^{\alpha\beta} H_{(\text{grav})\alpha} H_{(\text{grav})\beta}, \quad (5.2.2a)$$
$$h_\alpha = Z^\beta_\alpha H_\beta + \sqrt{G(X)} \partial_\beta T Z^\beta_\alpha, \quad (5.2.2b)$$

$H_{(\text{grav})}$ and $H_{(\text{grav})\alpha}$ being the usual scalar and momentum constraints, respectively, $P$ the projection of the rest mass current of the dust into the four velocity of the observers, and $P_\alpha = -PW_\alpha$. This way the Hamiltonian $h$ does not depend on the dust.

The quantization of this model is performed in the canonical way and yields, from equation (5.2.1a), the Hamiltonian constraint operator

$$\hat{H}^\uparrow = \hat{P}(X) + \hat{h}(X, \hat{h}_{\alpha\beta}, \hat{\Pi}_{\alpha\beta}) = 0. \quad (5.2.3)$$

This mechanism leads to a Schrödinger equation for the wave functional $\Psi = \Psi(\hat{T}, \hat{h})$

$$i \frac{\delta \Psi}{\delta \hat{T}} = \hat{h}\Psi. \quad (5.2.4)$$

The central point of this procedure is the independence of the effective Hamiltonian $h(X)$ on the dust; this allows a well posed spectral analysis formulation because $h$ commutes with itself. Furthermore, the Schrödinger equation can be split into a dust- (time-) dependent part and a truly gravitational one.

### 5.2.2 Evolutionary Quantum Gravity

In this section we remark some of the fundamental aspects of the evolutionary quantum gravity as presented in [380][362]. As a first step we analyze the implication of a Schrödinger formulation of the quantum dynamics for the gravitational field [235], and then we establish a dualism between time evolution and matter fields.

Let us assume that the quantum evolution of the gravitational field is governed by the smeared Schrödinger equation

$$i \partial_t \Psi = \hat{\mathcal{H}} \Psi = \int d^3x \left( N \hat{H} \right) \Psi \quad (5.2.5)$$

where the wave functional $\Psi$ is defined on the superspace, i.e. it is annihilated by the super-momentum operator $\hat{H}_\alpha$. Let us take the following expansion for the wave func-
5.2 The Problem of Time

\[ \Psi = \int D\epsilon \, \chi(\epsilon, \{h_{\alpha\beta}\}) \exp \left[ -i \int_{t_0}^{t} dt' \int_{\Sigma} d^3x (\mathcal{N}e) \right], \]

(5.2.6)

where \( D\epsilon \) is the Lebesgue measure on the space of the functions \( \epsilon(x) \). This expansion reduces the Schrödinger dynamics to an eigenvalue problem of the form

\[ \hat{H}\chi = \epsilon\chi, \quad \hat{H}n\chi = 0, \]

(5.2.7)

which outlines the appearance of a non-zero super-Hamiltonian eigenvalue.

In order to reconstruct the classical limit of the dynamical constraints (5.2.7), we replace the wave functional \( \chi \) by its corresponding zero-order WKB approximation \( \chi \sim e^{iS} \). In this case the eigenvalue problem (5.2.7) reduces to its classical counterpart

\[ \hat{H}_J S = \epsilon \equiv -2\sqrt{\hbar}T_{00}, \quad \hat{H}_{Jn} S = 0 \]

(5.2.8)

where \( \hat{H}_J \) and \( \hat{H}_{Jn} \) denote operators which, when applied to the phase \( S \), reproduce the super-Hamiltonian and super-momentum Hamilton-Jacobi terms, respectively. We see that the classical limit of the Schrödinger quantum dynamics is characterized by the appearance of a new matter contribution (associated with the non-zero eigenvalue \( \epsilon \)) whose energy density reads as

\[ \rho \equiv T_{00} = -\frac{\epsilon(x)}{2\sqrt{\hbar}}, \]

(5.2.9)

where by \( T_{ij} \) we refer to the new matter energy-momentum tensor.

Since the spectrum of the super-Hamiltonian has, in general, a negative component, then we can infer that, when the gravitational field is in its ground state, this matter comes out in the classical limit with a positive energy density. The explicit form of (5.2.9) is that of a dust fluid co-moving with the slicing of the three-hypersurfaces, i.e. the normal field \( n^i \) becomes the four-velocity of the appearing fluid (in other words, we deal with an energy-momentum tensor \( T_{ij} = \rho n_i n_j \)).

We stress how the space of the solutions can be turned into the Hilbert one and therefore a notion of probability density naturally arises, from the squared modulus of the wave functional.

Let us now consider the opposite sector, i.e. a gravitational system in the presence of a macroscopic matter source. In particular, we chose a perfect fluid with a generic equation of state \( p = (\gamma - 1)\rho \) (\( \rho \) being the pressure and \( \gamma \) the polytropic index). The energy-momentum tensor, associated to this system reads as

\[ T_{ij} = \gamma\rho u_i u_j - (\gamma - 1)\rho g_{ij}. \]

(5.2.10)

To fix the constraints when matter is included in the dynamics, let us make use of the relations

\[ G_{ij} n^i n^j = -\kappa \frac{H}{2\sqrt{\hbar}} \]

(5.2.11a)

\[ G_{ij} n^i \partial_a y^j = \kappa \frac{H_i}{2\sqrt{\hbar}}, \]

(5.2.11b)
where $\partial_{\alpha}y^i$ are the tangent vectors to the three-hypersurfaces, i.e. $n_i \partial_{\alpha}y^i = 0$. Equations (5.2.11a) and (5.2.11b), by (5.2.10) and identifying $u_i$ with $n_i$ (i.e. the physical space is filled by the fluid), rewrite as

$$\rho = -\frac{H}{2\sqrt{h}}, \quad H_i = 0,$$  

(5.2.12)

and furthermore, we get the equations

$$G_{ij}\partial_{\alpha}y^i\partial_{\beta}y^j \equiv G_{\alpha\beta} = \kappa(\gamma - 1)\rho h_{\alpha\beta}.$$  

(5.2.13)

The conservation law $\nabla_j T^j_i = 0$ implies the additional two conditions

$$\gamma \nabla_i (\rho u^i) = (\gamma - 1)u^i \partial_i \rho$$  

(5.2.14a)

$$u^i \nabla_j u_i = \left(1 - \frac{1}{\gamma}\right)\left(\partial_i \ln \rho - u_i u^j \partial_j \ln \rho\right).$$  

(5.2.14b)

With the space-time slicing, looking at the dynamics into the fluid frame (i.e. $n^i = \delta^i_0$), by the relation $n^i = (1/N, -N^k/N)$, the co-moving constraint implies the synchronous nature of the reference frame. Since a synchronous reference is also a geodesic one, the right-hand side of equation (5.2.14b) must identically vanish and, for a generic inhomogeneous case, this implies $\gamma \equiv 1$. Hence, equations (5.2.14a) yields $\rho = -\bar{\epsilon}(x)/2\sqrt{h}$ and substituted into (5.2.12), we get the same Hamiltonian constraints associated to the Evolutionary Quantum Gravity given above in eq.(5.2.7), as soon as the function $\bar{\epsilon}$ is turned into the eigenvalue $\epsilon$. In this respect, while $\bar{\epsilon}$ is positive by definition, the corresponding eigenvalue can also take negative values because of the structure of $H$.

Thus, we conclude that a dust fluid is a good choice to realize a clock in Quantum Gravity, because it induces a non-zero super-Hamiltonian eigenvalue into the dynamics; furthermore, for vanishing pressure ($\gamma = 1$), the equation (5.2.13) reduces to the proper vacuum evolution equation for $h_{\alpha\beta}$, thus outlining a real dualism between time evolution and the presence of a dust fluid.

For the cosmological applications of the above approach in the isotropic sector see [154, 381] and in a generic cosmological model see [382] and [44] where it is shown how, from a phenomenological point of view, an evolutionary quantum cosmology overlaps the Wheeler-DeWitt approach.

### 5.2.3 The Multi-Time Approach

The multi-time approach [314, 280] represents an alternative interesting way to get a Schrödinger quantum dynamics, even if deeply different from the one described above, since it is based on the ADM reduction of the dynamics. In fact, starting from equation (4.6.4),

$$P_A(x) + h_A(x, \chi, \phi, \pi) = 0,$$  

(5.2.15)

and performing a canonical quantization of the model, we obtain a Schrödinger-like equation

$$i\frac{\delta \Psi}{\delta \chi^A} = \hat{h}_A \Psi,$$  

(5.2.16)
5.3 The Minisuperspace Representation

where $\hat{h}_A$ is the operatorial version of the classical Hamiltonian density. Even if this approach and the evolutionary one (discussed in the previous subsection) seem to overlap each other when solving the problem of the frozen formalism, this is not the case. As matter of fact, the evolutionary quantum dynamics approach is based on a full quantization of the system. By the other hand, the multi-time approach relies on a quantization of only some degrees of freedom. In fact, the constraints are classically solved before implementing the quantization procedure, thus violating the geometrical nature of the gravitational field in view of real physical degrees of freedom. This fundamental difference between the two approaches is evident, for example, in a cosmological context. In fact, when we quantize a minisuperspace model in the ADM formalism, the scale factor of the Universe is usually chosen as a “time” coordinate, and therefore the dynamics is consequently expressed. By the other hand, in an evolutionary approach the scale factor is treated on the same footing of other variables, i.e. the anisotropies, and the evolution of the system is considered with respect to a privileged reference frame.

5.3 The Minisuperspace Representation

Although the full theory (“Quantum General Relativity”) is far from being reached, many approaches are properly treated in the context of the so-called minisuperspace, as for example quantum cosmology. In fact, only a finite number of gravitational degrees of freedom are invoked in the quantum theory, and the remaining ones are frozen out imposing some symmetries on the spatial metric. These space-times are, for instance, the homogeneous cosmological models.

In this sense quantum cosmology is a toy model for quantum gravity (with finite degrees of freedom) which is a simple arena to test ideas and constructions introduced in the full theory (a genuine quantum field theory). In particular, since on a classical level the Universe dynamics is described by such symmetric models, their quantization is required to answer the fundamental questions like the fate of the classical singularity, the inflationary expansion and the chaotic behavior of the Universe toward the singularity.

Moreover, as we will see in Section 6.1 in the general context of inhomogeneous cosmology, the spatial derivatives in the Ricci scalar are negligible with respect to the temporal ones, toward the singularity. This is the well-known BKL scenario [54, 57] where, as the singularity is approached (on a classical level), the spatial geometry can be viewed as a collection of small independent patches, in general Bianchi IX like models. Therefore a minisuperspace reduction of the dynamics is important also in the description of a generic Universe toward the classical singularity when restricted to each cosmological horizon.

5.4 On the Scalar Field as a Relational Time

Let us now discuss in some details the role of a matter field, in particular that of a scalar field $\phi$, used as a definition of time for the quantum dynamics of the gravitational field. As we have seen, when the canonical quantization procedure is applied, the usual Schrödinger equation is replaced by a Wheeler-DeWitt one in which the time coordinate is dropped from the formalism. One possible solution to this fundamental problem is adding a matter field in the dynamics and then let evolve the physical degrees of freedom
of the gravitational system with respect to it. This way the dynamics is described on a relational point of view, i.e. the matter field behaves as a relational time. Such an idea is essentially based on the absence of time at a fundamental level and therefore a field can evolve with respect to another one only (for more details on this approach see [435]).

In particular, in quantum cosmology, such choice appears as the most natural one. In fact, near the classical singularity, a monotonic behavior of a massless $\phi$ always appears as a function of the scale factor $a$ (more precisely the variable which describes the isotropic expansion of the Universe).

Let us consider the case of the Bianchi IX model in presence of a massless scalar field, whose Hamiltonian constraint in the Misner variables $(a \equiv e^\alpha, \beta_{\pm})$ has the form

$$H_{IX} + H_\phi = \kappa \left[ -\frac{p_a^2}{a} + \frac{1}{a^3} \left( p_+^2 + p_-^2 \right) \right] - \frac{a}{4\kappa} V(\beta_{\pm}) + \frac{p_\beta^2}{a^2} \approx 0,$$  \hspace{1cm} (5.4.1)

$V(\beta_{\pm})$ being the relative potential term.

When this system is canonically quantized, the associated Wheeler-DeWitt equation describes how the wave function $\Psi = \Psi(a, \beta_{\pm}, \phi)$ evolves with $\phi$. More precisely, from (5.4.1) we obtain

$$-\partial^2_\phi \Psi = \Xi \Psi, \quad \Xi \equiv \kappa \left[ -a^2 \partial_a^2 + \partial_+^2 + \partial_-^2 + \frac{a^4}{4\kappa^2} V(\beta_{\pm}) \right],$$  \hspace{1cm} (5.4.2)

behaving as a Klein-Gordon equation with $\phi$ playing the role of (relational) time and $\Xi$ of the spatial Laplacian. An explicit Hilbert space arises after performing the natural decomposition of the solution into positive and negative frequencies parts. In particular, the positive frequency sector offers the Schrödinger-like equation $-i \partial_\phi \Psi = \sqrt{\Xi} \Psi$.

We can analyze in which sense the scalar field can be regarded as a good time parameter for the dynamics. First of all, near the cosmological singularity $(a \to 0)$ the potential term $V(\beta_{\pm})$ can be neglected.\(^3\) In such approximation the (classical) equations of motion obtained from (5.4.1) read as

$$\dot{a} = \frac{a^2 p_a}{\sqrt{a^2 p_a^2 - p_\beta^2}}, \quad \dot{p}_a = -\frac{a p_a^2}{\sqrt{a^2 p_a^2 - p_\beta^2}}, \quad \dot{p}_+ = \dot{p}_- = 0,$$  \hspace{1cm} (5.4.3)

where $(\ldots) \equiv d(\ldots)/d\phi$ and $p_\beta^2 \equiv p_+^2 + p_-^2$. The solutions of system (5.4.3) have the form

$$a(\phi) = B \exp \left( \frac{A\phi}{\sqrt{A^2 - p_\beta^2}} \right), \quad p_a(\phi) = \frac{A}{B} \exp \left( -\frac{A\phi}{\sqrt{A^2 - p_\beta^2}} \right),$$  \hspace{1cm} (5.4.4)

$A$ and $B$ being integration constants and $p_\beta^2 = \text{const.}$

---

1. In fact, such behavior well approximates the one of an inflaton field when its potential is negligible at enough high temperature [140]. For a detailed discussion of the inflationary scenario within the framework of homogeneous cosmologies, see [331, 515, 226, 226, 132, 252, 449, 204, 62, 288, 117, 353].

2. The choice of the normal ordering is not important for the following discussion, thus we adopt the simplest one.

3. For a discussion on the consistency condition ensuring that the quasi-classical limit of the Universe dynamics is reached before the potential term becomes important, see [44].
5.5 Interpretation of the Universe Wave Function

We have recovered a monotonic dependence of the scalar field $\phi$ with respect to the isotropic variable of the Universe $a$ and therefore the massless $\phi$ shows to be a good (relational) time for the gravitational dynamics.

As we will see in Section 6.3, the dynamics toward the cosmological singularity of a generic inhomogeneous Universe is described, point by point, by the one of a Bianchi IX model. More precisely, the spatial points dynamically decouple toward the singularity and the spatial geometry can be viewed as a collection of small patches, each one independently evolving as a Bianchi IX model. From this point of view, the monotonic relation (5.4.4) is a proper general feature of the gravitational field, better clarifying the choice of the scalar field as a relational time.

5.5 Interpretation of the Universe Wave Function

In this Section we face the problem of the probabilistic interpretation of the Universe wave function, in agreement with the analysis developed in [502, 501] (for a different point of view see [298, 274, 223]). In fact, in quantum cosmology, the Universe is described by a single wave function $\Psi$ providing puzzling interpretations when analyzing the differences between ordinary quantum mechanics and quantum cosmology.

In quantum mechanics, given a wave function $\Psi(q_i, t)$ describing a system, the probability to find the system in a configuration-space element $d\Omega_q$ at time $t$ is given by

$$dP = |\Psi(q_i, t)|^2 d\Omega_q,$$

and it is positive semi-definite, i.e. $dP \geq 0$. On the other hand, the Universe wave function (which is a solution of the Wheeler-DeWitt equation) depends on the three-geometries, on the possible matter fields and no dependence on time appears. Therefore, the associated probability (here we denote whole the set of the superspace variables by $h$)

$$dP = |\Psi(h)|^2 |G|^{1/2} d^n h, \quad G = \det(G_{\alpha\beta\gamma\delta}),$$

($G$ being the supermetric) is not normalizable, because its integral over the whole superspace is diverging. Such behavior can be considered as the analogue of the quantum mechanical feature

$$\int |\Psi(q_i, t)| d\Omega_q dt = \infty.$$

In fact, in quantum cosmology, the “time” is included among the set of variables $h$.

An alternative definition of the Universe probability can be given in terms of conserved current [177] (for notation see Vilenkin[502])

$$\nabla_i j^i = 0, \quad j^i = -\frac{i}{2} G^{ij}(\Psi^* \nabla_j \Psi - \Psi \nabla_j \Psi^*).$$

This approach is limited as well since the corresponding probability to find the Universe in a surface element $d\Sigma_\alpha$ is

$$dP = j^\alpha d\Sigma_\alpha.$$

---

4This idea relies on the consideration that the WDW equation is nothing but a Klein-Gordon equation with variable mass.
and it can be negative, similarly to the problem of negative probabilities in the Klein-Gordon equation.

In order to correctly define a probability, i.e. a positive semi-definite one, we can proceed in two different ways: first we can consider a Universe, in which all the variables are treated semiclassically, then we can analyze a Universe where a quantum subsystem is taken into account, i.e. when some variables are pure quantum ones.

In the case of semiclassical variables, the wave function \( \Psi \) is given by

\[
\Psi = A(h)e^{iS(h)},
\]

which admits a WKB expansion and leads to a conserved current \( j^i = |A|^2 \nabla^i S \). The classical action \( S(h) \) describes a congruence of classical trajectories and we shall define probability distribution on the \((n-1)\)-dimensional equal-time surfaces. Requiring only single crossing between the trajectories and these equal-time surfaces, the probability (5.5.5) results to be positive semi-definite.

Let us now consider the case in which not all the superspace variables are semiclassical. We shall assume that the quantum variables are labeled by \( q \) and their effect on the dynamics of the semiclassical variables \( h \) can be neglected. Therefore, the WDW equation can be decomposed in a semiclassical part \( H_0 \), which corresponds to the one of the previous case, and a “quantum” one \( H_q \). The fact that the quantum subsystem is small is shown by the existence of a parameter \( \lambda \) (proportional to \( \hbar \)) such that

\[
H_q \Psi / H_0 \Psi = O(\lambda).
\]

Thus, since \( H_0 = O(\lambda^{-2}) \), therefore \( H_q = O(\lambda^{-1}) \). The superspace metric can then be expanded in terms of \( \lambda \) as

\[
G_{ij}(h, q) = G_{ij}^0(h) + O(\lambda),
\]

and the Universe wave function can be written as

\[
\Psi = A(h)e^{iS(h)}\chi(h, q),
\]

where the function \( \chi \) has to satisfy

\[
\left[ \nabla_0^2 + 2[\nabla_0(\ln A)]\nabla_0 + 2i(\nabla_0 S)\nabla_0 - H_q \right] \chi = 0,
\]

which can be written as a Schrödinger equation as \( i\partial_t \chi = NH_q \chi \) (we recall that \( \nabla_0 S \) coincides with the classical conjugate momentum to the semiclassical variable). Thus, we can get two different currents, one for the components in the classical subspace and one for those in the quantum one with the corresponding probability distribution written as

\[
\rho(h, q, t) = \rho_0(h, t) |\chi(q, h(t), t)|^2,
\]

where \( \rho_0(h, t) \) and \( |\chi|^2 \) are the probability distribution for the classical and the quantum variables, respectively. Considering the surface element on equal-time surfaces \( d\Sigma = d\Sigma_0 d\Omega_q \), for \( d\Sigma_0 \) defined from the metric \( g^0(h) \), the probability distribution (5.5.11) results to be normalizable.
By other words, we have recovered the standard interpretation of the wave function for a small subsystem of the Universe (only). This result agrees with the intrinsic approximate interpretation of the Universe wave function. In fact, in the interpretation of quantum mechanics, all realistic measuring devices have some quantum uncertainty. In particular, the bigger is the apparatus the smaller are the quantum fluctuations. In this sense, we are able to give a physical interpretation of the wave function of the Universe only in a domain in which some variables are semiclassical.

Finally, we recall two assumptions underlying this model:

(i) the analysis has been developed in the minisuperspace homogeneous models only;

(ii) the fundamental requirement of existence of a family of equal-time surfaces is taken as a general feature.

5.6 Quantization in the Misner Picture

In this Section we provide a quantum representation of the dynamics, relying on the adiabatic approximation ensured by the potential term, reduced to an infinite well and, according to C. W. Misner [368], we model the potential as an infinite square box with the same measure as in the original triangular picture. The volume-dependence of the wave function acquires increasing amplitude and frequency of oscillations as the Big Bang is approached and the occupation number grows, respectively.

For a review of the canonical quantization of Bianchi cosmologies in the WDW framework see [389, 403, 416, 112, 79, 339, 406, 317, 512, 373, 170, 354, 351, 399, 300, 269, 456, 253, 202, 201, 27, 511, 135, 96, 353, 503]. For a discussion on the quantization in a supersymmetric form of the Bianchi IX model, see [218, 221].

In a canonical framework, by replacing the canonical variables with the corresponding operators and implementing the Hamiltonian constraints we get the state function describing the system $\psi = \psi(\alpha, \beta_+, \beta_-)$.

Adopting the canonical representation in the configuration space we address the WDW equation

$$\hat{H}\psi = e^{-3\alpha} \left[ -\frac{\delta^2}{\delta \alpha^2} + \frac{\delta^2}{\delta \beta_+^2} + \frac{\delta^2}{\delta \beta_-^2} \right] \psi - e^\alpha V \psi = 0. \quad (5.6.1)$$

We can find a solution in the form

$$\psi = \sum_n \Gamma_n(\alpha) \phi_n(\alpha, \beta_+, \beta_-), \quad (5.6.2)$$

where the coefficients $\Gamma_n$ are $\alpha$-dependent amplitudes.

Thus, equation (5.6.1) is reduced to the ADM eigenvalue problem

$$\left[ -\frac{\partial^2}{\partial \beta_+^2} - \frac{\partial^2}{\partial \beta_-^2} + e^{4\alpha} V \right] \phi_n = E_n^2(\alpha) \phi_n. \quad (5.6.3)$$

According to [368], we approximate the triangular infinite walls of the potential by a box
having the same measure to find the eigenvalues $E_n$
\[
E_n(\alpha) = \pi \left( \frac{4}{3^{3/2}} \right)^{1/2} \frac{|n|}{\alpha},
\]
where $n^2 = n_+^2 + n_-^2$, and $n_+, n_- \in \mathbb{N}$ are the two independent quantum numbers corresponding to the variables $\beta_+, \beta_-$, respectively.

Substituting the expression for $\psi$ in equation (5.6.1) we get the differential equation for $\Gamma_n$
\[
\sum_n (\partial^2 \Gamma_n) \varphi_n + \sum_n \Gamma_n (\partial^2 \varphi_n) + 2 \sum_n (\partial \Gamma_n) (\partial \varphi_n) + \sum_n E_n^2 \Gamma_n \varphi_n = 0,
\]
which, in the limit of the Misner adiabatic approximation of neglecting $\partial \varphi_n$ (i.e. $\varphi \sim \phi(\beta_+, \beta_-)$), simplifies to
\[
\frac{d^2 \Gamma_n}{d\alpha^2} + \frac{k_n^2}{\alpha^2} \Gamma_n = 0
\]
where
\[
k_n^2 = \left( \frac{2\pi}{3} \right)^{3/2} |n|^2.
\]
The above equation is solved by $\Gamma_n(\alpha)$ in the form
\[
\Gamma_n(\alpha) = C_1 \sqrt{\alpha} \sin \left( \frac{1}{2} \sqrt{p_n} \ln \alpha \right) + C_2 \sqrt{\alpha} \cos \left( \frac{1}{2} \sqrt{p_n} \ln \alpha \right),
\]
where $\sqrt{p_n} = \sqrt{k_n^2 - 1}$. From (5.6.8) the self-consistency of the adiabatic approximation is ensured. Figure 5.1 shows the behavior of $\Gamma_n(\alpha)$ for various values of the parameter $k_n$.

Such wave function behaves like an oscillating profile whose frequency increases with occupation number $n$ and approaching the Big Bang, while the amplitude depends on the $\alpha$ variable only.

By this treatment, one finds [368] the interesting result that $n$ on average is constant toward the singularity and then if the initial state of evolution of the Universe is classical, extrapolating backwards it maintains a semiclassical character.

### 5.7 The quantum Universe in the Poincaré half-plane

The Misner representation provides a good insight in some qualitative aspects of the Mixmaster model quantum dynamics, and allows some physical considerations on the evolution toward the singularity. In this picture the potential walls move with time, and this is an obstacle toward a full implementation of a Schrödinger like quantization scheme. These difficulties can be by-passed as soon as MCI variables are adopted, characterized by static potential walls; in particular, we will choose the so-called Poincaré variables $(u, v)$, defined as

\[
\zeta = \frac{1 + u + u^2 + v^2}{\sqrt{3}v},
\]
\[
\theta = - \arctan \frac{\sqrt{3}(1 + 2u)}{-1 + 2u + 2u^2 + 2v^2}.
\]
5.7 The quantum Universe in the Poincaré half-plane

Figure 5.1: Behavior of the solution $\Gamma_n(\alpha)$ for three different values of the parameter $k_n = 1, 15, 30$. The bigger $k_n$, the higher the frequency of oscillation.

In the vicinity of the initial singularity, we have seen that the potential term behaves as a potential well and as soon as we restrict the dynamics to $\Pi_Q$, $H_{ADM} = \epsilon$ and we can rewrite (4.8.15) and (4.8.16) as

$$\delta S_{\Pi_Q} = \delta \int d\tau (p_\xi \ddot{\xi} + p_\theta \dot{\theta} - H_{ADM}) = 0 \quad (5.7.2a)$$

$$H_{ADM} = v \sqrt{p_u^2 + p_\theta^2}. \quad (5.7.2b)$$

The asymptotic dynamics is defined in a portion $\Pi_Q$ of the Lobatchevsky plane, delimited by inequalities

$$Q_1(u, v) = -u/d \geq 0 \quad (5.7.3a)$$

$$Q_2(u, v) = (1 + u)/d \geq 0 \quad (5.7.3b)$$

$$Q_3(u, v) = (u(u + 1) + v^2)/d \geq 0 \quad (5.7.3c)$$

$$d = 1 + u + u^2 + v^2, \quad (5.7.3d)$$

whose boundaries are composed by geodesics of the plane, i.e. two vertical lines and one semicircle centred on the absolute $v = 0$.

The billiard has a finite measure, and its open region at infinity together with the two points on the absolute $(0, 0)$ and $(-1, 0)$ correspond to the three cuspid of the potential in Fig. 4.3.

It is easy to show that, in the $u, v$ plane, (4.9.3) becomes

$$d\mu = \frac{1}{\pi} \frac{du \, dv \, d\phi}{v^2} \, 2\pi. \quad (5.7.4)$$
\[ \partial u + \partial (\dot{v} \rho) \partial v + \partial (\dot{p} \rho) \partial p u + \partial (\dot{p} \rho) \partial p v = 0, \] (5.8.1)

were the dot denotes the time derivative and the Hamilton equations associated to (5.7.2b) read as

\[ \dot{u} = \frac{\nu^2}{\epsilon} p u, \quad \dot{p} u = 0, \] (5.8.2a)

\[ \dot{v} = \frac{\nu^2}{\epsilon} p v, \quad \dot{p} v = -\frac{\epsilon}{\nu}. \] (5.8.2b)

From (5.8.1) and (5.8.2) we obtain

\[ \frac{\nu^2 p u \partial \rho}{\epsilon \partial u} + \frac{\nu^2 p v \partial \rho}{\epsilon \partial v} - \frac{\epsilon \partial \rho}{\nu \partial p v} = 0. \] (5.8.3)

The continuity equation provides an appropriate representation when we are sufficiently close to the initial singularity only, and the infinite-potential-wall approximation works. Such model corresponds to deal with the energy-like constant of motion, and fixes the microcanonical nature of the ensemble. From a dynamical point of view, this picture naturally arises because the Universe volume element monotonically vanishes (for non
stationary corrections to this scheme in the MCl variables, see [379].
Since we are interested to the distribution function in the \((u,v)\) space, we will reduce
the dependence on the momenta by integrating \(\rho(u,v,p_u,p_v)\) in the momentum space.
Assuming \(\rho\) to be a regular, vanishing at infinity in the phase-space, limited function, we
can integrate over \((5.8.3)\) getting the equation for "\(\tilde{w}(u,v;k)\)
\[
\frac{\partial \tilde{w}}{\partial u} + \sqrt{\left( \frac{E}{Cv} \right)^2 - 1} \frac{\partial \tilde{w}}{\partial v} + \frac{E^2 - 2C^2v^2}{Cv^2} \frac{\tilde{w}}{\sqrt{E^2 - (Cv)^2}} = 0 ,
\]
where the constant \(C\) appears, due to the analytic expression of the HJ solution, fixed
by the initial conditions. However, we deal with a distribution function that cannot con-
sider these initial conditions, and must be ruled out from the final result. We obtain the
following solution in terms of the generic function \(g\)
\[
\tilde{w}(u,v;C) = g \left( \frac{u + v\sqrt{E^2 - C^2v^2}}{v\sqrt{E^2 - C^2v^2}} - 1 \right) .
\]
The distribution function cannot contain the constant \(C\), and the final result is obtained
after the integration over it. We define the reduced distribution \(w(u,v)\) as
\[
w(u,v) \equiv \int_A \tilde{w}(u,v;k)dk ,
\]
where the integration is taken over the classical available domain for \(p_u \equiv C\)
\[
A \equiv \left[ -\frac{E}{v}, \frac{E}{v} \right] .
\]
In \((5.7.4)\) we proved demonstrated that the measure associated to it is the Liouville one;
the measure \(w_{mc}\) (after integration over the admissible values of \(\phi\)) corresponds to the
case \(g = \text{const.}\)
\[
w_{mc}(u,v) = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{1}{Cv^2 \sqrt{\frac{E^2}{C^2v^2} - 1}} dC = \frac{\pi}{v^2} .
\]
Summarizing, we have derived the generic expression of the distribution function fixing
its form for the microcanonical ensemble. This choice, in view of the energy-like constant
of motion \(H_{ADM}\), is appropriate to describe the Mixmaster system restricted to the con-
figuration space. This analysis reproduces in the Poincaré half-plane the same result as
the stationary invariant measure described in Section \(4.9\).

For completeness we report the explicit solution to \((2.4.21)\) to this model in the restricted
domain \(\Pi_Q\) as the Hamilton-Jacobi function for the point-Universe
\[
S_0(u,v) = Cu + \sqrt{\epsilon^2 - C^2v^2} - \epsilon \ln \left( 2 \frac{\epsilon + \sqrt{\epsilon^2 - C^2v^2}}{\epsilon^2v^2} \right) + D ,
\]
where \(C\) is the separation constant, and \(D\) is an integration one.
5 Quantum dynamics of the Mixmaster

5.9 Schrödinger dynamics

The Schrödinger quantum picture is obtained in the standard way, i.e. by promoting the classical variables to operators and imposing some boundary condition to the wave function. The first step is achieved as

\[ \hat{v} | \rangle = v | \rangle, \quad \hat{u} | \rangle = u | \rangle, \]
\[ \hat{p}_v \rightarrow -i \frac{\partial}{\partial v}, \quad \hat{p}_u \rightarrow -i \frac{\partial}{\partial u}, \quad \hat{p}_\tau \rightarrow -i \frac{\partial}{\partial \tau}, \quad (5.9.1) \]

while for the second one we will require the Dirichlet boundary conditions

\[ \Phi(\partial \Pi_Q) = 0. \quad (5.9.2) \]

The quantum dynamics for the state function \( \Phi = \Phi(u, v, \tau) \) obeys the Schrödinger equation

\[ i \frac{\partial \Phi}{\partial \tau} = \hat{H}_{ADM} \Phi = \sqrt{-v^2 \frac{\partial^2}{\partial u^2} - v^2 - a \frac{\partial}{\partial v} \left( v^a \frac{\partial}{\partial v} \right) } \Phi. \quad (5.9.3) \]

Here we have adopted a generic operator-ordering for the position and momentum parametrized by the constant \( a \), as soon as we have no indication on it providing a first problem. The other one is linked to the multi-time approach, i.e. to the non-locality of the Hamiltonian operator: when solving the Hamilton constraint with respect to one of the momenta, the ADM Hamiltonian contains a square root and consequently it might define a non-local dynamics.

The question of the correct operator-ordering is addressed the next Section comparing the classic evolution versus the WKB limit of the quantum-dynamics and requiring the overlapping of the two. On the other hand, we will assume the operators \( \hat{H}_{ADM} \) and \( \hat{H}_{ADM}^2 \) having the same set of eigenfunctions with eigenvalues \( E \) and \( E^2 \), respectively.

Under these assumptions, we will solve the eigenvalue problem for the squared ADM Hamiltonian given by

\[ \hat{H}_{ADM}^2 \Psi = \left[ -v^2 \frac{\partial^2}{\partial u^2} - v^2 - a \frac{\partial}{\partial v} \left( v^a \frac{\partial}{\partial v} \right) \right] \Psi = E^2 \Psi, \quad (5.9.4) \]

where \( \Psi = \Psi(u, v, E) \).

5.10 Semiclassical WKB limit

In order to study the WKB limit of equation \( 5.9.4 \), we separate the wave function into its phase and modulus\[ \]
\[ \Psi(u, v, E) = \sqrt{r(u, v, E)} e^{i \omega(u, v, E) / \hbar}. \quad (5.10.1) \]

\[ \text{The problems discussed by [296] do not arise here because in the domain } \Pi_Q \text{ the ADM Hamiltonian has a positive sign (the potential vanishes asymptotically).} \]

\[ \text{In this Section we restore } \hbar \text{ in the notation because we deal with the semiclassical limit.} \]
In Eq. (5.10.1) the function \( r(u,v) \) represents the probability density, and the quasi-classical regime appears in the limit \( \hbar \to 0 \); substituting (5.10.1) in (5.9.4) and retaining only the lowest order in \( \hbar \), we obtain the system

\[
v^2 \left[ \left( \frac{\partial \sigma}{\partial u} \right)^2 + \left( \frac{\partial \sigma}{\partial v} \right)^2 \right] = E^2 , \tag{5.10.2a}
\]

\[
\frac{\partial r}{\partial u} \frac{\partial \sigma}{\partial u} + \frac{\partial r}{\partial v} \frac{\partial \sigma}{\partial v} + r \left( \frac{\partial^2 \sigma}{\partial v^2} + \frac{\partial^2 \sigma}{\partial u^2} \right) = 0 . \tag{5.10.2b}
\]

In view of the HJ equation and of Hamiltonian (5.7.2b), we can identify the phase \( \sigma \) as the functional \( S_0 \).

Taking (5.8.9) into account, Eq. (5.10.2b) reduces to

\[
C \frac{\partial r}{\partial u} + \sqrt{\left( \frac{E}{v} \right)^2 - C^2 \frac{\partial r}{\partial v}} + \frac{a(E^2 - C^2 v^2) - E^2}{v \sqrt{E^2 - C^2 v^2}} r = 0 . \tag{5.10.3}
\]

Comparing (5.10.3) with (5.8.4), we see that they coincide for \( a = 2 \) only[61]. This correspondence is expectable for a suitable choice of the configurational variables; however, it is remarkable that it arises for the chosen operator-ordering only. Here arises the importance of the correspondence, which fixes a particular quantum dynamics for the system.

Summarizing, we have demonstrated from our study that it is possible to get a WKB correspondence between the quasi-classical regime and the ensemble dynamics in the configuration space, and we provided the operator-ordering when quantizing the Mixmaster model

\[
\hat{p}_u^2 \hat{p}_v^2 \to -\hbar^2 \frac{\partial}{\partial v} \left( v^2 \frac{\partial}{\partial v} \right) . \tag{5.10.4}
\]

### 5.11 The Spectrum of the Mixmaster

#### 5.11.1 Eigenfunctions and the vacuum state

Once fixed the operator ordering \( a = 2 \), the eigenvalue equation (5.9.4) rewrites as

\[
\left[ v^2 \frac{\partial^2}{\partial u^2} + v^2 \frac{\partial^2}{\partial v^2} + 2v \frac{\partial}{\partial v} + (E)^2 \right] \Psi(u,v,E) = 0 . \tag{5.11.1}
\]

By redefining \( \Psi(u,v,E) = \psi(u,v,E)/v \), we can reduce (5.11.1) to the eigenvalue problem for the Laplace-Beltrami operator in the Poincaré plane [484]

\[
\nabla_{LB} \psi(u,v,E) \equiv \nabla^2 \left( \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} \right) \psi(u,v,E) = E_s \psi(u,v,E) , \tag{5.11.2}
\]

which is central in the harmonic analysis on symmetric spaces and has been widely investigated in terms of its invariance under \( SL(2,\mathbb{C}) \) and its eigenstates and eigenvalues.
are

\[ \psi_s(u, v) = av^s + bv^{1-s} + \sqrt{v} \sum_{n \neq 0} a_n K_{s-1/2}(2\pi|n|v)e^{2\pi inu}, \quad a, b, a_n \in \mathbb{C}, \]  
\[ \nabla_{LB}\psi_s(u, v) = s(s-1)\psi_s(u, v), \]  
where \( K_{s-1/2}(2\pi n v) \) are the modified Bessel functions of the third kind[1] and \( s \) denotes the index of the eigenfunction. This is a continuous spectrum and the sum runs over every real value of \( n \).

The eigenfunctions for our model, then, read as

\[ \Psi(u, v, E) = av^{s-1} + bv^{-s} + \sum_{n \neq 0} a_n K_{s-1/2}(2\pi|n|v) e^{2\pi inu}, \]  
with eigenvalues

\[ E^2 = s(1-s). \]

To impose Dirichlet boundary conditions for the wave functions we will require a vanishing behaviour on the edges of the geodesic triangle of Fig. 5.2. Let us approximate[61] the domain with the one in Fig. 5.3; the value of the horizontal line \( v = 1/\pi \) provides the same measure for the exact as well as for the approximate domain

\[ \int_{\Pi Q} \frac{dudv}{v^2} = \int_{\text{Approx domain}} \frac{dudv}{v^2} = \pi. \]

Figure 5.3: The approximate domain where we impose the boundary conditions. The choice \( v = 1/\pi \) for the straight line preserves the measure \( \mu = \pi \) (from [61]).

The difficulty to deal with the exact boundary conditions relies in the sophisticated number theory is linked to these functions while the circle, that bounds from below the domain, furthermore mixes solutions with different indices \( s \).

The Laplace-Beltrami operator and the exact boundary conditions are invariant under parity transformation \( u \rightarrow -u - 1 \); however, the full symmetry group is \( C_{3v} \), and this can be seen in the disk representation of the Lobachewsky plane. \( C_{3v} \) has two one-
5.11 The Spectrum of the Mixmaster

dimensional irreducible representations and one two-dimensional representation \[158, 220].

The eigenstates transforming according to one of the two-dimensional representations are twofold degenerate, while the others are non-degenerate. The latter can be divided in two classes, either satisfying Neumann boundary conditions, or Dirichlet ones. We focus our attention to second case. The choice of the line \( v = 1/\pi \) approximates symmetry lines of the original billiard and corresponds to one-dimensional irreducible representations \[419, 158, 220].

The conditions on the vertical lines \( u = 0, u = -1 \) require to disregard the first two terms in (5.11.5); furthermore, we get the condition on the last term

\[
\sum_{n \neq 0} e^{2\pi i nu} \to \sum_{n=1}^{\infty} \sin(\pi nu),
\]

(5.11.8)

for integer \( n \). As soon as we restrict to only one of the two one-dimensional representations, we get

\[
\sum_{n \neq 0} e^{2\pi i nu} \to \sum_{n=1}^{\infty} \sin(2\pi nu),
\]

(5.11.9)

while the condition on the horizontal line implies

\[
\sum_{n > 0} a_n K_{s-1/2}(2n) \sin(2n\pi u) = 0, \quad \forall u \in [-1, 0],
\]

(5.11.10)

which in general is satisfied by requiring \( K_{s-1/2}(2n) = 0 \) only, for every \( n \). This last condition, together with the form of the spectrum (5.11.6), ensure the discreteness of the energy levels, thanks to discreteness of the zeros of the Bessel functions.

The functions \( K_{s}(x) \) are real and positive for real argument and real index, therefore the index must be imaginary, i.e. \( s = \frac{1}{2} + it \). In this case, these functions have (only) real zeros, and the corresponding eigenvalues turn out to be real and positive.

![Figure 5.4](image_url)

**Figure 5.4:** The intersections between the straight lines and the curves represents the roots of the equation \( K_{it}(n) = 0 \), where \( K \) is the modified Bessel function (from [61]).
The eigenfunctions \((5.11.5)\) exponentially vanish as infinite values of \(v\) are approached. The conditions \((5.11.10)\) cannot be analytically solved for all the values of \(n\) and \(t\), and the roots must be numerically worked out for each \(n\). There are several results on their distribution that allow one to find at least the first levels: a theorem\([404]\) on the zeros of these functions states that \(K_\nu(\nu x) = 0 \iff 0 < x < 1\); furthermore, the energy levels \((5.11.11)\) monotonically depend on the values of the zeros. Thus, one can search the lowest levels by solving Eq. \((5.11.10)\) for the firsts \(n\); in the next Section we will discuss some properties of the spectrum, while now we will discuss the ground state only.

A minimum energy exists, as follows from the quadratic structure of the spectrum and from the properties of the Bessel zeros, and its value is \(E_{20}^2 = 19.831\hbar^2\), and correspondingly the eigenfunction is plotted in Fig. 5.5, together with the probability distribution in Fig. 5.6 the eigenstate is normalized through the normalization constant \(N = 739.466\).

The existence of such a ground state has been numerically derived, but it can be inferred on the basis of general considerations about the Hamiltonian structure; the Hamiltonian, indeed, contains a term \(\vec{v}^2\vec{p}^2\) which has positive definite spectrum and does not admit vanishing eigenvalues.

\[
E^2 = t^2 + \frac{1}{4}.
\]  \(\text{(5.11.11)}\)

5.11.2 Distribution of the Energy Levels

In Table 5.1 we report the first ten “energy” levels evaluated solving \((5.11.10)\)\(^7\)

To study the distribution of the highest energy levels, we need to consider the asymptotic behavior of the zeros for the modified Bessel functions of the third kind. We will discuss the asymptotic regions of the \((t, n)\) plane in the two cases \(t \gg n\) and \(t \simeq n \gg 1\).

\(^7\)For a detailed numerical investigation of the energy spectrum of the standard Laplace-Beltrami operator, especially with respect to the high-energy levels, see\([158, 220]\), where the effects on the level spacing of deforming the circular boundary condition towards the straight line are numerically analyzed.
Table 5.1: The first ten energy eigenvalues, ordered from the lowest one.

| $E$ | 19.831 |
|-----|---------|
|    | 40.357 |
|    | 49.474 |
|    | 63.405 |
|    | 87.729 |
|    | 89.250 |
|    | 116.329|
|    | 128.234|
|    | 138.739|
|    | 146.080|

(i) For $t \gg n$, the Bessel functions admit the representation

$$K_{ilt} = \sqrt{\frac{2\pi e^{-t \pi/2}}{(t^2 - n^2)^{1/4}}} \left[ \sin a \sum_{k=0}^{\infty} \frac{(-1)^k}{t^{2k}} u_{2k} \left( \frac{1}{\sqrt{1 - p^2}} \right) + \cos a \sum_{k=0}^{\infty} \frac{(-1)^k}{t^{2k+1}} u_{2k+1} \left( \frac{1}{\sqrt{1 - p^2}} \right) \right], \quad (5.11.12)$$

where $a = \pi/4 - \sqrt{t^2 - n^2} + \tanh(t/n)$, $p \equiv n/t$ and $u_k$ are the polynomials

$$\begin{align*}
    u_0(t) &= 1, \\
    u_{k+1}(t) &= \frac{1}{2} t^2 (1 - t^2) u'_k(t) + \frac{1}{8} \int_0^1 (1 - 5t^2) u_k(t) dt . \quad (5.11.13)
\end{align*}$$

Retaining in the expression above only terms of order $o(n/t)$, the zeros are fixed by the relation

$$\sin \left[ \frac{\pi}{4} - t + t (\log(2) - \log(p)) \right] - \frac{1}{12t} \cos \left[ \frac{\pi}{4} - t + t (\log(2) - \log(p)) \right] = 0 . \quad (5.11.14)$$

In the limit $n/t \ll 1$, Eq. (5.11.14) can be recast as

$$t \log(t/n) = l\pi \Rightarrow t = \frac{l\pi}{\text{productlog} \left( \frac{ln}{n} \right)} , \quad (5.11.15)$$

where productlog(z) is a generalized function giving the solution of the equation $z = we^w$ and, for real and positive domain, is a monotonic function. In (5.11.15) $l$ is an integer number much greater than 1 in order to verify $n/t \ll 1$.

(ii) In case the difference between $2n$ and $t$ is $o(n^{1/3})$ for $t, n \gg 1$, we can evaluate the
first zeros $k_{s,v}$ by the relations\[^{29}\]

$$k_{s,v} \sim v + \sum_{r=0}^{\infty} (-1)^r s_r(a_s) \left( \frac{v}{2} \right)^{-(2r-1)/3},$$  \hspace{1cm} (5.11.16)

where $a_s$ is the $s$-th zero of $Ai((2/z)^{1/3})$, $Ai(x)$ is the Airy function\[^{15}\]$ and $s_i$ are some polynomials. From this expansion it results that, to lowest order

$$t = 2n + 0.030n^{1/3}.$$  \hspace{1cm} (5.11.17)

Eq. (5.11.17) provides the lowest zero (and therefore the energy) for a fixed value of $n$ and also the relation for the eigenvalues for high occupation numbers

$$E^2 \sim 4n^2 + 0.12n^{4/3}.$$  \hspace{1cm} (5.11.18)

Let us to discuss i.e. the completeness of the spectrum and the definition of a scalar product.

The problem of completeness can be faced by studying firstly the sine functions and then the Bessel ones. On the interval $[-1, 0]$, the set $\sin(2\pi nu)$ is not a complete basis, but as soon as we request the wave function to satisfy the symmetry of the problem, it becomes complete.

Let us take a value $n > 0$, thus functions (5.11.5) have the form $\Phi(u, v) = \sin(2\pi nu) g(v)$, which substituted in (5.11.1) provides

$$v^2 \left( \frac{\partial^2}{\partial u^2} + (2\pi n)^2 \right) g(v) = s(1-s) g(v),$$

whose solutions are exactly the Bessel functions.\[^{419}\]

This property together with the condition on the line $v = 1/\pi$ form a Sturm-Liouville problem and we deal with a complete of eigenfunctions.

Therefore, such eigenfunctions define a space of functions where we can introduce a scalar product, naturally induced by the metric of the Poincaré plane\[^{419}\]

$$\langle \psi, \phi \rangle = \int \psi(x, y) \phi^*(x, y) \frac{dxdy}{y^2},$$  \hspace{1cm} (5.11.19)

where $^*$ denotes complex conjugation.

Now we briefly discuss if the presence of a non-local function, like the square-root of a differential operator, can give rise to non-local phenomena. Following the work of Puzio\[^{419}\], a wavepacket which is non-zero in a finite region of the domain ($v < M$) and far from infinity fails to run to infinity in a finite time, i.e., the probability $P(v > M)$ to find the packet far away exponentially vanishes.

$$P(v > M) = \int_{-1}^{0} \int_{M}^{\infty} \left| v \sqrt{\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2}} \Psi(u,v) \right|^2 dv du <$$

$$< 4M^2 \frac{\pi}{2} \left( \sup \Psi \right)^2 \int_{-1}^{0} \int_{M}^{\infty} e^{-2v} dv du =$$

$$= 4M^2 \frac{\pi}{2} \left( \sup \Psi \right)^2 \left( \frac{e^{-2M}}{M} + \text{Ei}(-2M) \right) <$$

$$< 4 \sqrt{\frac{\pi}{2}} \left( \sup \Psi \right)^2 Me^{-2M}.$$  \hspace{1cm} (5.11.20)
5.12 Basic Elements of Loop Quantum Gravity

In this Section we will review some of the basic aspects of Loop Quantum Gravity (LQG) in a pedagogical manner for a non-expert reader. For a detailed and deeper approach, we refer to the textbooks [435, 485] and to some dedicated reviews [434, 486, 22, 467], while for a critical point of view we recommend [393].

LQG is an attempt to rigorously quantize General Relativity in a background independent manner, trying to define a quantum field theory just on a differential manifold \( M \) and not on a background space-time \( (M, g_0) \), i.e. independently of the choice of a fixed background metric \( g_0 \). However, a way to give a formulation of the theory independently of the possible topological changes of the underlying manifold has not been achieved so far in LQG.

In order to see how fundamental fixed background metric is, let us consider ordinary quantum field theory, whose whole framework, namely the Wightman axioms[234], breaks down as soon as the metric is no longer considered fixed but with a dynamical structure according to General Relativity. In fact we could only construct a rigorous quantum theory in the Minkowski background\(^8\) which implies a preferred notion of causality (locality) and a symmetry group, i.e. the Poincaré one.

LQG works in a Hamiltonian approach\(^9\) and it is able to overcome some of the problems of the older geometro-dynamical approach (described in the previous Sections) using new conceptual and technical ingredients.

Let us rewrite GR in the form of a \( SU(2) \) Yang Mills theory, so that the phase space is endowed with coordinates\(^10\) by a \( SU(2) \) connection \( A^i_\alpha \) and by an electric field \( E^\alpha_j \). These are related to the ADM variables \((h, K)\) by

\[
A^i_\alpha = \omega^i_\alpha + \gamma K_{\alpha\beta} e^{\beta j}, \quad E^\alpha_j = \sqrt{\text{he}}_\alpha^j, \tag{5.12.1}
\]

where \( \omega^i_\alpha = \frac{1}{2} \varepsilon^{\alpha\beta\gamma} \omega^j_{\beta\gamma} \) is the spin connection, \( K_{\alpha\beta} \) the extrinsic curvature and \( \gamma > 0 \) the so-called Immirzi parameter which does not affect the classical dynamics but brings to inequivalent quantum predictions [436]. The symplectic geometry is determined by the only non-trivial Poisson brackets

\[
\{ A^i_\alpha (x), E^j_\beta (x') \} = \kappa \gamma \delta^i_j \delta^\alpha_\beta \delta^3 (x - x'). \tag{5.12.2}
\]

Let us rewrite the constraints (2.4.14) in terms of these new variables, which in the phase

---

\(^8\)The only quantum fields in four dimensions fully understood to date are the free, or perturbatively interacting, fields.

\(^9\)For the covariant approach to LQG, i.e. the spin foams models, see [400, 408].

\(^10\)Here and in the following paragraphs on the LQG/C we will adopt \( i, j, k, \ldots = 1, 2, 3 \) as \( SU(2) \) indices.
phase satisfy the usual spatial diffeomorphism constraint

\[ H_\alpha = F^i_{\alpha\beta} E^\beta_i \approx 0, \quad (5.12.3a) \]

where \( F = dA + A \wedge A \) is the curvature of \( A \), and the scalar one

\[ H = \frac{\epsilon_{ijk} E^i_j E^k_E}{\sqrt{|\det(E)|}} \left[ F^i_{\alpha\beta} - (1 + \gamma^2) \epsilon_{imn} K^m_{\alpha} K^n_{\beta} \right] \approx 0, \quad (5.12.3b) \]

where \( \gamma K^i_{\alpha} = A^i_{\alpha} - \omega^i_{\alpha} \). In the connection formalism, with respect to the metric approach, we have the additional Gauss constraint

\[ G_i = D_\alpha E^\alpha_i = \partial_\alpha E^\alpha_i + \epsilon_{ijk} A^j_{\alpha} E^k_{\beta} \approx 0 \quad (5.12.4) \]

which gets rid of the \( SU(2) \) degrees of freedom. Since an observable is a gauge invariant function, it has to commute with all constraints.

As a second step we have to smear the fields \( A^i_{\alpha} \) and \( E^\alpha_i \) to overcome some of the problems arising in the direct approach. In fact, we switch from the connections \( A^i_{\alpha} \) to the holonomies as the basic variables. Given a curve on \( \Sigma \), i.e. an edge \( \ell \), a holonomy is defined as

\[ h_\ell[A] = \mathcal{P} \exp \left( \int_\ell A \right) = \mathcal{P} \exp \left( \int_\ell A^i_{\alpha} \tau^i dx^\alpha \right), \quad (5.12.5) \]

where \( \mathcal{P} \) denotes the path order and the \( \tau^i = \sigma^i / 2i \) form a basis of \( SU(2) \) and \( \sigma^i \) are the Pauli matrices. The holonomies \( h_\ell \) are elements of \( SU(2) \) and define the parallel transport of the connection \( A^i_{\alpha} \) along the edge \( \ell \). They are gauge invariant and have a one-dimensional support (rather than all \( \Sigma \)). The variable conjugate to the \( h_\ell[A] \) is the flux vector

\[ P^i_S[E] = \int_S *E^i = \int_S \epsilon_{\alpha\beta\gamma} E^i_{\alpha} dx^\beta \wedge dx^\gamma \quad (5.12.6) \]

through any two-dimensional surface \( S \subset \Sigma \), whose support is a two-dimensional submanifold of \( \Sigma \). In order to compute the Poisson brackets between these variables, let us consider an edge \( \ell \) that intersects a surface \( S \) in one point, thus obtaining

\[ \{ h_\ell[A], P^i_S[E] \} = \frac{K \gamma}{4} \alpha(e, S) \tau^i h_\ell[A], \quad (5.12.7) \]

where \( \alpha = 0 \) in the case of the edge not intersecting the surface and \( \alpha = \pm 1 \) when the orientation of the edge and surface are the same or the opposite, respectively. We note that the commutation relation (5.12.7) is non-canonical for the presence of \( h_\ell[A] \).

The quantum kinematics can be constructed promoting such variables to quantum operators obeying appropriate commutation relations. The essential feature of LQG is promoting the holonomies \( h_\ell[A] \) to operators rather than the connections \( A^i_{\alpha} \) themselves.

Let us investigate the kinematical Hilbert space \( \mathcal{H}_{\text{kin}} \) of LQG, i.e. that of the spin networks. These are defined as a graph \( \Gamma \) consisting of a finite number of edges and vertices with a given collection of spin quantum numbers \( j_\ell = 1/2, 1, 3/2, \ldots \), one for each edge, and of other quantum numbers \( I \), the intertwiners, one for each vertex. The wave function of
5.12 Basic Elements of Loop Quantum Gravity

The spin network, the so-called cylindric function, can thus be written as

\[ \Psi_{\Gamma, \psi}[A] = \psi(h_{\ell_1}[A], ..., h_{\ell_n}[A]). \]  

(5.12.8)

If the wave functions \( \psi \) are \( SU(2) \)-gauge invariant, they satisfy the Gauss constraint and vice versa. These functions are called cylindrical because they have a one-dimensional support, i.e. they probe the gauge connection on one-dimensional networks only. When promoted to quantum operators, the fundamental variables of the theory \( (h_{\ell}[A], P_S^E) \) act on the wave functions \( (5.12.8) \) as

\[ \hat{h}_{\ell}[A] \Psi_{\Gamma, \psi}(A) = h_{\ell}[A] \Psi_{\Gamma, \psi}(A) \]  

(5.12.9a)

\[ \hat{P}_S^E \Psi_{\Gamma, \psi}(A) = i\{P_S^E, \Psi_{\Gamma, \psi}(A)\}. \]  

(5.12.9b)

A key point in the LQG approach to the quantum gravity problem is the kinematical scalar product between two cylindric functions, since the main results of discretization of areas and volumes are based on it, which is defined as

\[ \langle \Psi_{\Gamma} | \Psi_{\Gamma'} \rangle = \begin{cases} 0 & \text{if } \Gamma \neq \Gamma' \\ \int \prod_{\ell \in \Gamma} dh_{\ell} \bar{\psi}_{\Gamma}(h_{\ell_1}, ...) \psi_{\Gamma'}(h_{\ell_1}, ...) & \text{if } \Gamma = \Gamma', \end{cases} \]  

(5.12.10)

where the integrals \( \int h_{\ell} \) are performed with the \( SU(2) \) Haar measure\[470\]. The definition is based on a strong uniqueness theorem \[324\]. The inner product vanishes if the graphs \( \Gamma \) and \( \Gamma' \) do not coincide and it is invariant under spatial diffeomorphisms, even if the states \( \Psi_1 \) and \( \Psi_2 \) themselves are not, because the information that the two graphs coincide is diffeomorphism invariant. The information on the position of the graphs, carried by the wave function, disappears in the scalar product \( (5.12.10) \).

Let us stress three relevant aspects:

(i) in contrast with the lattice gauge theory, where all quantities depend on the scale parameter, the “discretuum” of LQG is built via the construction of the scalar product \( (5.12.10) \). This feature is responsible for the failure of the Stone-von Neumann theorem \[234\]: LQG and WDW lead to different results, since the two quantizations procedures are not equivalent.

(ii) The obtained Hilbert space is not-separable, as it does not admit a countable basis, because the set of all spin networks is not numerable and two non-coincident spin networks are orthogonal with respect to \( (5.12.10) \).

(iii) States with negative norm are absent without imposing the constraints \( (5.12.3a), (5.12.3b), (5.12.4) \), in contrast with the usual gauge theories, where the negative norm states can be eliminated only after imposing the constraints. However, this kinematical Hilbert space is not relevant to solve the quantum constraints of LQG. Anyway, the area and volume operators (which we do not discuss here) are computed at this level and the discretization of the corresponding spectrum is related to this Hilbert space properties\[11\]

\[11\]The spectrum of the area operator \( A_S \) is computed applying it to a wave function \( \Psi \) defined in a given graph. Such a graph is refined in a way that the elementary surface \( S_1 \) is pierced only by the edge of the
The last step is to impose the constraint at a quantum level to obtain the physical states. These constraints are implemented firstly to express them in terms of holonomies and fluxes, and secondly to investigate their properties.

The Gauss constraint \((5.12.4)\) imposes several restrictions on the quantum numbers \(I\) of the cylindric functions. The diffeomorphism constraint \((5.12.3a)\) is more difficult to deal with and will not be treated in terms of an operatorial one. In fact, a diffeomorphism generator does not exist as an operator and diffeomorphism invariant states (with the exception of the empty spin network state \(\Psi = 1\)) do not exist in \(H_{\text{kin}}\). This constraint is imposed implementing a “group average method” in a way properly adapted to the scalar product \((5.12.10)\)\(^{[214]}\). A key step arises from solving the constraints on a larger space, i.e. the dual \(\text{Cyl}^*\) of the cylindric functions \(\text{Cyl}\), such that

\[
\text{Cyl} \subset H_{\text{kin}} \subset \text{Cyl}^*,
\]

which is the so-called Gel’fand triple\(^{[234]}\). An important feature of the new Hilbert space \(H_{\text{diff}}\) is of being separable, differently from \(H_{\text{kin}}\). The final challenge will be finding a space annihilated by all the constraints and defining a physical inner product which yields the final physical Hilbert space.

As mentioned in the WDW formalism, the main problem of all quantum gravity theories is to impose at a quantum level the scalar constraint. This difficulty appears also in the LQG approach and will be reflected also in the minisuperspace theory, i.e. the Loop Quantum Cosmology (LQC).

Let us rewrite the constraint \((5.12.3b)\) in terms of variables corresponding to a well defined quantum operator. This can be done using classical identities from which we can express the triads, the extrinsic curvature and the field strength in terms of holonomies and well-defined operators as the volume one. Then, similarly to quantum field theory, the Hamiltonian has to be regularized with a parameter \(\epsilon\) shrunk to zero at the end of the computation. This is a highly non trivial step and poses serious challenges. In fact, the regularisation \(\epsilon\) enters in the spin networks picture via a plaquette \(P(\epsilon)\), attached to a vertex and thus it modifies the underlying graph, but two wave functions supported on different networks are orthogonal by the scalar product \((5.12.10)\). In other words, for any cylindric function \(\Psi\), the limit \(\epsilon \to 0\) of \(\hat{H}_\epsilon \Psi\) does not exist on \(\text{Cyl}\). Usually one transfers the action of the scalar constraint to the dual space, adopting a weaker notion of limit. More specifically, the limit \(\epsilon \to 0\) is defined by

\[
\langle \hat{H}^* \chi | \Psi \rangle = \lim_{\epsilon \to 0} \langle \chi | \hat{H}_\epsilon \Psi \rangle
\]

for all \(\Psi \in \text{Cyl}\) and \(\chi \in V^* \subset \text{Cyl}^*\). The space \(V^*\) must be selected taking into account physical motivations. A natural choice is \(V^* = H_{\text{diff}}\), but this is not unique and furthermore poses several problems\(^{[393]}\).

The necessary use of the weaker limit \((5.12.13)\) is reflected on the quantum constraints network, therefore obtaining

\[
\hat{A}_S \Psi = \kappa \gamma \sum_p \sqrt{j_p(j_p + 1)} \Psi.
\]

The minimal accessible length appears to be of order of the Planck one and the spectrum discreteness is related to the structure of the spin networks. In fact, a further refinement of the area operator does not contribute to the result.
5.13 Isotropic Loop Quantum Cosmology

In fact, in LQG a weaker notion of algebra closure (with respect to the so-called off-shell closure) is formulated, requiring that equation

$$[\hat{H}^*, \hat{H}'^*] \chi = 0$$  \hspace{1cm} (5.12.14)

holds. The closure of the algebra is required only after the imposition of the constraints, and in this sense it is weaker. This is relevant when addressing the quantum space-time covariance, because only the off-shell closure exhibits this quantum gravity property and, relaxing the algebra closure, some crucial information may get lost.

Let us conclude noting that all the main results of LQG and LQC are related to the discretization of the spectrum of area and volume operators. The nature of this cut-off could be ambiguous[5,155], since it can be dynamically generated or imposed by hand when dealing with the compact SU(2) rather than the true gauge group of GR, i.e. the Lorentz one. In fact, in a covariant formalism, without imposing a time-gauge, the area spectrum is continuous [6], but for a discussion on this point of view we demand to [328] and references therein. For the recent interesting approaches to solve the scalar constraints problems mentioned above, see [211,212,213,487,240].

5.13 Isotropic Loop Quantum Cosmology

The Loop Quantum Cosmology is a minisuperspace model, i.e. a truncation of the phase space of classical GR, which is quantized according to the methods of LQG. Therefore LQC is not the cosmological sector of LQG, i.e. the inhomogeneous fluctuations are switched off by hand rather than being suppressed quantum mechanically. However the minisuperspace is an important arena to test a theory and in LQC the most spectacular results appear: the absence of the classical singularity [88], replaced by a Big-Bounce [23,24] in the isotropic settings, a geometrical inflation [89] and the suppression of the Mixmaster chaotic behavior toward the singularity [93].

In this Section we will analyze some basic aspects of the so-called isotropic Loop Quantum Cosmology and the fate of the classical singularity. For exhaustive discussions on this argument see [90,21].

In this case, the phase space of GR is two-dimensional, since the scalar factor $a = a(t)$ is the only degree of freedom of an isotropic model. Therefore, the variables (5.12.1) are reduced to

$$A = c^2 \omega^i \tau_i, \quad E = p \sqrt{\gamma} \epsilon_i \tau^i$$  \hspace{1cm} (5.13.1)

where a fiducial metric in $\Sigma$ is fixed by $h_{ab}$ and thus by the triad $\epsilon_i$ and co-triad $\omega^i$. Then, the phase space has coordinates $(c, p)$, which are conjugate variables satisfying \{c, p\} = $\kappa \gamma$. This connection formalism is related to the metric one via the relations

$$|p| = a^2, \quad c = \frac{1}{2}(k + \gamma \dot{a}),$$  \hspace{1cm} (5.13.2)

where $k = 0, \pm 1$ is the usual curvature parameter. Since the Gauss and the diffeomorphism constraints are already satisfied (with (5.13.1) they identically vanish), the scalar constraint

$$H^{(c,p)} = -\frac{3}{\kappa} \sqrt{|p|} \left( \frac{1}{\gamma^2} (c - \Gamma)^2 + \Gamma^2 \right) \approx 0,$$  \hspace{1cm} (5.13.3)
where $\Gamma \propto k$, is the only remaining. This is nothing but the Friedmann equation and reduces to a simple form in the flat case: $H_{k=0}^{(\ell,p)} = -\frac{3}{2\pi^2} c^2 \sqrt{|p|}$. We stress that $p \in (-\infty, +\infty)$ and the classical singularity appears for $p = 0$. Furthermore the changes in the sign of $p$ correspond to the changes in the orientation of the physical triad $e^\alpha_i$, related to $e^\beta_i$ via $\text{sign}(p) / \sqrt{|p|}$.

The quantization of this model follows the lines of LQG and therefore we have to construct $SU(2)$ holonomies and fluxes, in order to promote these variables to quantum operators, which become

$$h_i(c) = \cos \left(\frac{\mu c}{2}\right) + 2 \left(e^{i\alpha} \omega^i_\alpha\right) \tau_i \sin \left(\frac{\mu c}{2}\right), \quad P_\mu(p) = A_\mu p,$$

where $A_\mu$ is a factor determined by the background metric and $\mu \in (-\infty, +\infty)$ is a real continuous parameter, along which the holonomies are computed. The elements of the holonomies can be recovered from the almost periodic functions $N_\mu(c) = e^{i\mu c/2}$ and then the cylindric functions of this reduced model are given by

$$g(c) = \sum_j \xi_j e^{i\mu_j c/2} \in Cyl_S,$$

$Cyl_S$ being the space of the symmetric cylindric functions. The holonomy flux algebra is generated by $e^{i\mu c/2}$ and by $p_i$, i.e. we are in a hybrid representation between the Heisenberg $(p)$ and Weyl $(e^{i\alpha})$ ones.

The Hilbert kinematical space is now obtained requiring that the $N_\mu(c)$ form an orthonormal basis, i.e. $\langle N_\mu | N_{\mu'} \rangle = \delta_{\mu,\mu'}$, in analogy with the scalar product (5.12.10) of the full theory. From general theoretical considerations, the Hilbert space is necessarily $\mathcal{H}_S = L^2(\hat{R}_{\text{Bohr}}, \omega \mu)$, where $\hat{R}_{\text{Bohr}}$ is a compact Abelian group (the Bohr compactification of the real line). This is the space of the almost periodic function.

Let us stress that the construction of the Hilbert space is the key point of all the theory and of its main results. In fact, using $\hat{R}_{\text{Bohr}}$ one can introduce a new representation of the Weyl algebra. This is inequivalent to the standard Schrödinger representation and therefore leads to different results from the WDW theory.

In this Hilbert space the operators $\hat{N}_\mu$ and $\hat{p}$ act by multiplication and derivation, respectively. As usual, let us introduce the bra-ket notation $\langle c | \mu \rangle = \langle c | N_\mu(C) \rangle$. The volume operator $(V = |p|^{3/2})$ has a continuous spectrum $\hat{V} | \mu \rangle = V_\mu | \mu \rangle \propto |\mu|^{3/2} \sqrt{\mu} | \mu \rangle$, in contrast to LQG. In the reduced theory the spectrum is discrete in a weaker sense: all the eigenvectors are normalizable. Hence the Hilbert space can be expanded as a direct sum, rather than as a direct integral, of the one-dimensional eigenspaces of $\hat{p}$.

In view of the analysis of the singularity, we have to address the inverse scale factor operator which is a fundamental one because, at a classical level, the inverse scale factor $\text{sign}(p) / \sqrt{|p|}$ diverges toward the singularity. Let us express it in terms of holonomies and fluxes and then proceed to the quantization. We note that the following classical

---

12Note that this is a Kronecker-delta rather than the usual Dirac one.

13This feature can be attributed to the high degree of symmetry. In fact, in LQG the spin networks are characterized by a pair $(\ell, j)$ consisting of a continuous edge $\ell$ and a discrete spin $j$. Due to the symmetry, such pair now collapses to a single continuous label $\mu$. 

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Identity

\[
\frac{\text{sign}(p)}{\sqrt{|p|}} = \frac{4}{\kappa \gamma} \text{Tr} \left( \sum_i \tau^i h_i \left\{ h_i^{-1}, V^{1/3} \right\} \right),
\]

(5.13.6)

holds, where the holonomy \( h_i \) is evaluated along any given edge. In fact, since we have \( h_i h_i^{-1} \), the choice of the edge is not important, i.e. we do not introduce a regulator and the expression (5.13.6) is exact. With the scalar constraint the situation will be different.

We can proceed with the quantization of operator (5.13.6) in a canonical way. The eigenvalues are given by

\[
\left( \frac{\text{sign}(p)}{\sqrt{|p|}} \right) |\mu\rangle \propto \frac{1}{\gamma l_p} \left( V^{1/3}_\mu - V^{1/3}_{\mu-1} \right) |\mu\rangle,
\]

(5.13.7)

where \( V_\mu \) is the volume operator eigenvalue defined above, whose fundamental properties are to be bounded from above and to coincide with the operator \( 1/\sqrt{|p|} \) for \(|\mu| \gg 1\). The upper bound is obtained for the value \( \mu = 1 \) and therefore \( |p|^{-1/2} \sim l_p^{-1} \).

The physical situation emerging is intriguing. Although the volume operator admits a continuous spectrum and a zero volume eigenstate (the \(|\mu = 0\rangle\) state), the inverse scalar factor is non diverging at the classical singularity, but is bounded from above. This can indicate that, at a kinematical level, the classical singularity is avoided in a quantum approach. The semiclassical picture, i.e. the WDW behavior of the inverse scalar factor, appears for \(|\mu| \gg 1\) and therefore far from the fully quantum regime. Such a behavior contrasts with the WDW formalism where the inverse scale factor is unbounded from above and the differences reside in the non-standard Hilbert space adopted. In fact, differently from the WDW theory, all eigenvectors of \( p \) are normalizable in LQC, including the one with zero eigenvalue. Therefore, in order to define an inverse scale factor operator, one has to formulate the alternative procedure discussed above.

Let us stress that a key ingredient is the absence of the inhomogeneous fluctuations which conversely are present in the full theory. In fact \([100]\) computed in full LQC that the analogue of the inverse scale factor is unbounded from above on zero volume eigenstates. The boundedness of the inverse scale factor is neither necessary nor sufficient for the curvature singularity avoidance.

As a last point we have to impose the scalar constraint at a quantum level to discuss the fate of the singularity from a dynamical point of view.

In order to follow the lines of the the full theory, the starting point will be the constraint (5.12.3) and not the reduced one (5.13.3). In the expression (5.13.3), the connection \( c \) itself is present rather than the holonomies and the operator \( \hat{H}^{(c,p)} \) is not well defined at a quantum level. Let us investigate, for simplicity, the flat case. The two parts of (5.13.3) are then proportional to each other. Mimicking the procedure followed in the full theory \([485]\) we rewrite the constraint in terms of holonomies and fluxes as

\[
H_{\mu_0}^{(h,p)} = -\frac{4}{\kappa \gamma^3 \mu_0^2} \sum_{ijk} \epsilon^{ijk} \text{Tr} \left( h_{ij}^{\mu_0} h_{k}^{\mu_0} \left\{ (h_{k}^{\mu_0})^{-1}, V \right\} \right) + O(c_3^3 \mu_0),
\]

(5.13.8)

where \( h_{ij}^{\mu_0} \) denotes the holonomy computed around a square \( \alpha_{ij} \) with each side having

\(^{14}\)We recall that in this model the classical Ricci scalar curvature is given by \( R \sim 1/a^2 \) and therefore, from equation (5.13.7), at the classical singularity it does not diverge, assuming the value \( R \sim 1/l_p^2 \).
length $\mu_0$, i.e. $h_{ij} = h_i h_j^{-1} h_j^{-1}$. Differently from expression (5.13.6), the dependence on $\mu_0$ does not drop out and now plays the role of a regulator. However, at a classical level, we can take the limit $\mu_0 \to 0$ and verify that the resulting expression coincides with the classical Hamiltonian (5.13.3). As in the full theory, the problems arise at a quantum level. Let us investigate the action of the quantum operator $\hat{H}_{\mu_0}^{(h,p)}$ on the eigenstates which is

$$\hat{H}_{\mu_0}^{(h,p)}|\mu\rangle = \frac{3}{\kappa \gamma^3 \mu_0^3} (V_{\mu+\mu_0} - V_{\mu-\mu_0}) ((|\mu+4\mu_0\rangle - 2|\mu\rangle + |\mu-4\mu_0\rangle)).$$

The limit $\mu_0 \to 0$ fails to exist and the classical regulated version of equation (5.13.3) behaves as $H_{\mu_0}^{(h,p)} \to H^{(c,p)}$. Since it contains $c$, a limit at a quantum level does not exist because the operator $\hat{c}$ itself does not exist in the Hilbert space $\mathcal{H}_S$. As a matter of fact, in this reduced theory, there is no way to remove the regulator. This is resolved in comparison with the full theory. If we assume that the predictions of LQG are true, then the regulator $\mu_0$ can be shrunk until the minimal admissible length given by the area operator spectrum. In this sense, the $\mu_0 \to 0$ limit is physically meaningless. However, how this reduced theory (LQC) can see a minimal length coming out from LQG is not fully understood, since it is not the cosmological sector, but the usual cosmological minisuperspace phase space quantized through the LQG methods.

Let us investigate the physical states. As in the full theory, the physical states are those annihilated by all the constraints and live in some bigger space $Cyl_5$ and they do not need to be normalizable. A generic state $|\Psi\rangle \in Cyl_5$ can be expanded as

$$|\Psi\rangle = \sum_\mu \psi(\mu, \phi)|\mu\rangle,$$

where $\phi$ represents a generic matter field and satisfies the constraint equation

$$|\Psi\rangle \left( \hat{H}_{\mu_0}^{(h,p)} + \hat{H}_{\mu_0}^{(c,p)} \right) = 0$$

and therefore the equation for $\psi(\mu, \phi)$

$$(V_{\mu+5\mu_0} - V_{\mu+3\mu_0}) \psi(\mu, \phi) - 2(V_{\mu+\mu_0} - V_{\mu-\mu_0}) \psi(\mu, \phi) +$$

$$+ (V_{\mu-5\mu_0} - V_{\mu-3\mu_0}) \psi(\mu-4\mu_0, \phi) = -\frac{\kappa}{3} (\gamma^3 \mu_0^3)^2 \hat{H}_{\mu_0}^{(c,p)} \psi(\mu, \phi).$$

has to hold. This is nothing but a recurrence relation for the coefficients $\psi(\mu, \phi)$ which ensures that $|\Psi\rangle$ is a physical state. Even though $\mu$ is a continuous variable, it is given by (5.13.12) as an algebraic rather than by a differential equation as, for example, in the WDW theory.

Let us now briefly discuss what happens to the classical singularity at a dynamical level. It corresponds to the state $|\mu = 0\rangle$ and as we can see from equation (5.13.12), starting at $\mu = -4N\mu_0$ we can compute the coefficients $\psi(4\mu_0(n-N), \phi)$ for $n > 1$, all but $\psi(\mu = 0, \phi)$, because the generic coefficient vanishes if and only if $n = N$. Although the quantum evolution seems to break down right at the classical singularity, this is not the case, since the coefficient $\psi(\mu = 0, \phi)$ is decoupled from the others thanks to $V_{\mu_0} - V_{-\mu_0} = 15$ The notation $|\Psi\rangle$ is adopted to the eventuality of non-renormalizable states.
0 and to $\hat{H}_{\text{lo}}^\phi \psi(\mu = 0, \phi) = 0$ realizes. Therefore the coefficients in (5.13.12) are such that one can unambiguously evolve the states through the singularity even though $\psi(\mu = 0, \phi)$ is not determined and the classical singularity is solved in the LQC framework.

We conclude reporting that the previous results have been significantly extended [24] with a rigorous formulation of the physical Hilbert space, of the Dirac observables and of the semi-classical states. Furthermore, taking a massless scalar field as a relational clock for the system, the classical Big-Bang is replaced by a quantum Big-Bounce displaying in detail an intuitive picture of the Universe evolution in the Planckian era is displayed.

### 5.14 Mixmaster Universe in LQC

We review the basic aspects of the Mixmaster Universe in the LQC framework in this Section, while for the detailed analysis we demand to the literature [93, 95, 94].

As we have seen, the Bianchi IX evolution toward the singularity sees infinite sequences of Kasner epochs characterized by a series of permutations as well as by possible rotations of the expanding and contracting spatial directions. However, this infinite number of bounces within the potential, at the basis of chaos, is a consequence of an unbounded growth of the spatial curvature. When the theory offers a cut-off length and the curvature is bounded, the Bianchi IX model naturally shows a finite number of oscillations and in LQC a quantum suppression of the chaotic behavior appears close to the singularity.

Let us formulate in the connection formalism the vacuum Bianchi IX model. The spatial metric $dl^2 = a_I^2 (\omega^I)^2$ can be taken diagonal, leaving three degrees of freedom only. The basic variables for a homogeneous model are

$$A^I_k = c_{(I)} \Lambda^I_k \omega^I_k, \quad E^a_i = p^{(I)} \Lambda^I_i X^a_i,$$

where $\omega^I$ are the left-invariant 1-forms, $X_I$ are the left-invariant fields dual to $\omega^I (\omega^I (X_I) = \delta^I_J)$, the $SO(3)$-matrix $\Lambda$ contains the pure gauge degrees of freedom and $I, J, K, \ldots$ run as $1, 2, 3$. The physical information are expressed in terms of the gauge invariants $c_{(I)}$ and $p^{(I)}$ which satisfies the Poisson brackets $\{c_{I}, p^{J}\} = \gamma K \delta^I_J$. These variables are related to the scale factors $a_I$, the spin connections $\Gamma^I$ and the extrinsic curvature $K_I = -\frac{1}{2} \dot{a}_I$ by the relations

$$p^I = \text{sign}(a_I) |a_I a_K| \text{sign}(a_I), \quad c_I = \Gamma^I - \gamma K_I,$$

where

$$\Gamma^I = \frac{1}{2} \left( \frac{a_I}{a_K} + \frac{a_K}{a_I} - \frac{a_I^2}{a_J a_K} \right) = \frac{1}{2} \left( \frac{p^K}{p^I} + \frac{p^I}{p^K} - (p^I)^2 \right) .$$

The classical dynamics is governed by the scalar constraint (5.12.3b) which reads as

$$H = \frac{2}{\kappa} \left[ (\Gamma^I \Gamma_K - \Gamma_I) a_I - \frac{1}{4} a_I a_J a_K + \text{cyclic} \right] \approx 0 .$$

The particular case of the isotropic model, the open ($k = 1$) FRW, can be recovered setting $a_1 = a_2 = a_3 = a$. On the other hand, the Bianchi I model can be obtained for $\Gamma = 0$. The potential term from (5.14.4) is given by

$$W(p) = 2 \left( p^I p^J (\Gamma^I \Gamma_J - \Gamma_K) + \text{cyclic} \right)$$
which has infinite walls at small \( p^l \) due to the divergence of the spin connection components.

The loop quantization is performed straightforwardly as in the isotropic case. In fact, an orthonormal basis is given by the \( \hat{p}^l \)-eigenstates \( |\mu_1, \mu_2, \mu_3\rangle = |\mu_1\rangle \otimes |\mu_2\rangle \otimes |\mu_3\rangle \) and the Hilbert space is taken as a direct product of the isotropic ones, it is separable and is a subspace of the kinematical non-separable Hilbert space. As usual, the cylindric functions are given by a superposition of the functions \( \langle c|\mu\rangle \sim \exp(i\mu c/\hbar) \) and the basic quantum operators are the gauge invariant triad operators \( \hat{p}^l \) (fluxes) and the holonomies

\[
\hat{h}_l(c) = \cos\left(\frac{c_l}{2}\right) + 2\Lambda^l_j \tau_l \sin\left(\frac{c_l}{2}\right) .
\]

The \( \hat{p}^l \) and \( \hat{h}_l \) act as derivative and multiplication operators, respectively. In particular, the volume operator defined from \( \hat{p}^l \) as \( \hat{V} = \sqrt{[\hat{p}^1 \hat{p}^2 \hat{p}^3]} \), acts on the eigenstates \( |\mu_1, \mu_2, \mu_3\rangle \) as

\[
\hat{V} |\mu_1, \mu_2, \mu_3\rangle = \left(\frac{1}{2}\kappa \gamma\right)^{3/2} \sqrt{|\mu_1\mu_2\mu_3|} |\mu_1, \mu_2, \mu_3\rangle ,
\]

and it has a continuous spectrum.

From these basic operators we can obtain, similarly to the isotropic case, the inverse triad operator. Since it is diverging toward the classical singularity, we are interested to its behavior at a quantum level. Conceptually its construction in the homogeneous cosmological sector is the same as in the isotropic one, the only difference residing in the computations and in the appearance of some quantization ambiguities, as in particular the half-integer \( j \) and a continuous parameter \( l \in (0,1) \). Nevertheless, all the results are independent on them. This behavior mimics the quantization ambiguities present either in LQG or in the isotropic sector of LQC. While in the full theory we find an ambiguous choice of the spin number \( j \) associated to a given edge of the spin network, in the isotropic LQC it is reflected on the choice of the Hamiltonian regulator \( \mu_0 \). Nevertheless, this is but a parameter that we can neither shrunk to zero, neither fix in some way in the context of LQC theory itself but it outcomes from keeping some prediction of another theory (usually LQG). In the inverse scale factor of isotropic LQC none quantization ambiguity appears.

Since we can express \( |p^l|^{-1} \) in terms of holonomies and volumes via a classical identity, it can be canonically quantized as follows

\[
|p^l|^{-1} |\mu_1, \mu_2, \mu_3\rangle = A_{i,j,l}(\mu_1) |\mu_1, \mu_2, \mu_3\rangle ,
\]

where

\[
f_{j,l}(\mu_1) = \left( \sum_{k=-j}^{j} k |\mu_1 + 2k| \right)^{1/1-l} \]

and \( A_{i,j,l} \) is a function of the quantization ambiguities, i.e. \( j \) and \( l \). The values \( f_{j,l}(\mu) \) decrease for \( \mu < 2j \) and we have \( f_{j,l}(0) = 0 \) and therefore \( |p^l|^{-1}|\mu_1 = 0\rangle = 0 \). Thus, the inverse triad operator annihilates the state corresponding to the classical singularity \( |\mu_1 = 0\rangle \).

Fundamental properties of the eigenvalues of the operator \( (5.14.8) \) can be extracted from the asymptotic expansions of \( \hat{F}_{j,l}(\mu_1) \equiv A_{i,j,l}(\mu_1) \). For large \( j \), \( F_{j,l}(\mu_1) = F_l(\nu_1) \),
with \( v_I = \mu_I/2J \), and no dependence on \( j \) appears, in particular

\[
F_I(v_I) = \begin{cases} 
\frac{1}{v_I} & \text{if } v_I \gg 1 \quad (\mu_I \gg j) \\
\left( \frac{v_I}{I + 1} \right)^{1/4} & \text{if } v_I \ll 1 \quad (\mu_I \ll j).
\end{cases}
\] (5.14.10)

The classical behavior for the inverse triad components is obtained for \( v_I \gg 1 \) and the loop quantum modifications arise for \( v_I \ll 1 \). Rewriting the spin connection in the triad representation, the potential (5.14.5) is given by

\[
W_{i,j}(\nu) = 2(\gamma\kappa j)^2 \left( v_I v_J (\Gamma_I\Gamma_J - \Gamma_K) + \text{cyclic} \right),
\] (5.14.11)

where

\[
\Gamma_I(v_I) = \frac{1}{2} \left[ v_K \text{sign}(v_I) F_I(v_I) + v_J \text{sign}(v_K) F_I(v_K) - v_I v_J F_I^2(v_I) \right].
\] (5.14.12)

The loop quantization of the scalar constraint is different in the homogeneous case. In fact, unlike the full theory, the spin connections are tensors due to the homogeneity symmetry and cannot vanish as in LQG, thus the holonomies will depend also on them and the quantum scalar operator leads to a partial difference equation, like in isotropic LQC, for which we refer to [95].

Let us discuss the Mixmaster Universe in the LQC framework, analyzing its behavior at a semiclassical level, considering the modifications induced in the dynamics by the loop quantization. Since an effective Hamiltonian must arise from the underlying quantum evolution, we will proceed in two steps.

i) For a slow varying solution, the differences equation is specialized, in the continuum regime \( \mu_I \sim p^I/\gamma\kappa \gg 1 \),\(^{16}\) thus obtaining the Wheeler-DeWitt equation

\[
\left( \kappa^2 p^I p^J \frac{\partial^2}{\partial p^I \partial p^J} |S(p)\rangle + \text{cyclic} \right) + W_{i,j}(p) \sqrt{|p^I p^J p^K|} |S(p)\rangle = 0,
\] (5.14.13)

where \( \phi \) denotes a generic matter field.

\[\text{ii) We take the WKB limit of the wave function } T(p) = \sqrt{|p^I p^J p^K|} |S(p)\rangle, \text{ i.e. } T = e^{i\Lambda/\hbar}, \text{ leading to the Hamilton-Jacobi equation for the phase } \Lambda \text{ to zero-th } \hbar \text{ order.}\]

We have obtained the classical dynamics plus the quantum loop corrections. The key point for the classical analysis of the effective Hamiltonian is that the classical region \( \mu_I \gg 1 \) can be separated in two subregions. In fact, remembering the \( p \)-dependence in the WDW equation (5.14.13) given by \( \mu_I/2J \sim p^I/\gamma\kappa j \), we obtain the condition \( \mu_I \gg 1 \) for \( p^I \gg j\gamma\kappa (j \gg \mu_I \gg 1) \) and \( p^I \gg j\gamma\kappa (\mu_I \gg j \gg 1) \).

The second subregion \( (\mu_I \gg j \gg 1) \) is the purely classical one, i.e. where the Misner picture is still valid. From expansion (5.14.10), the eigenvalues of the inverse triad operator correspond to the classical values. On the other hand, the region where \( j \gg \mu_I \gg 1 \) is

\(^{16}\)The eigenvalues of the triad operator \( \hat{p}^I \) are given by \( \hat{p}^I |\mu_1, \mu_2, \mu_3\rangle = p^I |\mu_1, \mu_2, \mu_3\rangle \), where \( p^I \sim \gamma\kappa \mu_I \).
characterized by loop quantum modifications. In fact, the inverse triad operator eigenvalues have a power law dependence. The quantum modifications of the classical dynamics are controlled by the parameter $j$: if it is large enough, one can move the quantum effects within the effective potential into the semi-classical domain. On the other hand, the WKB limit ($\hbar \to 0$) is strictly valid in the Misner region ($\mu_1 \gg j \gg 1$), because in the first region a dependence on $(\gamma \kappa)^{-1}$, appears in the potential term. We assume the validity of such approximation in the ($j \gg \mu_1 \gg 1$)-region, because the inverse triads vanish as $\pi_1 \to 0$.

A qualitative study of the modified classical dynamics, arises from analyzing the potential term, whose explicit expression is more complex than the original one, making the analysis of the dynamics tricky. The volume variable is regarded as a time variable and in general the dependence on it does not factorize. Nonetheless, in the second region, the Misner potential is restored.

Considering the particular case $q_- = 0$ (the Taub Universe\textsuperscript{17}), we can qualitatively study the effective (loop) potential. In this case we get $\nu_2 = \nu_3 \equiv \nu$ and $\nu_1 \equiv \rho = V^2 / ((2\pi)^3 \nu)$ and therefore $\Gamma_2 = \Gamma_3$. The wall is seen for $\nu \gg 1$ so that $F_1(\nu) \sim \nu^{-1}$, but $\rho$ not negligible, i.e. the relation $F_1(\rho) \sim \rho^2$ holds and the potential wall (5.14.11) becomes

$$W_{j,l} \sim \frac{V^4}{j \rho^2} F_1^2 \rho (3 - 2 \rho F_1(\rho)),$$

where $V$ denotes the volume. For $\rho \gg 1$, $F_1(\rho) \sim \rho^{-1}$ and the classical wall $e^{4\alpha - 8\beta_+}$ is restored. The key difference with the Misner case relies in the wall finite height. As the volume decreases, the wall moves inwards and its height decreases as well. In the following evolution the wall completely disappears. In particular it gets its maximum for $\beta_+ = -\alpha$ and vanishes as $e^{12\alpha} \propto V^4$ toward the classical singularity ($\alpha \to -\infty$).

This peculiar behavior shows that the Mixmaster evolution stops at a given time and therefore chaos disappears. In fact, the point-Universe, when the volume is so small that the quantum modifications arise, will never bounce against the potential wall and the Kasner epochs will continue without any replacement. This behavior predicted by the LQC framework produces (qualitatively) the same results of the influence of a scalar filed on the Universe dynamics: in fact, also in that case, at a given time the particle performs the last bounce and then it freely moves (see Section 4.13).

For a discussion of the Bianchi cosmologies in this new canonical first order formalism see [307, 308, 25, 355, 216, 222, 309, 94, 165, 111, 110, 128, 129].

### 5.15 On the GUP and the Minisuperspace Dynamics

This paragraph is devoted to explain some results obtained in a recent approach [45, 46] (see also [496, 401, 497]) to quantum cosmology, in which the notion of a minimal length naturally appears. In particular, the purpose is to quantize a cosmological model by using a modified Heisenberg algebra, which reproduces a Generalized Uncertainty Principle (GUP)

$$\Delta q \Delta p \geq \frac{1}{2} \left( 1 + \beta (\Delta p)^2 + \beta (p)^2 \right),$$

\textsuperscript{17} The Taub model is nothing but a particular case of the Bianchi IX one in which $\beta_- = 0$ [446].
where $\beta$ is a “deformation” parameter. The uncertainty principle (5.15.1) can be obtained by considering an algebra generated by $q$ and $p$ obeying the commutation relation

$$[q, p] = i \left( 1 + \beta p^2 \right). \quad (5.15.2)$$

Such deformed Heisenberg uncertainty principle appeared in studies on string theory [227, 508, 7] and leads to a fundamental minimal scale. From this point of view, a minimal observable length is a consequence of the limiting scale given by the string one. However, we stress that the minimal scale predicted by the GUP is different from the one predicted by other approaches. In fact, equation (5.15.1) implies a finite minimal uncertainty in position

$$\Delta q_{\text{min}} = \sqrt{\beta}. \quad (5.15.3)$$

This way, we will introduce a minimal scale in the quantum dynamics of a cosmological model.

The appearance of a non-zero uncertainty in position poses some difficulty in the construction of a Hilbert space, as position eigenstates cannot be physically constructed. An eigenstate of an observable necessarily has to have a vanishing uncertainty. Although it is possible to construct position eigenvectors, they are formal but not physical states. In order to recover information on position, we consider the so-called quasiposition wave functions

$$\psi(\zeta) = N \int_{-\infty}^{+\infty} \frac{dp}{(1 + \beta p^2)^{3/2}} \exp \left( i \frac{\zeta}{\sqrt{\beta}} \arctan \left( \sqrt{\beta} p \right) \right) \psi(p), \quad (5.15.4)$$

where $\zeta$ is the quasiposition defined by the main value of the position $q$ on appropriate functions, i.e. $\langle q \rangle = 1$ and $N$ is a normalization factor. The quasiposition wave function (5.15.3) represents the probability amplitude to find a particle maximally localized around the position $\zeta$, i.e. with standard deviation $\Delta q_{\text{min}}$. For more details on quantum mechanics in this framework we recommend [291, 290].

The GUP approach relies on a modification of the canonical prescription for quantization and can be applied to any dynamical system. Moreover, such formalism allows us to analyze some peculiar features of string theory in the minisuperspace dynamics.

Let us investigate the consequences of a Heisenberg deformed algebra (5.15.2) of the quantum dynamics of the flat ($k = 0$) FRW model in presence of a massless scalar field $\phi$. We are interested on the fate of the classical singularity. In the following we summarize the discussion and results reported in [45, 46].

The Hamiltonian constraint for this model has the form

$$H_{\text{grav}} + H_{\phi} = -9\kappa p^2 x + \frac{p^2_{\phi}}{x} \approx 0, \quad x \equiv a^3, \quad (5.15.5)$$

where $a$ is the scale factor. In the classical theory, the phase space is four-dimensional, with coordinates $(x, p_x; \phi, p_{\phi})$, and the physical volume of the Universe vanishes at $x = 0$ and the singularity appears. Moreover each classical trajectory can be specified in the $(x, \phi)$-plane, i.e. $\phi$ can be considered as a relational time. The dynamical trajectories read as

$$\phi = \pm \frac{1}{3\sqrt{\kappa}} \ln \left| \frac{x}{x_0} \right| + \phi_0, \quad (5.15.5)$$

where $x_0$ and $\phi_0$ are integration constants. In equation (5.15.5), the plus sign corresponds
to a Universe expanding from the Big-Bang, while the minus sign to a contracting one into the Big-Crunch. The classical cosmological singularity is for $\phi = \pm \infty$ and every classical solution, in this model, reaches it.

The canonical approach (the WDW theory) does not solve the singularity problem. In fact, we can construct a state localized at some initial time. Then, in the backward evolution, the peak of the wave packet will move along the classical trajectory (5.15.5) falling in the classical singularity[86], so that the latter is not tamed by quantum effects.

This picture is radically changed in the GUP framework and the modifications can be realized in two steps. Firstly, we can show how the probability density $|\Psi(\zeta, t)|^2$ to find the Universe around $\zeta \simeq 0$ (around the Planckian region) can be expanded as

$$|\Psi(\zeta, t)|^2 \simeq |A(t)|^2 + \zeta^2|B(t)|^2, \quad (5.15.6)$$

where $t$ is a dimensionless time $t = 3\sqrt{\kappa}\phi$ and the wave packets

$$\Psi(\zeta, t) = \int_0^\infty d\epsilon \, g(\epsilon) \Psi_\epsilon(\zeta) e^{i\epsilon t} \quad (5.15.7)$$

are such that the state is initially peaked at late time, i.e. the weight function $g(\epsilon)$ is a Gaussian distribution centered at some $\epsilon^* \ll 1$ (at energy much less then the Planck one $1/l_P$). Of course, $\Psi_\epsilon(\zeta)$ represents the quasiposition eigenfunctions (5.15.3) of this problem.

Near the Planckian region, the probability density to find the Universe is $|A(t)|^2$, which is very well approximated by a Lorentzian function peaked in $t = 0$, which corresponds to the classical time when $x(t) = x_0$. For $x_0 \sim O(1/l_P^3)$, the probability density to find the Universe in a Planck volume has a maximum around the corresponding classical values and vanishes for $t \to -\infty$, where the classical singularity appears. In this sense the classical cosmological singularity is solved.

The more interesting differences between the WDW and the GUP approaches relies on the wave packets dynamics. If we consider a wave packet initially peaked at late time, once numerically evolved backward, the integration results in a probability density, at different fixed values of $\zeta$, still approximated by a Lorentzian function. The width of this function remains the same as the states evolve from large $\zeta$ ($\sim 10^3$) to $\zeta = 0$, while its peaks move along the classically expanding trajectory (5.15.5) for values of $\zeta$ larger than $\sim 4$. Near the Planck region, i.e. when $\zeta \in [0, 4]$, we observe a modification of the trajectory of the peaks since they follow a power-law up to $\zeta = 0$, reached in a finite time interval and they escape from the classical trajectory toward the singularity (see Figure 5.7). The peaks of the Lorentzian at fixed time $t$ slowly evolve remaining close to the Planck region. Such behavior outlines how the Universe has a stationary approach to the cutoff volume, accordingly to Figure 5.7, and is different from other approaches.

In fact, it was shown how the classical Big-Bang is replaced by a Big-Bounce in the framework of LQC [24]. Qualitatively, one expects that the bounce (and the consequently repulsive features of the gravitational field in the Planck regime) are consequence of a Planckian cut-off length, but this is not the case. We can observe from Figure 5.7 that there is not a bounce for the quantum Universe. The main difference between the two approaches resides in the quantum modification of the classical trajectory. In fact, in LQC we observe a “quantum bridge” between the expanding and contracting Universes, while in our approach the probability density of finding the Universe reaches the Planck region in a stationary way.
5.16 Quantum Chaos

In the previous section we have widely discussed the chaotic features of the Mixmaster dynamics; as usual in chaotic systems, we expect that this classical behavior is maintained also at a quantum level. Several attempts were made over the years to characterize the “quantum chaos” of the Bianchi IX model, analyzing the evolution of the shape of the wave functions [205, 206, 63] or the distribution of the energy levels [158, 220, 219].

The numerical simulation performed in [205, 206] is focused on a wave packet initially peaked in the center of the \((\beta_+, \beta_-)\) plane and is a solution of the WDW equation. The evolution is numerically computed as a multiple-reflection problem of the wave-packet within moving potential walls. The quantized Mixmaster model possessing a quantum mixing property can also be seen as a quantum chaotic system. The mixing operates on the expectation values of the scale factors, which tend to an equilibrium value without any help of the matter field or of the cosmological term. A self-similar structure of the distribution of probability density emerges, strongly suggesting the existence of a fractal structure.

From [63] one finds another feature of the classical chaos emerging at a quantum level. Adopting a path-integral representation of the dynamics, a Monte Carlo simulation of the dynamics shows how the anisotropy potential at the origin of the classical chaos yields

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**Figure 5.7:** The peaks of the probability density \(|\Psi(\zeta, t)|^2\) are plotted as functions of \(t\) and \(\ln(\zeta)\). The points (resulting from numerical computation) are fitted by a logarithm \(0.050 \ln(\zeta) + 0.225\) for \(\zeta \geq 4\) and by a power law \(0.067 \zeta^{1.060}\) for \(\zeta \in [0, 4]\) (from [43]).

Finally, we emphasize two points: i) the above result on the singularity-free behavior of the GUP (FRW) Universe is confirmed by the more general Taub model (for a discussion about the Taub Universe in the GUP framework we refer to [46]). Also in this case the singularity is probabilistically suppressed. ii) In the GUP Taub Universe, the wave packets favour the establishment of a quantum isotropic Universe with respect to those in the WDW theory.

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From [63] one finds another feature of the classical chaos emerging at a quantum level. Adopting a path-integral representation of the dynamics, a Monte Carlo simulation of the dynamics shows how the anisotropy potential at the origin of the classical chaos yields
a quantum mechanical correlation between large universe volume and high anisotropy, although the peak at zero anisotropy is significant as well. This result suggests a possible failure of the quantized Mixmaster cosmology to represent the very Early Universe, or it might be a consequence of neglecting non gravitational fields.

A different point of view is addressed in [158, 220], where the quantum chaos is outlined when studying the distribution of the energy levels of the quantized dynamics, assuming Dirichlet boundary conditions. In the Poincaré upper half-plane representation, the authors evaluate approximately the first $10^3$ eigenvalues, their distribution and how the energy levels are influenced by the deformation of the circular side of the bounding triangle.
6 Inhomogeneous Mixmaster Model

This Section is devoted to the generalization of the Mixmaster dynamics to the inhomogeneous case and to its multidimensional extensions. We firstly provide the construction of the generic cosmological solution of the Einstein equations in the neighborhood of the Big Bang and then we discuss the so-called fragmentation process. The Hamiltonian formulation of the inhomogeneous Mixmaster is reviewed with particular attention to the role played by the Ricci scalar and the quantum picture is then briefly analyzed. We close this review showing how the chaos is a dimensional phenomenon summarizing the most important results obtained in the multidimensional extensions of GR.

6.1 Formulation of the generic cosmolological problem

We will focus our attention on the generic behavior of the Einstein equations near the Big Bang, i.e., we will discuss the properties of their general cosmological solution, meaning with it a solution that possesses the right number of physical arbitrary functions allowing to specify arbitrary initial conditions on a generic non-singular space-like hypersurface at a fixed instant \( t \), thus four arbitrary functions in vacuum, or eight if a perfect fluid is a source [319] (for a discussion in presence of inflationary matter see [489]).

Belinskii, Khalatnikov and Lifshitz in the 70’s derived such a solution and how its dynamics resembles the one of the homogeneous indices of types VIII and IX [51, 56, 57] (see also [73, 70]). The construction can be achieved firstly considering the generic solution for the individual Kasner epoch, and then providing a general description of the alternation of two successive epochs. The answer to the first question is given by the so-called generalized Kasner solution, while to the latter is found to be in close analogy to the replacement rule in the homogeneous indices.

For a general view on inhomogeneous cosmologies, see [108, 459, 3, 109, 241, 438, 439, 440, 441, 300, 72, 405].

6.1.1 The Generalized Kasner Solution

The homogeneous indices of types VIII and IX provide the prototypes for the construction of the generic (non-homogeneous) solution of the Einstein equations in the neighbourhood of the singularity. In [294], it is shown that the Kasner solution can be generalized to the inhomogeneous case and near the singularity, as

\[
\begin{align*}
\langle dl^2 &= h_{\alpha\beta}dx^\alpha dx^\beta, \\
h_{\alpha\beta} &= a^2l_\alpha l_\beta + b^2m_\alpha m_\beta + c^2n_\alpha n_\beta,
\end{align*}
\]

where

\[
a \sim t^{p_i}, \quad b \sim t^{p_m}, \quad c \sim t^{p_n},
\]

(6.1.1)

(6.1.2)
and \(p_l, p_m, p_n\) are functions of spatial coordinates subjected to the conditions
\[
p_l(x^\gamma) + p_m(x^\gamma) + p_n(x^\gamma) = p_l^2(x^\gamma) + p_m^2(x^\gamma) + p_n^2(x^\gamma) = 1. \tag{6.1.3}
\]
Differently from the homogeneous indices, the frame vectors \(l, m, n\) are now arbitrary functions of the coordinates (subject to the conditions imposed by the Einstein equations \(0a\)).

The behaviour (6.1.1) cannot last up to the singularity, unless a further condition is imposed on the vector \(l\) (i.e., the one corresponding to the negative index \(p_1\))
\[
l \cdot \nabla \wedge l = 0. \tag{6.1.4}
\]

This condition reduces to three the number of arbitrary functions, i.e. one less than the generic solution: in fact, (6.1.1) possesses twelve arbitrary functions of the coordinates (nine components of the Kasner axes and three indexes \(p_i(x^\gamma)\)), and satisfies the two Kasner relations (6.1.3), the three 0\(\alpha\) Einstein equations, the three conditions from the invariance under three-dimensional coordinate transformations, and (6.1.4).

The generalized Kasner solution (6.1.1) does not require any additional condition, since the individual Kasner epoch lasts only for a finite interval of time, and contains, for example, four arbitrary functions in vacuum.

### 6.1.2 Inhomogeneous BKL indices

Let us now generalize our scheme by investigating the implications of the remaining conditions (6.1.4). This analysis leads to the inhomogeneous BKL indices.

We assume that the factors that determine the order of magnitude of the components of the spatial metric tensor (6.1.1) can be included in the functions \(a, b, c\), which change with time according to (6.1.2), i.e. the vectors \(l, m, n\) define the directions of the Kasner axes. For non homogeneous spaces there is no reason to introduce a fixed set of frame vectors, which would be independent of Kasner axes.

The time interval of applicability of solution (6.1.1) is determined by conditions which follow from the Einstein equations. Near the singularity, the matter energy-momentum tensor in the 00- and \(\alpha\beta\)-components may be neglected
\[
-R^0_0 = \frac{1}{2} \dot{x}^a + \frac{1}{4} \lambda^a \lambda^b = 0 , \tag{6.1.5a}
\]
\[
-R^\beta_\alpha = \frac{1}{2 \sqrt{h}} \partial_t \left( \sqrt{h} \chi^\beta_\alpha \right) + P^{\beta}_\alpha = 0 . \tag{6.1.5b}
\]

Solution (6.1.1)-(6.1.3) is obtained neglecting the three-dimensional Ricci tensor \(P^{\beta}_\alpha\) in (6.1.5b) and its validity is easily formulated in terms of the projections of the tensors along the directions \(l, m, n\), which must satisfy the conditions
\[
p_l^l, p_m^m, p_n^n \ll t^{-2} , \quad P_l^l \gg P_m^m, P_n^n . \tag{6.1.6}
\]

The off-diagonal projections of (6.1.5b) determine the off-diagonal projections of the metric tensor \((\eta_{lm}, \eta_{ln}, \eta_{mn})\), which should only be small corrections to the leading terms of the metric, as given by (6.1.1). In the latter, the only non-vanishing projections are the
diagonal \((\eta_{ll}, \eta_{mm}, \eta_{nn})\), and satisfy

\[
\eta_{lm} \ll \sqrt{\eta_{ll} \eta_{mm}}, \quad \eta_{ln} \ll \sqrt{\eta_{ll} \eta_{nn}}, \quad \eta_{mn} \ll \sqrt{\eta_{mm} \eta_{nn}},
\]  

(6.1.7)

and consequently

\[
P_{lm} \ll ab/t^2, \quad P_{ln} \ll ac/t^2, \quad P_{mn} \ll bc/t^2.
\]  

(6.1.8)

In this case, the off-diagonal components of (6.1.5b) can be disregarded to leading order. The Ricci tensor \(P_{\beta \alpha}\) for the metric (6.1.1) is given in Appendix D of [294].

The diagonal projections \(P_{ll}, P_{mm}, P_{nn}\) contain the terms

\[
\frac{1}{2} \left( \frac{a l \nabla \wedge (a l)}{abc(l \cdot [m \times n])} \right) \sim \frac{k^2 a^2}{b^2 c^2} = \frac{k^2 a^4}{\Lambda^2 l^2},
\]  

(6.1.9)

and analogous terms with \(a l\) replaced by \(b m\) and \(c n\), where \(1/k\) denotes the order of magnitude of spatial distances over which the metric significantly changes, and \(\Lambda\) is the same as in (3.6.5). In (6.1.9), all the vectorial operations are performed as in the Euclidean case.

According to (6.1.6), we get the inequalities

\[
a \sqrt{k/\Lambda} \ll 1, \quad b \sqrt{k/\Lambda} \ll 1, \quad c \sqrt{k/\Lambda} \ll 1,
\]  

(6.1.10)

which are not only necessary, but also sufficient conditions for the existence of the generalized Kasner solution. After conditions (6.1.10) are satisfied, all other terms in \(P_{ll}, P_{mm}, P_{nn}\), as well as \(P_{lm}, P_{ln}, P_{mn}\), automatically satisfy (6.1.6) and (6.1.8) as well.

An estimate of these terms leads to the conditions

\[
\frac{k^2}{\Lambda^2} (a^2 b^2, \ldots, a^3 b, \ldots, a^2 b c, \ldots) \ll 1,
\]  

(6.1.11)

containing on the left-hand side the products of powers of two or three of the quantities which enter in (6.1.10), and therefore are a fortiori true if the latter are satisfied. Inequalities (6.1.11) moreover represent a natural generalization of those which already appearing in the oscillatory regime in the homogeneous case.

As \(t\) decreases, an instant \(t_{tr}\) may eventually occur when one of the conditions (6.1.10) is violated (the case when two of these are simultaneously violated can happen when the exponents \(p_1\) and \(p_2\) are close to zero, corresponding to the case of small oscillations). Thus, if during a given Kasner epoch the negative exponent refers to the function \(a(t)\), i.e., \(p_l = p_1\), then at \(t_{tr}\), we have

\[
a_{tr} = \sqrt{\frac{k}{\Lambda}} \sim 1.
\]  

(6.1.12)

Since during that epoch the functions \(b(t)\) and \(c(t)\) decrease with \(t\), the other two inequalities in (6.1.10) remain valid and at \(t \sim t_{tr}\) we shall have

\[
b_{tr} \ll a_{tr}, \quad c_{tr} \ll a_{tr}.
\]  

(6.1.13)

At the same time all conditions (6.1.11) continue to hold, and all off-diagonal projections of (6.1.5b) may be disregarded. In the diagonal projections (6.1.9), only terms containing
\(a^4/t^2\) become relevant. In such remaining terms we have
\[
(a l \cdot \nabla \wedge (a l)) = a (l \cdot [\nabla a \times l]) + a^2 (l \cdot \nabla \wedge l) = a^2 (l \cdot \nabla \wedge l) ,
\]
i.e., the spatial derivatives of \(a\) drop out.

As a result, we obtain the following equations for the replacement of two Kasner epochs
\[
\begin{align*}
-R_l^l &= \frac{\dot{a} \cdot \dot{c}}{abc} + \lambda^2 \frac{a^2}{2b^2c^2} = 0 , \\
-R_m^m &= \frac{\dot{a} \cdot \dot{c}}{abc} - \lambda^2 \frac{a^2}{2b^2c^2} = 0 , \\
-R_l^l &= \frac{\dot{a} \cdot \dot{c}}{abc} , \\
-R_0^0 &= \frac{\ddot{a}}{a} + \frac{\ddot{b}}{b} + \frac{\ddot{c}}{c} = 0 ,
\end{align*}
\]
which differ from the corresponding ones of the homogeneous indices \((3.6.2-3.6.3)\) only for the quantity
\[
\lambda(x) = \frac{l \cdot \nabla \wedge l}{l \cdot [m \times n]} ,
\]
o longer being a constant, but a function of the space coordinates. Since \((6.1.15c)\) is a system of ordinary differential equations with respect to time where space coordinates enter parametrically only, such difference does not affect at all the solution of the equations and the following map. Similarly, the law of alternation of exponents derived for homogeneous indices remains valid in the general inhomogeneous case. Numerical evidences support the point-like dynamics of the generic cosmological solution at the basis of the BKL conjecture.

### 6.1.3 Rotation of the Kasner axes

Even if the dynamics is quite similar to that of the homogeneous indices in vacuum, the new feature of the rotation of the Kasner axes emerges. If in the initial epoch the spatial metric is given by \((6.1.1)\), then in the final one we have
\[
h_{\alpha\beta} = a^2 l_\alpha' l_\beta' + b^2 m_\alpha' m_\beta' + c^2 n_\alpha' n_\beta' ,
\]
with \(a, b, c\) given by a new set of Kasner indexes, and some vectors \(l', m', n'\). If we project all tensors (including \(h_{\alpha\beta}\)) in both epochs onto the same directions \(l, m, n\), the turning of the Kasner axes can be described as the appearance, in the final epoch, of off-diagonal projections \(\eta_{lm}, \eta_{ln}, \eta_{mn}\), which behave in time as linear combinations of the functions \(a^2, b^2, c^2\). Such projections do indeed appear, and induce the rotation of the Kasner axes.

The main effects can be reduced to a rotation of the \(m-\) and \(n-\) axis by a large angle, and a rotation of the \(l-\) axis by a small one, thus neglecting the small changes of \(l\) the new Kasner axes are related to the old ones as
\[
l' = l , \quad m' = m + \sigma_m l , \quad n' = n + \sigma_n l ,
\]
6.2 The fragmentation process

where the $\sigma_m, \sigma_n$ are of order unity, and are given by

$$\sigma_m = -\frac{2}{p_2 + 3p_1} \left\{ \left[ l \times m \right] \cdot \nabla \frac{p_1}{\lambda} + \frac{2p_1}{\lambda} m \cdot \nabla l \right\} \frac{1}{l \cdot \left[ m \times n \right]} ,$$

$$\sigma_n = \frac{2}{p_2 + 3p_1} \left\{ \left[ n \times l \right] \cdot \nabla \frac{p_1}{\lambda} - \frac{2p_1}{\lambda} n \cdot \nabla l \right\} \frac{1}{l \cdot \left[ m \times n \right]} ,$$

(6.1.19a)

and can be inferred also from the $0 - \alpha$ Einstein equations which play the role of constraints to the space functions.

The rotation of the Kasner axes (that appears for a matter-filled homogeneous space only) is inherent in the inhomogeneous solution already in the vacuum case. The role played by the matter energy-momentum tensor can be mimicked by the terms due to inhomogeneity of the spatial metric in the Einstein equations. As in the generalized Kasner solution, in the general inhomogeneous approach to the singularity the presence of matter is exhibited in the relations between the arbitrary spatial functions which appear in the solution only.

6.2 The fragmentation process

We will now qualitatively discuss a further mechanism that takes place in the inhomogeneous Mixmaster indices in the limit towards the singular point: the so-called fragmentation process [301, 299, 374].

The extension of the BKL mechanism to the general inhomogeneous case contains the physical restriction of the “local homogeneity”: in fact, the general derivation is based on the assumption that the spatial variation of all spatial metric components possesses the same characteristic length, described by a unique parameter $k$, which can be regarded as an average wavenumber. Nevertheless, such local homogeneity could cease to be valid, as a consequence of the asymptotic evolution towards the singularity. The conditions (6.1.3) do not require that the functions $p_a(x^\gamma)$ have the same ordering in all points of space. Indeed, they can vary their ordering throughout space an infinite number of times without violating conditions (6.1.3), in agreement with the oscillatory-like behaviour of their spatial dependence. Furthermore, the most important property of the BKL map evolution is the strong dependence on initial values, which produces an exponential divergence of the trajectories resulting from its iteration.

Given a generic initial condition $p_a^0(x^\gamma)$, the continuity of the three-manifold requires that, at two nearby space points, the Kasner index functions assume correspondingly close values. However, for the mentioned property, the trajectories emerging from these two values exponentially diverge and, since the $p_a(x^\gamma)$ vary within the interval $[-1/3, 1]$ only, indeed the spatial dependence acquires an increasingly oscillatory-like behaviour.

In the simplest case, let us assume that, at a fixed instant of time $t_0$, all the points of the manifold are described by a generalized Kasner metric, the Kasner index functions have the same ordering point by point, and $p_1(x^\gamma), p_2(x^\gamma), p_3(x^\gamma)$ are described throughout the whole space, by a narrow interval of $u$-values, i.e. $u \in [K, K + 1]$ for a generic integer $K$. We refer to this situation as a manifold composed by one “island”. We introduce the remainder part of $u(x^\gamma)$ as

$$X(x^\gamma) = u(x^\gamma) - [u(x^\gamma)], \quad X \in [0, 1) \quad \forall x \in \Sigma ,$$

(6.2.1)
where the square brackets indicate the integer part. Thus the values of the narrow interval can be written as \( u^0(x^\gamma) = K^0 + X^0(x^\gamma) \). As the evolution goes by, the BKL mechanism induces a transition from an epoch to another; the \( n \)-th epoch is characterized by an interval \([K - n, K - n + 1]\), until \( K - n = 0 \); then the era comes to an end and a new one begins. The new \( u^1(x^\gamma) \) starts from \( u^1 = 1/X^0 \), i.e., takes value in the interval \([1, \infty)\).

Only very close points can still be in the same “island” of \( u \) values; distant ones in space will be described by very different integer \( K \) and will experience eras of different length. As the singular point is reached, more and more eras take place, causing the formation of a greater and greater number of smaller and smaller “islands”, providing the “fragmentation” process. Our interest is focused to the value of the parameter \( k \), which describes the characteristic length and increases as the islands get smaller. This implies the progressive increase of the spatial gradients and in principle could deform the BKL mechanism.

We argued that this is not the case with a qualitative explanation: the progressive increase of the spatial gradients produces the same qualitative effects on all the terms present in the three-dimensional Ricci tensor, including the dominant ones. In other words, for each single value of \( k \), in every island, a condition of the form

\[
\frac{\text{inhomogeneous term}}{\text{dominant term}} \sim \frac{k^2 t^{2K_i} f(t)}{K^2 t^{4p_1}} \ll 1,
\]

\[K_i = 1 - p_i \geq 0, \quad f(t) = O(\ln t, \ln^2 t), \quad t \ll 1,
\]

is still valid, where we call inhomogeneous the terms containing spatial gradients of the scale factors, which are evidently absent from the dynamics of the homogeneous cosmological indices.

From this point of view, the fragmentation process does not produce any behaviour capable of stopping the iterative scheme of the oscillatory regime.

### 6.3 Hamiltonian formulation and dry turbulence

As mentioned above, a generic cosmological solution is represented by a gravitational field with all its degrees of freedom and, therefore, allowing to specify a generic Cauchy problem.

In the ADM formalism, the three-metric tensor corresponding to such a generic indices reads as

\[
h_{\alpha\beta} = \delta_{\alpha\beta}O^a_bO^b_c\partial_\alpha y^a\partial_\beta y^c,
\]

where \( q^a = q^a(x, t) \) and \( y^b = y^b(x, t) \) are six scalar functions and \( O^a_b = O^a_b(x) \) is a SO(3) matrix. Thus the action for the gravitational field is

\[
S = \int_{\Sigma \times \mathbb{R}} dt d^3x \left( p_a \partial_a q^a + \Pi_\alpha \partial_\alpha y^\alpha - NH - N^a H_a \right),
\]

\[
H = \frac{1}{\sqrt{h}} \left[ \sum_a (p_a)^2 - \frac{1}{2} \left( \sum_b p_b \right)^2 - h^{-1} R \right],
\]

\[
H_a = \Pi_\alpha \partial_\alpha y^a + p_a \partial_a q^a + 2p_a (O^{-1})^a_b \partial_a O^a_b,
\]

where \( p_a \) and \( \Pi_\alpha \) are the conjugate momenta of the variables \( q^a \) and \( y^\alpha \), respectively.
The ten independent components of a generic metric tensor are represented by the three scale factors $q^a$, the three degrees of freedom $y^a$, the lapse $N$ and the shift-vector $N^a$; by the variation of the action (6.3.2a) with respect to $p_a, \Pi_a$, the relations

$$\partial_t y^d = N^a \partial_a y^d$$  \hspace{1cm} (6.3.3)

$$N = \frac{\sqrt{\eta}}{\sum_a p_a} \left( N^a \partial_a \left( \sum_b q^b - \partial_t \sum_b q^b \right) \right)$$  \hspace{1cm} (6.3.4)

hold.

We remind that a wide class of cosmological models resembling the behavior of the inhomogeneous Mixmaster is the so-called Gowdy cosmology[228, 279].

### 6.3.1 Solution of the super-momentum constraint

By the usual Hamiltonian constraints (6.3.2b) and (6.3.2c), the super-momentum can be solved by choosing the function $y^a$ as space coordinates, taking $\eta = t$, and $y^a = y^a(t, x)$, getting

$$\Pi_b = -p_a \frac{\partial q^a}{\partial y^b} - 2p_a (O^{-1})^a_b \frac{\partial O^a}{\partial y^b}.$$  \hspace{1cm} (6.3.5)

and furthermore

$$q^a(t, x) \rightarrow q^a(\eta, y)$$  \hspace{1cm} (6.3.6a)

$$p_a(t, x) \rightarrow p'_a(\eta, y) = p_a(\eta, y) / |J|$$  \hspace{1cm} (6.3.6b)

$$\frac{\partial}{\partial t} \rightarrow \frac{\partial y^b}{\partial t} \frac{\partial}{\partial y^b} + \frac{\partial}{\partial \eta}$$  \hspace{1cm} (6.3.6c)

$$\frac{\partial}{\partial \chi^a} \rightarrow \frac{\partial y^b}{\partial \chi^a} \frac{\partial}{\partial y^b}.$$  \hspace{1cm} (6.3.6d)

where $|J|$ denotes the Jacobian of the transformation, relation (6.3.6a) in general holds for all the scalar quantities, while (6.3.6b) for all the scalar densities and action (6.3.2a) rewrites as

$$S = \int_{\Sigma \times \mathbb{R}} d\eta d^3 y \left( p_a \partial_\eta q^a + 2p_a (O^{-1})^a_b \partial_\eta O^a_b - NH \right).$$  \hspace{1cm} (6.3.7)

### 6.3.2 The Ricci scalar

In this scheme, the potential term appearing in the super-Hamiltonian reads as

$$U = \frac{D}{|J|^2} (3) R = \sum_a \lambda_a^2 D^2 Q_a + \sum_{b \neq c} D^{Q_b+Q_c} \left( \partial q, (\partial q)^2, y, \eta \right)$$  \hspace{1cm} (6.3.8)

where $D = h|J|$, $h \equiv \exp \sum_a q^a$, the $Q_a$ are the anisotropy parameters (4.5.4) and $\lambda$ are the functions

$$\lambda_a^2 \equiv \sum_{k,j} \left( O^c_b \tilde{\nabla} O^a_c \left( \tilde{\nabla} y^c \wedge \tilde{\nabla} y^b \right)^2 \right).$$  \hspace{1cm} (6.3.9)
Assuming \( y^a(t, x) \) smooth enough (which implies smoothness of the coordinates system as well), then all the gradients appearing in the potential \( U \) are regular, in the sense their behavior is not as strongly divergent as to destroy the billiard representation. It was shown [299] that the spatial gradients logarithmically increase in the proper time along the billiard’s geodesics and result of higher order. Thus, as \( D \to 0 \) the spatial curvature \( ^{(3)}R \) diverges and the cosmological singularity appears; in this limit, the first term of \( U \) dominates all the remaining ones and can be indexed by the potential

\[
U = \sum_a \Theta(Q_a),
\]  

(6.3.10)

resembling the behavior of the Bianchi IX indices. By (6.3.10) the Universe dynamics independently evolves in each space point; the point-University moves within the dynamically-closed domain \( \Pi_Q \) and near the singularity we have \( \partial p_a / \partial \eta = 0 \). Thus, the term \( 2p_a(O^{-1})^a_b \partial_\eta O^b_c \) in (6.3.7) behaves as an exact time-derivative and can be ruled out of the variational principle.

The same analysis developed for the homogeneous Mixmaster model in Section 4.8 can be straightforwardly implemented in a covariant way (i.e. without any gauge fixing for the lapse function or for the shift vector).

The super-Hamiltonian constraint is solved in the domain \( \Pi_Q \) as

\[-p_\tau \equiv \mathcal{H}_{ADM} = \sqrt{(\xi^2 - 1)p_\xi^2 + \frac{p_\theta^2}{\xi^2 - 1}} \]  

(6.3.11)

and the reduced action reads as

\[\delta S_{\Pi_Q} = \delta \int d\eta d^3y \left( p_\xi \partial_\eta \xi + p_\theta \partial_\eta \theta - \mathcal{H}_{ADM} \partial_\eta \tau \right) = 0. \]  

(6.3.12)

By the asymptotic limit (6.3.10) and the Hamilton equations associated with (6.3.12) we get \( d\epsilon / d\eta = d\epsilon / d\eta = 0 \) and therefore \( \mathcal{H}_{ADM}(y^a) \) is a constant of motion even in the non-homogeneous case.

### 6.4 The Iwasawa decomposition

We will now briefly discuss the generalization of the technique due to Chitré and Misner introduced in [164]. This technique was adopted by the authors to study the dynamics of the multi-dimensional Einstein equations coupled to dilatons and \( p \)-forms in the neighborhood of a generic singularity (see last section of this chapter). We will limit our discussion to the four dimensional case only.

The Iwasawa decomposition of the spatial metric \( h_{\alpha\beta} \) is based on the choice of a unique oriented orthonormal spatial coframe \( \{ \omega^a \} \), \( \omega^a = e^a_\alpha dx^\alpha \) defined by the relations

\[ e^a_\alpha = \sum_{\beta} D^a_\beta M^b_\alpha \]  

(6.4.1)
\[ (D^a_b) = \begin{pmatrix} e^{-b^1} & 0 & 0 \\ 0 & e^{-b^2} & 0 \\ 0 & 0 & e^{-b^3} \end{pmatrix}, \quad (M^a_b) = \begin{pmatrix} 1 & m_1 & m_2 \\ 0 & 1 & m_3 \\ 0 & 0 & 1 \end{pmatrix}, \] (6.4.2)

resulting in the following expression for \( h_{\alpha\beta} \)

\[ h_{\alpha\beta} = \sum_a \exp(-2b^a)M^a_\alpha M^a_\beta \] (6.4.3)

The existence and the uniqueness of this frame is a consequence of the uniqueness of the QR decomposition in linear algebra; furthermore the matrix \( M \) can be viewed as representing the Gram-Schmidt orthogonalization of the spatial coordinate coframe.

In this variables, the Lagrangian of the gravitational field reads

\[ L = \sqrt{h}N \left[ \sum_a b^a b^a - \left( \sum_b b^b \right)^2 + \frac{1}{2} \sum_{c<d} \exp[2(b^d - b^c)]M^c_\alpha \left( \dot{M}^d_\alpha \right)^2 \right] + \sqrt{h}N^3R, \] (6.4.4)

where \( \dot{M} \) denote the inverse matrix of \( M \).

As soon as the Legendre transformation is taken and the momenta \( \pi_a \) and \( P^a_\alpha \) introduced, the gravitational Hamiltonian in vacuum is obtained

\[ H = N \left[ \frac{1}{4} \left( \sum_a \pi_a \pi_a - \frac{1}{2} \left( \sum_b \pi_b \right)^2 \right) + \frac{1}{2} \sum_{c<d} \exp[2(b^d - b^c)]M^c_\alpha \left( \dot{M}^d_\alpha \right)^2 \right] - g^3R. \] (6.4.5)

In [164] it is argued that, as soon as the existence of a space-like singularity in the past is hypothesized, \( b^a \) is expected to be timelike in the vicinity of this singularity (in the sense of the associated Minkowskian metric that endows the \( b^a \)-space). This allows to introduce a new set of variables, \( \lambda \) and the "orthogonal angular variables" \( \gamma_a \) in which the Hamiltonian reads (the lapse function has been rescaled and set equal to \( \exp(2\lambda) \))

\[ H = \frac{1}{4} \left[ -\pi_\lambda^2 + \sum_a (\pi_\gamma_a) \right] + e^{2\lambda} \sum_A c_A \exp(-2w_A(\gamma)e^{\lambda}); \] (6.4.6)

here \( c_A \) denotes some functions of spatial derivatives of the metric, off-diagonal metric variables, and momenta; \( w_A(\gamma) \) denote linear forms of the variables \( \gamma_a \), i.e. \( w_A(\gamma) = \sum_b (w_A)_b \gamma_b \). It is expected the singularity to appear in the limit \( \lambda \to \infty \); in this limit, each term of the summation becomes an infinite wall, and can be described by the usual generalized \( \Theta \) function. Like in Chit`e-Misner picture, the are three dominant terms (in the vacuum case) that describe the billiard table. The coefficients \( c_A \) are non negative functions of the variables, but "generically" they are positive [164]. The three dominant terms \( c_A e^{2\lambda} \exp(-2w_A(\gamma)e^{\lambda}) \) are assumed to be the only relevant contributions for the asymptotic dynamics, while the other are subdominant and dropped away. The limiting Hamiltonian then reads

\[ H_{\text{asymptotic}} = \frac{1}{4} \left[ -\pi_\lambda^2 + \sum_a (\pi_\gamma_a) \right] + \sum_{A=1}^{3} \Theta[-2w_A(\gamma)] \] (6.4.7)
As in the previous sections, this Hamiltonian is independent of \( M, P^a_\alpha \) and \( \lambda \), suggesting the existence of asymptotic constants of the motion. The remaining variables describe free motion on the hyperbolic space, constrained by the three walls.

This Hamiltonian formulation of Einsteinian theory was adopted in the cosmological framework by Uggla and collaborators in a series of papers [250, 493, 8]. In particular, they split the field equations into decoupled equations for the conformal factor (by means of the conformal Hubble-normalization) and a coupled system of dimensionless equations for quantities associated with the dimensionless conformal metric. This reduced dimensionless system carries the essential information about the problem, while the dimensional one allows to recover the physical metric. One of the main advantages of Hubble-normalization lies in the behaviour of the dynamical variables as the cosmological singularity is reached: the Hubble-normalized variables remain bounded despite the standard field ones do not (for further details see the recent review [250]. When this formalism is applied to the generic field equations in the vicinity of the initial singularity, it can be demonstrated the existence of the so-called billiard attractor [493]. The main feature of this attractor is to give a precise meaning to the notion of piece-wise BKL approximation. This way the space-like cosmological singularity is silent, denoting the decoupling of space points on the causal horizon [8]. Furthermore it was established the existence of a duality of such framework with the cosmological billiard approach of Damour et al. [164].

There are some other interesting features, which we mention here as a reference although demanding to the literature for details. For the Bianchi type IX there is a very strong limit on global vorticity, caused by the difficulty of “fitting in” a vortex in the type IX compact geometry [246, 145, 39, 34]. Moreover, in the inhomogeneous case arises a linearisation instability [43], i.e. linearisations around the killing vectors of compact spaces are not stable and series expansions around them in general do not form the leading order terms of a series converging to a true solution of the Einstein equations, unless satisfying further constraints.

### 6.5 Inhomogeneous quantum Mixmaster

Since the spatial gradients of the configurational variables don’t play a relevant dynamical role in the asymptotic limit \( \tau \to \infty \) (indeed the spatial curvature behaves as a potential well), then the quantum evolution takes independently place in each space point and the total wave function of the Universe can be represented as

\[
\Xi(\tau, u, v) = \Pi_{x_i} \xi_{x_i}(\tau, u, v)
\]

where the product is (heuristically) taken over all the points of the spatial hypersurface. However, in the spirit of the long-wavelength approximation, the physical meaning of a space point must be recovered on the notion of a cosmological horizon; in fact, we are dealing with regions where the inhomogeneity effects are negligible and this corresponds to super-horizon sized spatial gradients. Even if this request is statistically well confirmed to classical level [299], in the quantum sector it acquires a precise meaning if we refer the dynamics to a lattice indexing the space-time in which the spatial gradients of the configurational variables become real potential terms. In this respect, the geometry of the space-time is expected to acquire a discrete structure on the Planck scale and we
believe that a regularization of our approach could arrive from a loop quantum gravity treatment [91].

Despite this local homogeneous framework of investigation, the appearance near the singularity of high spatial gradients and of a space-time foam (like as outlined in classical dynamics [299, 374]) can be recognized in the above quantum picture too. In fact, the probability that in $n$ different space points (horizons) the variables $u$ and $v$ take values within the same narrow interval decreases with $n$ as $p^n$, $p$ being the probability in a single point; all probabilities are identical to each other and no interference phenomenon takes place. From a physical point of view, this consideration indicates that a smooth picture of the large scale Universe is forbidden on a probabilistic level and different causal regions are expected to be completely disconnected from each other during their quantum evolution. Therefore, if we start with a strongly correlated initial wave function $\Xi_0(u, v) \equiv \Xi(\tau_0, u, v)$, its evolution toward the singularity induces increasingly irregular distributions, approaching (6.5.1) in the asymptotic limit $\tau \to \infty$.

6.6 Multidimensional oscillatory regime

Let us consider a $(d + 1)$-dimensional space-time $(d \geq 3)$, whose associated metric tensor obeys a dynamics described by a generalized vacuum Einstein equations

$$\left( d+1 \right) R_{ik} = 0 , \quad (i, k = 0, 1, \ldots, d) , \quad (6.6.1)$$

where the $(d + 1)$-dimensional Ricci tensor takes its natural form in terms of the metric components $g_{ik}(x^l)$.

In [173], it is shown that the inhomogeneous Mixmaster behaviour finds a direct generalization in correspondence to any value of $d$. Moreover, in correspondence to $d > 9$, the generalized Kasner solution acquires a generality character, in the sense of the number of arbitrary functions, i.e. without a condition analogous to (1 $\lambda_{\text{gen}}$).

In a synchronous reference (described by the usual coordinates $(t, x^\gamma)$), the time-evolution of the $d$-dimensional spatial metric $h_{\alpha\beta}(t, x^\gamma)$ singles out an iterative structure near the cosmological singularity ($t = 0$). Each single stage consists of intervals of time (Kasner epochs) during which $h_{\alpha\beta}$ takes the generalized Kasner form

$$h_{\alpha\beta}(t, x^\gamma) = \sum_{a=1}^{d} t^{2p_a} l^{a}_{\alpha} l^{a}_{\beta} , \quad (6.6.2)$$

where the Kasner indeces $p_a(x^\gamma)$ satisfy

$$\sum_{a=1}^{d} p_a(x^\gamma) = \sum_{a=1}^{d} p_a^2(x^\gamma) = 1 , \quad (6.6.3)$$

and $l^{1}(x^\gamma), \ldots, l^{d}(x^\gamma)$ denote $d$ linear independent 1-forms $l^{a} = m^{a}_{\alpha} dx^{\alpha}$, whose components are arbitrary functions of the spatial coordinates.

In each point of space, the conditions (6.6.3) define a set of ordered indexes $\{ p_a \} (p_1 \leq p_2 \leq \ldots \leq p_d)$ which, from a geometrical point of view, fixes one point in $\mathbb{R}^d$, lying on a connected portion of a $(d - 2)$-dimensional sphere. We note that conditions (6.6.3)
require \( p_1 \leq 0 \) and \( p_{d-1} \geq 0 \), where the equality takes place for the values \( p_1 = \ldots = p_{d-1} = 0 \) and \( p_d = 1 \) only. The following \( d \)-dimensional BKL map, linking the old Kasner exponents \( p_a \) to the new ones \( q_{ar} \), holds \[\tag{6.6.4}
q_1 = \frac{-p_1 - P}{1 + 2p_1 + P}, \quad q_2 = \frac{p_2}{1 + 2p_1 + P}, \quad \ldots, \quad q_{d-2} = \frac{p_{d-2}}{1 + 2p_1 + P}, \quad q_{d-1} = \frac{p_{d-1} + 2p_1 + P}{1 + 2p_1 + P}, \quad q_d = \frac{p_d + 2p_1 + P}{1 + 2p_1 + P}
\] where \( P = \sum_{a=2}^{d-2} p_a \).

As shown in \[\tag{174, 261}\] (see also \[299, 302\]), each single step of the iterative solution is stable, in a given point of the space, if
\[
\lim_{t \to 0} t^2 (d) R^b_a = 0. \quad \tag{6.6.6}
\]
The limit \[\tag{6.6.6}\] is a sufficient condition to disregard the dynamical effects of the spatial gradients in the Einstein equations. An elementary computation shows how the only terms capable to perturb the Kasner behavior in \( t^2 (d) R^{b}_{a} \) contain the powers \( t^2 \alpha_{abc} \), where \( \alpha_{abc} \) are related to the Kasner exponents as
\[
\alpha_{abc} = 2p_a + \sum_{d \neq a,b,c} p_d, \quad (a \neq b,a \neq c,b \neq d), \quad \tag{6.6.7}
\]
and for generic \( l^a \), all possible powers \( t^2 \alpha_{abc} \) appear in \( t^2 (d) R^b_a \). This leaves two possibilities for the vanishing of \( t^2 (d) R^b_a \) as \( t \to 0 \). Either the Kasner exponents can be chosen in an open region of the Kasner sphere defined in \[\tag{6.6.3}\], so as to make \( \alpha_{abc} \) positive for all triples \( a, b, c \), or the conditions
\[
\alpha_{abc}(x^r) > 0 \quad \forall (x^1, \ldots, x^d) \quad \tag{6.6.8}
\]
are in contradiction with \[\tag{6.6.3}\], and one must impose extra conditions on the functions \( l \) and their derivatives. The second possibility occurs, for instance, for \( d = 3 \), since \( \alpha_{abc} \) is given by \( 2p_{a} \), and one Kasner exponent is always negative, i.e. \( \alpha_{1,d-1,d} \). Thus \[\tag{6.6.3}\] is a solution of the vacuum Einstein equations to leading order if and only if the vector \( l^1 \) obeys the additional condition
\[
l_1 \cdot \nabla \land l_1 = 0, \quad \tag{6.6.9}
\]
and this kills one arbitrary function.

It can be shown \[\tag{174, 261}\] that, for \( 3 \leq d \leq 9 \), at least the smallest of the quantities \[\tag{6.6.7}\], i.e. \( \alpha_{1,d-1,d} \) results to be always negative (excluding isolated points \( \{ p_i \} \) in which it vanishes); for \( d \geq 10 \) an open region exists of the \((d-2)\)-dimensional Kasner sphere where \( \alpha_{1,d-1,d} \) takes positive values, the so-called Kasner Stability Region (KSR).

For \( 3 \leq d \leq 9 \), the evolution of the system to the singularity consists of an infinite number of Kasner epochs, while for \( d \geq 10 \), the existence of the KSR, implies a profound modification in the asymptotic dynamics. In fact, the indications presented in \[173, 302\] in favor of the “attractivity” of the KSR, imply that in each space point (excluding sets of zero measure) a final stable Kasner-like regime appears.

In correspondence to any value of \( d \), the considered iterative scheme contains the right
6.6 Multidimensional oscillatory regime

number of \((d + 1)(d - 2)\) physically arbitrary functions of the spatial coordinates, required to specify generic initial conditions (on a non-singular space-like hypersurface). In fact, we have \(d^2\) functions from the \(d\) vectors \(l\) and \(d - 2\) Kasner exponents; invariance under spatial reparametrizations allows to eliminate \(d\) of these functions, and other \(d\) because of the 0\(\alpha\) Einstein equations. This piecewise solution describes the asymptotic evolution of a generic inhomogeneous multidimensional cosmological indices. For a cosmological application of the eleven space-times models see \[383\]. A wide analysis of the dynamics concerning homogeneous and inhomogeneous multidimensional cosmologies see \[336, 42, 337, 312, 478, 176, 491, 30, 412, 123, 334, 333, 335, 332, 331, 330\].

We summarize some properties about the insertion of \(p\)-forms and dilatons in the gravitational dynamics. This is a wide topic, and for review we refer to \[164\].

The inclusion of massless \(p\)-forms, in a generic multi-dimensional indices \[160, 161, 163\], can restore chaos when it is otherwise suppressed. In particular, even though pure gravity is non-chaotic in 11 space-time dimensions, the 3-forms of \(d + 1 = 11\) supergravity \[172\] make the system chaotic (those \(p\)-forms are part of the low-energy bosonic sector of superstring/M-theory indices \[161, 160\]).

The billiard description in the four dimensional case is quite general and can be extended to higher space-time dimensions, with \(p\)-forms and dilatons \[281, 162, 340\]. If there are \(n\) dilatons, the billiard is a region of the hyperbolic space \(\Pi_{d+n-1}\), and in the Hamiltonian each dilaton is equivalent to the logarithm of a new scale factor.

The other ingredients that enter the billiard definition are the different types of the walls bounding it: symmetry walls related to the off-diagonal components of the spatial metric, gravitational walls related to the spatial curvature, and \(p\)-form walls (electric and magnetic). All of them are hyper-planar, and the billiard is a convex polyhedron with finitely many vertices, some of which are at infinity.

For the cosmological application of the brane framework \[344\], see \[243, 498, 141\], in which the homogeneous models and the Mixmaster chaos are discussed.
7 Conclusions

By this work, we resumed many of the key efforts made over the last four decades to characterize, as accurate as possible, the nature of the asymptotic behavior of the Universe when it approaches the singularity. In particular, the description of the oscillatory regime for the Bianchi VIII and IX models outlines that the singular character of the solution survives also when the isotropy condition is relaxed, but the detailed features of the dynamics can be deeply altered, driving up the smooth behavior of the FLRW scale factor to a chaotic evolution of the no longer equivalent directions.

However, the astonishing result consists of the possibility to extend the oscillatory regime to the generic inhomogeneous case, as far as a sub-horizon sized geometry is concerned, especially in view of the stability this picture acquires with respect to the presence of a matter fluid. We think that this very general dynamics does not provide only the important, but somehow academical, proof about the existence of the singularity (as a general feature of the Einstein equations under cosmological hypotheses), but it also represents the real physical arena to implement any reliable theory of the Universe birth. Indeed, both from a classical and from a quantum point of view, the inhomogeneous Mixmaster offers a scenario of full generality to investigate the viability of a theoretical conjecture, without the serious shortcoming of dealing with specific symmetries (in principle even not appropriate to the aim of the implementation, i.e. consider the use of the minisuperspace when the quantization is performed, disregarding causality). In this sense, the results we presented here are only the basic statements for future developments on the nature of the generic singularity. An important issue will be to fix the chaotic features as expectable properties of the Universe origin, when a convincing proposal for the quantization of gravity will acquire the proper characteristics of a Theory. Of course, in a quantum picture, the chaotic nature of the Universe would be translated into certain indicators of the state arrangements. The transition to the classical limit of an expanding Universe must be addressed as a crucial stage for the early cosmology investigation.

On the basis of the material included in this work and in view of the present knowledge of fundamental interactions, we can formulate the following proposal for the origin of the actual Universe from the generic singularity. Far from being a definitive picture of the Universe birth, it better represents the course grain that would be useful, in our opinion, as a guideline for future investigations in this field.

We summarize our point of view into the following individual, but correlated, steps:

- The Universe was born in a quantum configuration, in which the gravitational field and the kinetic term of the scalar inflaton field are the only important degrees of freedom. In this scenario, the scalar field would play the role of a time variable (in a relational sense) and a Big-Bounce could be inferred.

- The presence of the scalar field, as well as other pure quantum effects, would imply the absence of real quantum chaos features. Thus the Universe could reach configuration of semiclassical nature, as far as regions of enough large volume are explored.
However, we could infer that, without an additional contribution, the classical limit could not arise. Two main terms can be suggested as good candidates for this scope, the quadratic potential of small oscillations and a cosmological constant term; we propose that these two terms could act as synergic ones to each other.

- After the classical limit is established, the achievement of an isotropic and homogeneous Universe, up to a large scale, is got by the action of the classical slow-rolling phase of the scalar field. In this respect it is crucial that the cosmological term can act before the three-scalar of curvature becomes important enough, for instance during a long era of small oscillations or in the damped oscillation of small anisotropies.

However, we have to stress that the reliability of this picture is concerned with a strong cosmological term, to some extents, significantly greater than the one expected by the current theory of inflation. Thus the profile of the inflationary Universe has, in this perspective, to be modified even to include aspects eventually related to a quantum, or semi-classical de-Sitter phase.

Finally, we emphasize that the traced ideas rely on the assumption, made in this review article, to deal only with the Einstein-Hilbert action. More general proposals for the quantum interaction of gravity and matter fields could fix different character for the Universe birth, but eventually enforce the presented point of view.

We would like to thank all the colleagues who gave valuable feedback on our work, and in particular, John Barrow, Dieter Lorenz-Petzold and Henk van Elst
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