thp Institute for Theoretical Physics University of Cologne

Quantum Fate of Singularities in Anisotropic Cosmological Models

Inaugural-Dissertation

zur
Erlangung des Doktorgrades
der Mathematisch-Naturwissenschaftlichen Fakultät
der Universität zu Köln
vorgelegt von

Nick Kwidzinski

aus Unna

Köln, 17.04.2020

1. Gutachter:	Prof. Dr. Claus Kiefer
2. Gutachter:	Prof. Dr. Alexander Altland
Tag der mündlichen Prüfung:	30.06.2020

Abstract

This thesis studies the possibility of the quantum avoidance of gravitational singularities in anisotropic cosmological models.

For that purpose, we review the fundamentals of spatially homogeneous cosmological models and quantum cosmology based on the Wheeler-DeWitt equation in minisuperspace. Furthermore, we introduce a generalized dynamical system which is designed to emulate some of the main features of the cosmological models. After studying its geometric properties, we start to investigate how one can approach the canonical quantization of such a system. The main focus of our analysis is on the factor ordering problem in the Wheeler-DeWitt equation. The considerations motivate us to formulate criteria for singularity avoidance, that respect the conformal geometry of the configuration space of the spatially homogeneous models.

We then go on by studying some specific models with and without matter. In particular we examine classical and quantum properties of the Bianchi type I, II and IX and the Kantowski-Sachs universe. The criteria we developed previously are applied to see under which circumstances singularities can be avoided. If the potential terms are negligible when compared against the velocity terms in the gravitational action, the approach towards the singularity is called asymptotically velocity term dominated. We find that such singularities can be resolved, if the dimension of the minisuperspace is sufficiently large. The underlying mechanism is a spreading of wave packets in minisuperspace.

We also consider the non-diagonal Bianchi IX model with tilted dust. This model is relevant in the context of the BKL scenario. We pay particular attention to the asymptotic regime close to the singularity and the temporal behavior of curvature invariants in this regime.

Zusammenfassung

In dieser Arbeit untersuchen wir die Möglichkeit der Vermeidung von Singularitäten in anisotropen kosmologischen Modellen.

Zu diesem Zweck wiederholen wir die Grundlagen der räumlich homogenen kosmologischen Modelle und der Quantenkosmologie basierend auf der Wheeler-DeWitt-Gleichung im Minisuperraum. Des Weiteren führen wir ein verallgemeinertes dynamisches System ein, welches entworfen wurde um die Haupteigenschaften der kosmologischen Modelle nachzuahmen. Nachdem wir dessen geometrische Eigenschaften studiert haben, beginnen wir zu untersuchen wie dieses System kanonisch quantisiert werden kann. Das Hauptaugenmerk unserer Analyse liegt dabei auf dem Faktorordnungsproblem in der Wheeler–DeWitt–Gleichung. Unsere Betrachtungen motivieren uns dazu, Kriterien für die Singularitätenvermeidung zu formulieren, welche die konforme Geometrie des Konfigurationsraumes der räumlich homogenen Modelle berücksichtigen.

Wir fahren fort indem wir spezifische Modelle, mit und ohne Materie, untersuchen. Insbesondere behandeln wir die klassischen und quantenmechanischen Eigenschaften der Bianchi I, II und IX-Modelle sowie die des Kantowski-Sachs Universums. Wir verwenden dabei die im Vorigen entwickelten Kriterien, um zu prüfen, unter welchen Umständen Singularitäten vermieden werden können. Wir zeigen, dass Singularitäten, bei welchen die Potential Terme in der Wirkung vernachlässigbar klein sind, vermieden werden können, wenn die Dimension des Minisuperraums hinreichend groß ist. Der zugrundeliegende Mechanismus ist ein Zerfließen von Wellenpaketen.

Des Weiteren betrachten wir ein mit Staub gefülltes nicht-diagonales Bianchi IX-Modell, welches im Kontext des BKL Szenarios relevant ist. Wir untersuchen insbesondere das Regime, in welchem sich die Dynamik asymptotisch der Singularität annähert, und studieren unter anderem das zeitliche Verhalten von Krümmungsinvarianten in diesem Regime.

Notation and conventions

Symbols:

$:=$	Definition, e.g. $f(x) := x^2$ or equivalently $x^2 =: f(x)$.
$\equiv$	$f(x) \equiv 0$ is a shorthand notation for $f(x) = 0$ for all x.
$\approx$	$f(x) \approx 1$ states that the relation $f(x) \approx 1$ holds approximately.
$\simeq$	Since "$\approx$" is already reserved we shall use $f(x) \simeq 0$ in order to indicate that $f(x)$ vanishes weakly in the Dirac sense.
$\propto$	$f(x) \propto x$ denotes that $f(x)$ is proportional to x.
$\otimes$	Tensor product.
$\wedge$	Wedge product.
d	Exterior derivative, e.g. $\mathrm{d}f = \frac{\partial f}{\partial x^\mu}\mathrm{d}x^\mu$.
$\lrcorner$	Interior product, e.g. $\frac{\partial}{\partial x^\nu} \lrcorner \mathrm{d}x^\mu = \delta^\mu_\nu$.
$(\,.\,)^*$	Complex conjugation, e.g. $(x + \mathrm{i}y)^* = x - \mathrm{i}y$ for $x, y \in \mathbb{R}$.
∂_μ	Shorthand notation for $\frac{\partial}{\partial x^\mu}$.

Indices:

- Greek letters $(\mu, \nu, \lambda, \ldots)$ denote spacetime indices, e.g. $\mu = 0, 1, 2, 3$.
- Small latin letters $(i, j, k, l, \ldots)$ denote spatial indices, e.g. $i = 1, 2, 3$.
- Capital latin letters $(A, B, C, D, \ldots)$ denote minisuperspace indices.

We employ the Einstein summation convention everywhere if not stated otherwise. Furthermore, we will use the same type of letters for holonomic and anholonomic indices. The meaning of indices should become clear from the context. If both, holonomic and anholonomic indices, are in use at the same time we will employ hats, e.g. i and $\hat{\imath}$, for a distinction.

Symmetrization and antisymmetrization of Tensor components: Let $T_{\mu\nu}$ be the components of a $\binom{0}{2}$–tensor. For symmetrization and antisymmetrization of tensor indices we use the notations

$$T_{(\mu\nu)} := \frac{1}{2!}\left(T_{\mu\nu} + T_{\nu\mu}\right)$$
$$T_{[\mu\nu]} := \frac{1}{2!}\left(T_{\mu\nu} - T_{\nu\mu}\right) \ ,$$

and the corresponding generalizations for more than 2 indices. In addition, we introduce the notation

$$T_{(\mu|\lambda|\nu)} := \frac{1}{2!}\left(T_{\mu\lambda\nu} + T_{\nu\lambda\mu}\right)$$

and its generalizations (see e.g. [1] for details).

Convention for the curvature tensor: Let M be a differentiable manifold, ∇ be a connection on M and $\boldsymbol{v} = v^\mu \partial_\mu \in TM$. We will use the following convention for the components of the curvature tensor:

$$R^\mu{}_{\nu\lambda\sigma} v^\nu := [\nabla_\lambda, \nabla_\sigma] v^\mu \ .$$

In other words

$$R^\mu{}_{\nu\lambda\sigma} = \partial_\lambda \Gamma^\mu_{\nu\sigma} - \partial_\sigma \Gamma^\mu_{\nu\lambda} + \Gamma^\mu_{\lambda\alpha}\Gamma^\alpha_{\nu\sigma} - \Gamma^\mu_{\sigma\alpha}\Gamma^\alpha_{\nu\lambda} \,,$$

where $\Gamma^\mu_{\nu\lambda}$ are the components of the connection ∇. Furthermore, we use the convention

$$R_{\mu\nu} := R^\lambda{}_{\mu\lambda\nu} \ .$$

Contents

Chapter 1

Introduction

1.1 Quantum Gravity

Einstein's theory of general relativity (GR), developed more than 100 years ago, has unambiguously passed all observational and experimental tests so far. It is highly successful in describing the physics at the scales of our solar system. Apart from that, GR also consistently describes the expansion of the universe and forms the basis of current cosmology [2]. More recently the direct detection of gravitational waves by the LIGO observatories confirmed not only the existence of binary black hole systems but also the linearized, long-range behavior of vacuum GR.

The theory, however, also predicts its own breakdown due to the occurrence of spacetime singularities. The most famous examples of such singularities are the Big Bang singularities encountered in the homogeneous and isotropic Friedmann models and the singularity at the center of the spherically symmetric Schwarzschild black hole. Such singularities are not an artifact of the highly symmetrical nature of these solutions. Indeed the singularity theorems first proven by Hawking and Penrose [3, 4] state that solutions to the Einstein field equations possess singularities under quite general assumptions.

All known interactions, apart from gravity, are well described within quantum field theory. Indeed quantum theory seems to be a universal framework to describe nature. Gravity, nevertheless, has resisted so far any attempts that try to formulate it within a quantum framework. In addition, quantum gravitational effects also seem to be currently out of the experimental and observational reach. There is a widespread belief that the issue of singularities will be resolved within a quantum theory of gravity.

Attempts at formulating a quantum theory of gravity are mostly pursued from two directions. One might either start from a classical theory of gravity, that is, general relativity or some alternative/modification of the former and apply quantization rules, leading to ‘quantum general relativity’ or ‘quantum geometrodynamics’. Alternatively one might attempt to formulate a unified theory of all interactions and then try to recover quantum general relativity in an appropriate limit. The most prominent example of the latter approach is string theory. In this thesis we will follow the former direction.

The first attempts to directly quantize general relativity were undertaken by DeWitt in the pioneering series of papers [5–7]. While [5] deals with the canonical approach, [6, 7] deal with the covariant one. We will follow the canonical approach. The 3+1 decomposition of spacetime $M = \mathbb{R} \times \Sigma$ allows for the application of the Dirac-Bergmann algorithm. This yields a Hamiltonian formulation of general relativity

$$H = N\mathcal{H} + N^i\mathcal{H}_i \simeq 0 \ . \tag{1.1}$$

The Hamiltonian constraint $\mathcal{H} \simeq 0$ and the momentum (or diffeomorphism) constraints $\mathcal{H}_i \simeq 0$ together with the Hamiltonian field equations are then equivalent to the Einstein field equations. The infinite dimensional configuration space of the theory was first studied by Wheeler in [8], where it was named superspace. Superspace is the quotient space $S(\Sigma) := \mathrm{Riem}\,\Sigma \,/\, \mathrm{Diff}\,\Sigma$ where $\mathrm{Riem}\,\Sigma$ is the space of all three metrics h_{ij} on Σ and we factored out all spatial diffeomorphism $\mathrm{Diff}\ \Sigma$. Applying now the Dirac quantization method, with the three metric chosen as the configuration variable, yields the Wheeler-DeWitt equation and a quantum version of the momentum constraints. In the vacuum case the equations read

$$\hat{\mathcal{H}}\Psi[h_{ij}] = \left[-16\pi G\hbar^2 \mathcal{G}_{ijkl}\frac{\delta^2}{\delta h_{ij}\delta h_{kl}} - \frac{\sqrt{h}}{16\pi G}{}^{(3)}R\right]\Psi[h_{ij}] = 0 \tag{1.2}$$

$$\hat{\mathcal{H}}_k\Psi[h_{ij}] = -2D_j h_{ik}\frac{\hbar}{\mathrm{i}}\frac{\delta}{\delta h_{ij}}\Psi[h_{ij}] = 0 \ . \tag{1.3}$$

The wave functional is a map $\Psi : \mathrm{Riem}\,\Sigma \to \mathbb{C}$. The equations (1.2) and (1.3) are second order and first order partial functional differential equations, respectively. The dynamical content of quantum geometrodynamics is provided by the Wheeler-DeWitt equation. The momentum constraints, on the other hand, ensure that the wave functional is invariant under spatial coordinate transformations [9]. The so-called DeWitt metric $\mathcal{G}^{ijkl}$ has Lorentzian signature and thus the Wheeler-DeWitt equation (1.2) resembles the form of a Klein-Gordon equation. The Wheeler-DeWitt approach to Quantum Gravity comes with severe problem which are of both mathematical and conceptual nature.

To begin with, the Wheeler-DeWitt equation as written in equation (1.2) is ill-defined. More precisely, second order functional derivatives evaluated at the same point in space contain infinities in the form "$\delta(0)$". Thus the Wheeler-DeWitt equation requires a regularization. Several proposals for regularization have been introduced in the literature (see e.g. the references in [10] and the recent paper [11]). The problem of regularization, however, remains open.

In ordinary quantum theory time is an external parameter while in GR time is dynamical. Thus Quantum Gravity certainly requires a novel concept of time. In the canonical approach under consideration this manifests itself in the fact that, unlike the Schrödinger equation, the Wheeler-DeWitt equation is a timeless equation. The usual concept of time emerges only as an approximate notion in the semi-classical limit [10]. Deeply connected to the problem of time is the problem of Hilbert space. Because of the lack of a well defined Lebesgue measure in the functional case one might at best define an inner product formally. The most popular options are a Schrödinger or a Klein-Gordon type inner product. Both options, however, come with additional problems [10]. To this end it is not even clear if a Hilbert space structure is needed at all for a quantum theory of gravity. After all the concept of Hilbert space might only be emergent in the semi classical limit. The lack of a Hilbert space structure and the problem of time lead to obstacles for the interpretation of the wave functional since we are missing the notions of probability and unitary time evolution.

Due to the ambiguity in factor ordering there is no unique way of writing the Wheeler-DeWitt equation. The factor ordering problem is intimately connected to the other problems as well. Given a Hilbert space, for example, one might demand the Hamiltonian operator to be symmetric with respect to the inner product. This might fix the ordering or at least result in an admissible sub-class of factor orderings. The relation between the factor ordering problem and the problem of time is less obvious but we will try to convince the reader that they are indeed directly connected.

Another path to canonical Quantum Gravity is provided by Loop Quantum Gravity (LQG) [10, 12]. In this approach one starts from a different set of canonical variables, the so called Ashtekar variables. The choice of these variables makes GR look closer to a Yang-Mills type theory. The kinematic structure of the theory seems to be more or less settled. This includes that a Hilbert space can be rigorously defined. One of the main open problems is the quantum implementation of the Hamiltonian constraint. This step might also require a regularization or renormalization.

Both the Wheeler-DeWitt approach and LQG have in common that the question of the fate of singularities remains to be open [13].

1.2 Quantum Cosmology

Soon after Einstein published his theory of general relativity physicists started to investigate its consequences for cosmology. Einstein himself proposed a static universe model in 1917. Mostly driven by mathematical curiosity some cosmological solutions to the vacuum field equations were already derived and studied in 1921 by Kasner [14]. In 1924 Friedmann dropped the assumption of a static universe and allowed the spatial volume to be dynamic while preserving spatial homogeneity and isotropy. The same model was studied independently by Lemaitre in 1927. Robertson and Walker should later prove that the line elements under consideration are the unique line elements compatible with the spatial homogeneity and isotropy in 3+1 dimensions. Today these models are known as the Friedmann-Lemaitre-Robertson-Walker (FLRW) models.

The discovery of Edwin Hubble in 1929 that the universe is expanding showed on the one hand that the Einstein's static universe was untenable from an observational point of view. On the other hand it signaled that the FLRW models are indeed physically relevant. Today the standard model of cosmology [2] gives a highly consistent picture of the history of our universe.

The FLRW models are among the simplest solutions of the Einstein field equations. The simplicity stems from the drastic assumptions of homogeneity and isotropy. For the models we study in this thesis we drop the assumption of isotropy. The fact that the CMB is almost isotropic together with the fundamental result of Ehlers, Geren and Sachs [15] implies that the Universe is almost FLRW at recent times. It was shown, however, by Wald [16] that certain classes of spatially homogeneous models tend to isotropize at late times if a positive cosmological constant is present in the Einstein field equations. This signals that an inflationary era can in principle cause anisotropies to die out. Hence anisotropic models could still be relevant for the physics of the early universe.[1]

On the other hand homogeneous anisotropic models are interesting from a purely theoretical point of view for several reasons. The assumption of homogeneity leads to a drastic simplifica-tion of the Einstein field equations. Instead of a set of coupled partial differential equations one has to only deal with a set of coupled ordinary differential equations. Furthermore, the symmetry reduction to spatial homogeneity leads to the concept of minisuperspace. The term "minisuperspace" is due to Misner [17] and refers to the finite dimensional configuration space of the symmetry reduced model. The models are in that context often called minisuperspace models and we will also adopt this terminology.

The main idea behind Quantum Cosmology is to apply quantization procedures to a

[1] Constraints on anisotropy are discussed in [18].

minisuperspace model. This idea was applied by DeWitt himself in [5]. The focus of this thesis lies on the minisuperspace Wheeler-DeWitt equation, that is, the equation which is obtained by applying the Dirac quantization procedure to the symmetry reduced model. The Wheeler-DeWitt equation in minisuperspace is then no longer a functional partial differential equation but only a usual partial differential equation. In other words: After a canonical quantization we will only have to deal with a quantum mechanical problem instead of quantum field theoretical one. Most importantly the Wheeler-DeWitt equation is no longer ill defined. It is, however, questionable if this so called minisuperspace "approximation" is anyhow some valid approximation of a full theory of Quantum Gravity. After all the freezing out of infinitely many degrees of freedom identically violates the Heisenberg uncertainty principle. Furthermore, there is so far no way to consistently perform such a symmetry reduction at the level of the full Wheeler-DeWitt equation. The validity of the minisuperspace approximation was for example discussed by Kuchař and Ryan in [19]. Nevertheless, even if the minisuperspace approximation was invalid there are still good motivations to pursue the path of Quantum Cosmology. Firstly the minisuperspace approximation allows us to study the conceptual issues which are already present in the full theory at the level of a simplified setup. These conceptual issues include the problem of time, the Hilbert space problem, the factor ordering problem, and the interpretation of the wave function Ψ. The problems can be investigated without the mathematical issues of the full theory at the level of a heavily simplified setup. Moreover, one can easily compare different quantization schemes within the context of minisuperspace. Secondly there remains the hope that the results obtained within the framework of Quantum Cosmology somehow reflect the results of a full theory of Quantum Gravity. Quantum cosmological models can usually be attacked with standard methods. This allows one to investigate several aspects as for example the emergence of a classical world through decoherence [20, 21]. Furthermore, it is expected that Quantum Gravity plays an important role in the early phases of the universe. Thus it is natural to discuss for example Quantum Gravity correction to the CMB anisotropy spectrum in a quantum cosmological framework [22, 23].

Last but not least we can address the issue of singularity avoidance within the minisuperspace approximation. In the context of the Wheeler-DeWitt framework this program was initiated by the work [24] followed by a series of papers [25–27] all dealing with certain singularities in isotropic cosmological models. The results all signal towards the avoidance of such singularities in Quantum Cosmology. One of the main goals of this thesis is the extension of this work to spatially homogeneous but anisotropic cosmological models. An important role in this regard is played by the Belinski-Kalatnikov-Lifshitz (BKL) conjecture

[28]: During the approach to a generic spacelike singularity the dynamics of neighboring spacelike separated points approximately decouples and can effectively be described by a homogeneous cosmological model (usually Bianchi VIII or IX). If the BKL conjecture turned out to also hold true at the quantum level it might be possible to extend results on singularity avoidance to the more realistic inhomogeneous cases and finally to the full theory.

1.3 Structure of the thesis

This thesis is organized as follows: Chapter 2 is divided into two parts. We first provide some general considerations regarding the spatially homogeneous cosmological models at the classical level. We introduce the Bianchi models and discuss the Lagrangian and Hamiltonian formulations of their general relativistic dynamics. Furthermore, we introduce a generalized dynamical system 2.1.5. This model is designed to generalize the dynamics of the minisuperspace models while still capturing their main features. In the second part of chapter 2 we discuss the Wheeler-DeWitt equation in minisuperspace and develop criteria for the avoidance of singularities. Chapter 3 is devoted to the study of specific models with and without matter. We study both their classical and quantum aspects. Particular attention is given to the avoidance of singularities in terms of the criteria developed in chapter 2. We start with the consideration of the Bianchi I model, where we examine the vacuum case, the case of ideal fluids and the case of a minimally coupled electromagnetic field. Afterwards we will investigate the Kantowski-Sachs universe, first, with a cosmological constant and an electromagnetic field and, second, with a minimally coupled massless scalar field. It follows a short section on the Bianchi II model, in which we restrict our attention to the vacuum case. In the end of chapter 3 we consider the Bianchi IX universe. In particular we examine the non-diagonal model filled with a tilted dust field and study the dynamical regime asymptotically close to the singularity. The thesis is concluded with a summary and an outlook in chapter 4.

Chapter 2

General considerations

2.1 Spatially homogeneous cosmological models

In this section we aim to provide the basics required to prepare ourselves for the discussion of the Quantum Cosmology of spatially homogeneous models. It is possible to provide a unified picture of the spatially homogeneous cosmological models and their general relativistic dynamics. This is feasible because of fundamental work which has been done in the middle of the last century. The history of the beginnings of this formalism is presented in [29]. The work of Jantzen [30] can be regarded as an important step towards a complete understanding of the spatially homogeneous dynamics. For a collective treatment of all spatially homogeneous models see the paper [31]. Jantzen's approach is nowadays often referred to as the *orthonormal frame bundle approach*. It allows for a study of the spatially homogeneous dynamics from a group theoretical perspective. We will also introduce the notion of *homogeneity preserving diffeomorphism* [32–35, 37] which connects the dynamical point of view with a spacetime point of view.

While [31] served as a main guideline for this thesis there are certainly many other resources which will provide different perspectives and add insights which are beyond the scope of this thesis [35, 36, 38]. We will also not consider any of the observational aspects of the spatially homogeneous models (see for example [18]).

2.1.1 Homogeneous spaces

In the following let Σ be a (simply connected) manifold and G be a Lie group. A group representation G is said to act *transitively* on a space Σ if for all $x, y \in \Sigma$ there exists a $g \in G$ such that $gx = y$. The space Σ is then called *homogeneous* with respect to G. In other words, the group orbit $Gx = \{gx \mid g \in G\}$ of every point $x \in \Sigma$ is Σ itself. The group is said to act *simply transitively* if for all $x \in \Sigma$ it follows that if $gx = hx$ then $g = h$. [1] Given a basis $\{\boldsymbol{\xi}_i\}$ of the Lie algebra $\mathfrak{g}$ of G their Lie bracket can be written as

$$[\boldsymbol{\xi}_i, \boldsymbol{\xi}_j] = C^k_{ij}\boldsymbol{\xi}_k \ , \tag{2.1}$$

where C^k_{ij} are the structure coefficients of the Lie algebra $\mathfrak{g}$ in the basis $\{\boldsymbol{\xi}_i\}$. The $\boldsymbol{\xi}_i$ are linearly independent if and only if G acts simply transitively. Given a group representation G acting simply transitively on a manifold Σ we aim to construct a metric $\mathrm{d}l^2$ on Σ that respects the homogeneity. In other words, the vector fields $\boldsymbol{\xi}_i$ should be Killing vector fields of the metric dl^2. We now construct an invariant basis $\{\boldsymbol{e}_i\}$ of $T\Sigma$. We therefore pick an arbitrary point $x \in \Sigma$ and set $\boldsymbol{e}_i(x) = \boldsymbol{\xi}_i(x)$. Using the flow of the $\boldsymbol{\xi}_i$ this allows us to Lie drag the vectors $\boldsymbol{e}_i(x)$ from x to all other points in Σ by demanding that the basis is invariant, that is

$$\mathcal{L}_{\boldsymbol{\xi}_i}\boldsymbol{e}_j = [\boldsymbol{\xi}_i, \boldsymbol{e}_j] = 0 \ . \tag{2.2}$$

This procedure yields a basis $\{\boldsymbol{e}_i\}$ of the tangent bundle $T\Sigma$ which obeys

$$[\boldsymbol{e}_i, \boldsymbol{e}_j] = C^k_{ij}\boldsymbol{e}_k \ . \tag{2.3}$$

The structure coefficients of the basis $\{\boldsymbol{e}_i\}$ agree with the structure constants of the Lie algebra $\mathfrak{g}$. The coframe $\{\boldsymbol{\sigma}^i\}$ dual to $\{\boldsymbol{e}_i\}$ obeys the relation

$$\mathrm{d}\boldsymbol{\sigma}^i = -\frac{1}{2}C^i_{jk}\boldsymbol{\sigma}^j \wedge \boldsymbol{\sigma}^k \ , \tag{2.4}$$

which is nothing but the Maurer-Cartan equation that determines the anti-symmetric part of the Levi-Civita connection on Σ. We define now the spatial metric

$$\mathrm{d}l^2 = h_{ij}\boldsymbol{\sigma}^i \otimes \boldsymbol{\sigma}^j \tag{2.5}$$

where h_{ij} is real valued and symmetric with Euclidean signature. Since $\mathcal{L}_{\boldsymbol{\xi}_i}\mathrm{d}l^2 = 0$ by construction the group G is the isometry group of the Riemannian manifold $(\Sigma, \mathrm{d}l^2)$. As we aim to evolve the metric in time according to Einstein's theory we define the spacetime manifold $M = \mathbb{R} \times \Sigma$ and equip it with the Lorentzian metric

$$\mathrm{d}s^2 = -\mathrm{d}t^2 + \mathrm{d}l^2 = -\mathrm{d}t^2 + h_{ij}\boldsymbol{\sigma}^i \otimes \boldsymbol{\sigma}^j \ , \tag{2.6}$$

[1] Since any Lie group acts simply transitively on itself some authors (e.g. Jantzen [31]) choose to identify the homogeneous space with $\Sigma = G$ (or the component of G connected to the identity).

where the h_{ij} are functions of the comoving time t now. The basis on the spatially homogeneous spacetime M is $\{\boldsymbol{e}_\mu\} := \{\partial_t, \boldsymbol{e}_i\}$. The *comoving condition* $[\partial_t, \boldsymbol{e}_i] = 0$ is satisfied by construction.

Note that we have made an important choice on the topology in the construction above. We chose the hypersurfaces Σ such that they can be identified with the connected component of the isometry group G. As shown in [32], the number of degrees of freedom is in general not uniquely determined by the isometry group but depends in addition on the choice of topology.

2.1.2 The Bianchi-Schücking-Behr classification

As we have seen in the previous section homogeneous spaces can be constructed based on symmetry considerations. Classifying homogeneous spaces is therefore equivalent to a classification of Lie algebras. The first to work out a classification of 3–dimensional symmetry groups was Luigi Bianchi in 1898 [39]. The scheme we shall present here is usually referred to as the Bianchi-Behr classification of 3 dimensional Lie algebras [31, 40]. Engelbert Schücking, however, played a major role in its development [29].

The starting point of the scheme is the fact that the structure coefficients can be decomposed into a $(2,0)$–tensor density n^{ij} and a covector v_i as follows:

$$\begin{aligned} C^k_{ij} &= \varepsilon_{ijl} n^{kl} + 2 v_l \delta^l_{[i} \delta^k_{j]} \ , \quad \text{where} \\ n^{ij} &= \frac{1}{2} C^{(i}_{kl} \varepsilon^{j)kl} \quad \text{and} \quad v_i = \frac{1}{2} C^j_{ij} \ . \end{aligned} \tag{2.7}$$

Inserting the basis vectors $\boldsymbol{e}_i$ into the Jacobi identity yields that

$$C^m_{i[l} C^l_{jk]} = 0 \ . \tag{2.8}$$

After a further contraction of the Jacobi identity one finds that n^{ij} and v_j must obey the relation

$$n^{ij} v_j = 0 \ , \tag{2.9}$$

that is, either $v_i = 0$ or n^{ij} has at least one zero eigenvalue. The basis $\boldsymbol{e}_i$ is of course not unique. Letting $\mathbf{A} = \{A_i{}^j\} \in GL(3,\mathbb{R})$ we can transform to a new basis via $\bar{\boldsymbol{e}}_i = A_i{}^j \boldsymbol{e}_j$. Such a basis change induces a transformation of the structure constants according to

$$C^k_{ij} \mapsto \bar{C}^k_{ij} = (A^{-1})^k{}_m A_j{}^n A_i{}^l C^m_{ln} \ , \tag{2.10}$$

which in terms of n^{ij} and v_i reads

$$n^{ij} \mapsto \bar{n}^{ij} = \frac{1}{\det(\mathbf{A})}(A^{-1})^i{}_k(A^{-1})^j{}_l n^{kl} \quad \text{and} \quad v_i \mapsto \bar{v}_i = A_i{}^j v_j \ . \tag{2.11}$$

Note that n^{ij} transforms like a tensor density of weight 2 and v_i transforms like a co-vector. One can now use a suitable transformation to bring the structure coefficients into the so called *standard diagonal form*

$$\{n^{ij}\} = \operatorname{diag}\left(n^{(1)}, n^{(2)}, n^{(3)}\right) \quad \text{and} \quad v_i = v\delta_i^3 \quad \text{with} \quad v \geq 0 \ . \tag{2.12}$$

A Bianchi type Lie algebra is now said to be of class A if $v = 0$ and of class B otherwise. For class B models we can define an additional scalar h via the relation

$$v_i v_j = h\varepsilon_{ikl}\varepsilon_{inm}n^{kn}n^{lm} \ , \tag{2.13}$$

which becomes $v^2 = hn^{(1)}n^{(2)}$ when C^k_{ij} is in standard diagonal form. Furthermore, we can assume, without any loss of generality, that the non-zero $n^{(i)}$ are normalized such that $|n^{(i)}| = 1$. Modulo permutations of the $n^{(i)}$ and the transformation $n^{ij} \mapsto -n^{ij}$ we finally obtain the table 2.1 classifying all 3-dimensional Lie algebras.[2]

Class	Bianchi type	$n^{(1)}$	$n^{(2)}$	$n^{(3)}$	v	h
A	I	0	0	0	0	$\diagdown$
	II	0	0	1	0	$\diagdown$
	VI_0	1	-1	0	0	0
	VII_0	1	1	0	0	0
	VIII	1	1	-1	0	0
	IX	1	1	1	0	0
B	V	0	0	0	1	$\diagdown$
	IV	1	0	0	1	$\diagdown$
	$\mathrm{III}{:=}\mathrm{VI}_{-1}$	1	-1	0	1	-1
	$\mathrm{VI}_{h\neq 0,-1}$	1	-1	0	v	$-v^2$
	$\mathrm{VII}_{h\neq 0}$	1	1	0	v	v^2

Table 2.1: Bianchi-Schücking-Behr classification of 3-dimensional Lie algebras. The roman numerals are due to Bianchi who used a different classification scheme [39].

If the structure constants are in standard diagonal form the commutation relations for the

[2]To my knowledge the table appeared in this form first in a paper by Ellis and MacCallum [41].

basis vectors reads

$$\begin{aligned} &[\boldsymbol{e}_1, \boldsymbol{e}_2] = n^{(3)}\boldsymbol{e}_3 - ve_2 \ , \quad [\boldsymbol{e}_2, \boldsymbol{e}_3] = n^{(1)}\boldsymbol{e}_1 \ , \\ &[\boldsymbol{e}_3, \boldsymbol{e}_1] = n^{(2)}\boldsymbol{e}_2 + v\boldsymbol{e}_3 \ . \end{aligned} \tag{2.14}$$

The only case that is not covered by this classification is the Kantowski-Sachs spacetime for which the symmetry group $G = \mathbb{R} \times SO(3, \mathbb{R})$ is 4-dimensional. Its representation is irreducable and acts transitively but not simply transitively on the spatial hypersurfaces which can be identified by, e.g. $\Sigma = \mathbb{R} \times S^2$. Hence the model requires a separate treatment (see section 3.2 of this thesis or the appendix of [31]).

The automorphism group $\mathbf{Aut}_{\boldsymbol{e}}(\mathfrak{g})$

An important ingredient for the description of spatially homogeneous cosmological models is the automorphism group $\mathrm{Aut}_{\boldsymbol{e}}(\mathfrak{g}) \subset \mathrm{GL}(\mathfrak{g})$ of the Lie algebra $\mathfrak{g}$ with respect to the basis $\{\boldsymbol{e}_i\}$. The Automorhism group $\mathrm{Aut}_{\boldsymbol{e}}(\mathfrak{g})$ can be defined as the subgroup of the general linear group formed by the transformations $\bar{\boldsymbol{e}}_i \mapsto \bar{\boldsymbol{e}}_i = A_i{}^j \boldsymbol{e}_j$ that preserve the structure constant components, that is,

$$C^k_{ij} \mapsto \bar{C}^k_{ij} = (A^{-1})^k{}_m A_j{}^n A_i{}^l C^m_{ln} = C^k_{ij} \ . \tag{2.15}$$

To find the generators of the component of automorphism group connected to the identity we consider a path $\gamma : \ \mathbb{R} \to \mathrm{Aut}_e(\mathfrak{g})$, $t \mapsto A_i{}^j(t)$ through the identity $A_i{}^j(0) = \delta^j_i$ and differentiate equation (2.15) to obtain

$$C^k_{il} a^j_k = a^k_i C^j_{kl} + a^k_l C^j_{ik} \tag{2.16}$$

where a^j_i is identified as a tangent vector to the path γ at the identity. The general solution to equation (2.16) thus yields the Lie algebra of $\mathrm{Aut}_{\boldsymbol{e}}(\mathfrak{g})$, which we denote by $\mathfrak{aut}_{\boldsymbol{e}}(\mathfrak{g})$.

A set of particular solutions to (2.16) is given by the matrices

$$a^k_j = [\boldsymbol{k}_i]^k{}_j := C^k_{ij} \ . \tag{2.17}$$

The subgroup which is generated by the subalgebra $\{\boldsymbol{k}_i\}$ is called the *inner automorphism group*. We denote this Lie subgroup by $\mathrm{In}\,\mathrm{Aut}_{\boldsymbol{e}}(\mathfrak{g})$ and its Lie algebra by $\mathrm{In}\,\mathfrak{aut}_{\boldsymbol{e}}(\mathfrak{g})$. The remaining solutions to (2.16), that is, those which cannot be written as structure coefficients, generate the so-called *outer automorphism group*. We utilize here the notations $\mathrm{Out}\,\mathrm{Aut}_{\boldsymbol{e}}(\mathfrak{g})$ and $\mathrm{Out}\,\mathfrak{aut}_{\boldsymbol{e}}(\mathfrak{g})$ for this Lie group and its Lie algebra, respectively.

The automorphism group not only plays an important role for the efficient description and the analysis of the classical dynamics of the Bianchi models. We will also see that it is of relevance for the corresponding quantum theory. Particularly relevant are the dimensions dim (In $\mathrm{Aut}_e(\mathfrak{g})$) and dim (Out $\mathfrak{aut}_e(\mathfrak{g})$). They turn out to determine the number of linearly independent momentum constraints and possible constants of motion of the dynamics. The dimensions can be read off from the table 2.2. We will further elaborate on the role of the automorphisms after the discussion of the general relativistic dynamics of the Bianchi models.

Type	I	II	III	V	IV, VI, VII	VIII, IX
dim ($\mathrm{Aut}(\mathfrak{g})$)	9	6	4	6	4	3
dim ($\mathrm{InAut}(\mathfrak{g})$)	0	2	2	3	3	3

Table 2.2: Dimensions of the automorphsim group and the inner automorphism group for all Bianchi models. This table was taken from [31].

2.1.3 Kinematics and dynamics of the Bianchi class A models

The ADM form of the metric is given by

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + h_{ij}\left(N^i\mathrm{d}t + \sigma^i\right) \otimes \left(N^j\mathrm{d}t + \sigma^j\right). \tag{2.18}$$

In order to make use of the preferred foliation defined by the homogeneous hypersurfaces we restrict the Lapse function N and the shift vector N^i to be spatially homogeneous as well, that is, $N = N(t)$ and $N^i = N^i(t)$. While N controls the time gauge, N^i controls the foliation. Both N and N^i will not be determined by any dynamical equations of the theory and they can in fact be chosen freely (with the constraint that $N > 0$). Their choice, however, will influence the dynamics of the spatial metric.

The components of the spatial metric h_{ij} contain all the degrees of freedom of the theory and are functions of the coordinate time t only. If h_{ij} stays diagonal during the temporal evolution we speak of a diagonal model. This is, however, in general not the case and h_{ij} is only diagonalizable at a fixed instant of time t.

Furthermore, we shall from now on mostly restrict our attention to the Bianchi class A models. The reason for this are certain well known problems with the Hamiltonian formulation of the class B models, which we shall comment on later.

Diagonal/off-diagonal decomposition

It is well known that the symmetry reduction to spatially homogeneous models reduces the Einstein field equations to a system of ordinary differential equations. In order to get insights into the dynamics it is desirable to introduce an appropriate parametrization of the minisuperspace such that the form of the dynamical equations assumes a simple form. By minisuperspace we mean here the unconstrained configuration space $\mathcal{M}$ which consists of all 3–dimensional matrices $\{h_{ij}\}$ that are symmetric with Euclidean signature.[3]

Recall the fact that any symmetric matrix is diagonalizable. The main idea is now to split the minisuperspace $\mathcal{M}$ into a diagonal part which coincides with the scale group $\mathrm{Diag}(3,\mathbb{R})^+$ and an unimodular 3–parameter diagonalizing matrix group $\hat{G}$ (a Lie group) such that $\mathcal{M} \cong \mathrm{Diag}(3,\mathbb{R})^+ \times \hat{G}$. For that purpose we write

$$h_{ij} = S_i{}^k S_j{}^l \bar{h}_{kl} \tag{2.19}$$

with $\mathbf{S} = \{S_i{}^j\} \in \hat{G}$ being unimodular and $\{\bar{h}_{kl}\} \in \mathrm{Diag}(3,\mathbb{R})^+$. Equation (2.19) can be thought of as a map $\mathrm{Diag}(3,\mathbb{R})^+ \times \hat{G} \to \mathcal{M}$ which we now specify further in order to provide a suitable parametrization of $\mathcal{M}$. In practice this map will be used to pullback the equations of motion from $\mathcal{M}$ to $\mathrm{Diag}(3,\mathbb{R})^+ \times \hat{G}$ where they should be easier to study. It is convenient to introduce a suitable parametrization of the diagonal matrix $\{\bar{h}_{kl}\}$. We will mostly work here with the so called Misner variables [42, 43] which we denote by α, β_+ and β_-.[4] The diagonal part of the metric is parametrized as

$$\{\bar{h}_{ij}\} = \mathrm{e}^{2\alpha}\ \mathrm{diag}\left(\mathrm{e}^{2\beta_+ + 2\sqrt{3}\beta_-}, \mathrm{e}^{2\beta_+ - 2\sqrt{3}\beta_-}, \mathrm{e}^{-4\beta_+}\right)\ . \tag{2.20}$$

Note that due to these choices $\sqrt{h} := \sqrt{\det(\{h_{ij}\})} = \mathrm{e}^{3\alpha}$, that is, the variable α alone describes the temporal evolution of the spatial volume of the universe. We will therefore call e^{α} the *scale factor* of the universe (in full analogy to the Friedmann models). The variables $\beta_\pm$ control the "shape" of the universe and might therefore be called *anisotropy factors*. The unimodular matrix $\mathrm{diag}\left(\mathrm{e}^{2\beta_+ + 2\sqrt{3}\beta_-}, \mathrm{e}^{2\beta_+ - 2\sqrt{3}\beta_-}, \mathrm{e}^{-4\beta_+}\right)$ is sometimes called the *anisotropy matrix*. Choosing the Misner variables has the virtue that the kinetic term in the Einstein-Hilbert action will be partially in canonical form. Note that the decomposition of the degrees of freedom into a scale and shape part corresponds to an unimodular decomposition of the spatial metric.

Let us now turn to the question of how to construct the diagonalizing matrix $\mathbf{S}$. Let us denote the Lie algebra of the diagonalizing group by $\hat{\mathfrak{g}}$. In order to parametrize the connected component of $\hat{G}$ we can use the exponential map $\exp : \hat{\mathfrak{g}} \to \hat{G}$. We will therefore start by constructing a matrix representation of a basis $\{\boldsymbol{\kappa}_i\}$ of $\hat{\mathfrak{g}}$. Let $\mathbf{e}^i{}_j$ be the 3×3-matrix with the only non-vanishing component being a 1 in the i^{th} row and the j^{th} column. Then $\{\mathbf{e}^i{}_j\}$

[3]Our notion of minisuperspace is not the true analogue of superspace. A notion which appears to be closer to the notion of superspace in the full theory is provided by Jantzen [30].

[4]Note that instead of α Misner originally introduced the variable $\Omega = -\alpha$ [42, 43].

constitutes a natural basis of $\mathfrak{gl}(3,\mathbb{R})$ and satisfies the relations $\left[\mathbf{e}^i{}_j, \mathbf{e}^k{}_l\right] = \delta^k_j \mathbf{e}^i{}_l - \delta^i_l \mathbf{e}^k{}_j$. We can now decompose the generators of the diagonalizing matrix group into

$$\boldsymbol{\kappa}_i = [\boldsymbol{\kappa}_i]^j{}_k \mathbf{e}^k{}_j \ . \tag{2.21}$$

The diagonalizing matrix is then obtained via the exponential map

$$\mathbf{S} = \mathrm{e}^{\theta^1 \boldsymbol{\kappa}_1} \mathrm{e}^{\theta^2 \boldsymbol{\kappa}_2} \mathrm{e}^{\theta^3 \boldsymbol{\kappa}_3} \ , \tag{2.22}$$

where the θ^i variables are "generalized angles" which serve as a parametrization of $\hat{G}$ (or more precisely the component of $\hat{G}$ connected to the identity). It is required that the algebra closes and that the generated group is unimodular, that is,

$$\mathrm{Tr}\,(\boldsymbol{\kappa}_i) = 0 \quad \text{and} \quad [\boldsymbol{\kappa}_i, \boldsymbol{\kappa}_j] = -\hat{C}^k_{ij} \boldsymbol{\kappa}_k \ . \tag{2.23}$$

For any $\{h_{ij}\} \in \mathcal{M}$ to be diagonalizable by $\mathbf{S}$ it is required that $\{\boldsymbol{\kappa}_i\}$ is an ordered basis with the property that $\boldsymbol{\kappa}_i \in \operatorname{span}\left\{\mathbf{e}^j{}_k, \mathbf{e}^k{}_j\right\}$ for any cyclic permutation (i,j,k) of $(1,2,3)$. Now consider

$$\mathbf{S}^{-1}\mathrm{d}\mathbf{S} =: \boldsymbol{\kappa}_i \hat{\boldsymbol{\sigma}}^i \tag{2.24}$$

where the 1-forms on the right hand side can be expanded as

$$\hat{\boldsymbol{\sigma}}^i = W^i{}_j \mathrm{d}\theta^j \ . \tag{2.25}$$

After denoting the inverse of $W^i{}_j$ by $(W^{-1})_i{}^j$ we can define the dual vector fields

$$\hat{\boldsymbol{e}}_i := \left(W^{-1}\right)_i{}^j \frac{\partial}{\partial \theta^j} \ . \tag{2.26}$$

We can then convince ourselves[5] that

$$[\hat{\boldsymbol{e}}_i, \hat{\boldsymbol{e}}_j] = \hat{C}^k_{ij} \hat{\boldsymbol{e}}_k \quad \text{and} \quad \mathrm{d}\hat{\boldsymbol{\sigma}}^i = -\frac{1}{2}\hat{C}^i_{jk} \hat{\boldsymbol{\sigma}}^j \wedge \hat{\boldsymbol{\sigma}}^k \ . \tag{2.27}$$

Consequently $\{\hat{\boldsymbol{e}}_i\}$ is a left invariant basis frame of $T\hat{G}$ and $\{\hat{\sigma}^i\}$ its dual frame on $T^*\hat{G}$. Analogously one might construct a right invariant basis [31]. We will only make use of the left invariant one in this thesis. For completeness we remark that

$$\hat{C}^k_{ij} = -4 (W^{-1})_{[i}{}^l (W^{-1})_{j]}{}^n \partial_l W^k{}_n \ . \tag{2.28}$$

[5] Compute the exterior derivative of equation (2.24).

Examples: A particular example of a diagonalizing matrix group is $\hat{G} = SO(3,\mathbb{R})$ interpreted as rotations of the principal axes. This is the canonical choice for the diagonalizing matrix group in the case of the Bianchi IX spacetime. Note that in this case the symmetry group and the diagonalizing group incidentally coincide. One might parametrize the group $SO(3,\mathbb{R})$ using three Euler angles θ, ϕ, ψ. The diagonalizing matrix is then given by the Euler matrix

$$\mathbf{S} = \left\{O_i{}^j\right\} = O_\theta O_\phi O_\psi \in SO(3)\ , \quad \text{where}$$
$$O_\psi = \begin{pmatrix} \cos(\psi) & \sin(\psi) & 0 \\ -\sin(\psi) & \cos(\psi) & 0 \\ 0 & 0 & 1 \end{pmatrix}\ , \quad O_\theta = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & \sin(\theta) \\ 0 & -\sin(\theta) & \cos(\theta) \end{pmatrix}\ , \tag{2.29}$$
$$O_\phi = \begin{pmatrix} \cos(\phi) & \sin(\phi) & 0 \\ -\sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}\ .$$

This diagonalization has been used by Ryan [44–47]. Ryan, however, diagonalized all Bianchi models using $SO(3,\mathbb{R})$. This is impractical for all types other than I and IX.

Another particular choice would be to pick the Heisenberg group, that is, choose $\mathbf{S}$ as an upper triangular matrix with diagonal elements being equal to 1. This corresponds to the Iwasawa decomposition of the triads (see e.g. [48]). While this choice was found to be useful to reveal hidden Kac-Moody symmetries in gravitational theories, it is, however, rather impractical for the study of the dynamics of most of the Bianchi class A models at the Hamiltonian level.

Diagonalization via the special automorphism subgroup: The question remains how to choose the diagonalizing group such that our kinematical picture is tailored for the study of the dynamics arising from Einsteins theory. As has been pointed out by Jantzen [31] there is an advantageous choice of $\hat{G}$ for this purpose. This is to take a suitable 3 parameter subgroup of the special automorphism group

$$\hat{G} \subseteq S\mathrm{Aut}_{\mathbf{e}}(\mathfrak{g}) = \{\boldsymbol{A} \in \mathrm{Aut}_{\mathbf{e}}(\mathfrak{g}) \mid \det(\boldsymbol{A}) = 1\}\ , \tag{2.30}$$

of the Bianchi model under consideration. In particular the inner automorphism group should be contained as a subgroup in $\hat{G}$. The advantage of this choice will be revealed in the Hamiltonian formulation. In particular the form of the momentum constraints and the three–curvature will be drastically simplified. In the case of the diagonalization of Bianchi class A models with structure constants being in standard diagonal form, $\mathbf{S} \in S\mathrm{Aut}_{\mathbf{e}}(\mathfrak{g})$

simply means that

$$n^{ij}\left(S^{-1}\right)_i{}^k\left(S^{-1}\right)_j{}^l = n^{kl} \quad \text{and} \quad \det(\mathbf{S}) = 1 \; . \tag{2.31}$$

Let us now turn to the construction of the Lie algebra basis $\{\boldsymbol{\kappa}_i\}$. We first define the matrices

$$\boldsymbol{k}_i := C^k_{ij}\mathbf{e}^j{}_k \; , \tag{2.32}$$

where $C^k_{ij} = \epsilon_{ijl}n^{lk}$ are the structure constants of the Bianchi class A model in standard diagonal form. Recall that the $\boldsymbol{k}_i$ are the generators of the inner automorphism group.

Diagonalization of types VII$_0$, VIII and IX: The following construction is suitable for the diagonalization of the type VII$_0$, VIII and IX models. We define the *scale matrix*

$$\left\{\sqrt{\mathrm{Tr}\left(\boldsymbol{k}_i\boldsymbol{k}_j^T\right)/2}\right\} = \frac{1}{\sqrt{2}}\,\mathrm{diag}\left(\sqrt{\left[n^{(2)}\right]^2+\left[n^{(3)}\right]^2}, \sqrt{\left[n^{(3)}\right]^2+\left[n^{(1)}\right]^2}, \sqrt{\left[n^{(1)}\right]^2+\left[n^{(2)}\right]^2}\right) \tag{2.33}$$

and set

$$\boldsymbol{\kappa}_i := \frac{1}{\sqrt{\mathrm{Tr}\left(\boldsymbol{k}_i\boldsymbol{k}_i^T\right)/2}}\,\boldsymbol{k}_i \; . \tag{2.34}$$

By construction the basis $\{\boldsymbol{\kappa}_i\}$ satisfies

$$\begin{gathered}\mathrm{Tr}\left(\boldsymbol{\kappa}_i\right) = \hat{C}^j_{ij} = 0 \quad \text{and} \quad \left[\boldsymbol{\kappa}_i, \boldsymbol{\kappa}_j\right] = \hat{C}^k_{ij}\boldsymbol{\kappa}_k \; , \quad \text{where} \quad \hat{C}^k_{ij} = \epsilon_{ijl}\hat{n}^{lk} \\ \text{with} \quad \left\{\hat{n}^{ij}\right\} = \mathrm{diag}\left(\hat{n}^{(1)}, \hat{n}^{(2)}, \hat{n}^{(3)}\right) \; .\end{gathered} \tag{2.35}$$

The parameters $\hat{n}^{(i)}$ are given by

$$\hat{n}^{(1)} = \frac{n^{(1)}}{\sqrt{2}\sqrt{\left[n^{(2)}\right]^2+\left[n^{(3)}\right]^2}} \; , \quad \hat{n}^{(2)} = \frac{n^{(2)}}{\sqrt{2}\sqrt{\left[n^{(3)}\right]^2+\left[n^{(1)}\right]^2}} \; , \quad \hat{n}^{(1)} = \frac{n^{(3)}}{\sqrt{2}\sqrt{\left[n^{(1)}\right]^2+\left[n^{(3)}\right]^2}} \; . \tag{2.36}$$

The matrices $\boldsymbol{\kappa}_i$ can be explicitly written as

$$\boldsymbol{\kappa}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \hat{n}^{(3)} \\ 0 & -\hat{n}^{(2)} & 0 \end{pmatrix} \; , \quad \boldsymbol{\kappa}_2 = \begin{pmatrix} 0 & 0 & -\hat{n}^{(3)} \\ 0 & 0 & 0 \\ \hat{n}^{(1)} & 0 & 0 \end{pmatrix} \; , \quad \boldsymbol{\kappa}_3 = \begin{pmatrix} 0 & \hat{n}^{(2)} & 0 \\ -\hat{n}^{(1)} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \; , \tag{2.37}$$

Diagonalization of types I, II, VI$_0$: Note that $\{\hat{n}^{ij}\}$ is not well defined for the Bianchi class A types I, II and IV$_0$. As already mentioned the above construction only works for types VII_0, XIII and IX. For the other types it is convenient to pick the generators $\boldsymbol{\kappa}_i$ in the span of the non-vanishing $\boldsymbol{k}_i$ and find a suitable candidate for the remaining $\boldsymbol{\kappa}_i$ in such a way that the algebra closes and that the generated group is unimodular. For Bianchi type I, for example, the special automorphism group is $\mathrm{SL}(3,\mathbb{R})$. In this case one might pick any suitable 3–parameter matrix subgroup to diagonalize the metric, e.g. $SO(3,\mathbb{R})$.

For later usage we also define the (possibly singular) matrix ${\rho_i}^j$ via the relation

$$\boldsymbol{k}_i = {\rho_i}^j \boldsymbol{\kappa}_j \ . \tag{2.38}$$

The matrix ${\rho_i}^j$ is non-singular for Bianchi types VIII and IX. For all other types it is singular with at least one zero eigenvalue. In the case of Bianchi I the vanishing of the structure coefficients implies that ${\rho_i}^j = 0$.

Remarks on other suitable variables: We decide in this thesis to mostly work with Jantzen's orthonormal frame approach and to use the Misner variables for the parameterization of the diagonalized metric. There are of course other variables on the market which are tailored for certain applications.

The Hubble normalized variables are a set of dimensionless variables which allow for the application of certain methods from the theory of dynamical systems. This has been used to obtain rigorous results concerning the dynamics of the Bianchi models and even beyond (see e.g. [18, 48–50]). Hubble normalized variables are also useful for the application of numerical methods. The variables are, however, not suitable for quantization.

Another interesting set of variables solely constructed for the application to spatially homogeneous cosmologies was introduced in [51]. According to the authors these three variables "completely and irreducibly, determine a spatial three geometry". The variables are invariant under the action of special automorphisms and in particular well suited for applications in Quantum Cosmology.

Lagrangian and Hamiltonian formulation

The topic of this section is the Hamiltonian formulation of the vacuum Bianchi class A models. One aim is to find a suitable representation of the dynamics by using the diagonal/off-diagonal decomposition. We presuppose that a class A model has been picked from the table 2.1 and that a basis $\{\boldsymbol{\kappa}_i\}$ has been constructed according to the previous section such that we obtain a diagonalizing matrix $\mathbf{S} \in \hat{G} \subseteq S\mathrm{Aut}_{\mathbf{e}}(\mathfrak{g})$. Our starting point is the Einstein-Hilbert action

$$\mathcal{S}_{\mathrm{EH}} = \frac{1}{16\pi G} \int_{\mathcal{M}} \mathrm{d}^4x \sqrt{-g}(R - 2\Lambda) - \frac{1}{8\pi G} \int_{\partial\mathcal{M}} \mathrm{d}^3x \sqrt{h} K \ . \tag{2.39}$$

The coupling of matter will not be discussed in this section. While a discussion of minimally coupled scalar fields is straightforward, a general prescription of the coupling of more complicated forms of matter is rather non-trivial and will only be discussed in this thesis based on the examples of specific models in chapter 3. The Einstein-Hilbert action can be cast into the well known ADM form

$$\mathcal{S}_{\mathrm{EH}} = \frac{1}{16\pi G} \int\limits_{\Sigma} \boldsymbol{\sigma}^1 \wedge \boldsymbol{\sigma}^2 \wedge \boldsymbol{\sigma}^3 \int \mathrm{d}t \ N\sqrt{h} \left[\left(h^{ik}h^{jl} - h^{ij}h^{kl} \right) K_{ij}K_{kl} + {}^{(3)}R \right] \ , \tag{2.40}$$

where $K_{ij} = \frac{1}{2N}\left(\dot{h}_{ij} - 2D_{(i}N_{j)}\right)$ is the extrinsic curvature and ${}^{(3)}R$ is the Ricci scalar on the spatially homogeneous hypersurfaces Σ. The covariant derivative on Σ is denoted by D. The connection 1-forms on the spatial hypersurfaces Σ are given by $\boldsymbol{\sigma}^i{}_j = {}^{(3)}\Gamma^i_{jk}\boldsymbol{\sigma}^k$ and are uniquely determined via the two equations

$$\begin{aligned} \mathrm{d}\boldsymbol{\sigma}^i + \boldsymbol{\sigma}^i{}_j \wedge \boldsymbol{\sigma}^j &= 0 \qquad && \text{(vanishing torsion)} \\ h_{ik}\boldsymbol{\sigma}^k{}_j + h_{jk}\boldsymbol{\sigma}^k{}_i &= 0 && \text{(metricity)} \ . \end{aligned} \tag{2.41}$$

The anti-symmetric part of the connection is completely determined by demanding vanishing torsion. The symmetric part on the other hand is determined by the demand for metricity. The solution to the two equations is given by

$${}^{(3)}\Gamma^k_{ij} = -\frac{1}{2}C^k_{ij} + h^{kl}C^m_{l(i}h_{j)m} \ . \tag{2.42}$$

We will from now choose our units such that $\frac{1}{16\pi G}\int \boldsymbol{\sigma}^1 \wedge \boldsymbol{\sigma}^2 \wedge \boldsymbol{\sigma}^3 = \frac{1}{12}$. The DeWitt metric

$$\mathrm{d}\mathcal{S}^2 := \mathcal{G}^{ijkl}\mathrm{d}h_{ij} \otimes \mathrm{d}h_{kl} \ , \tag{2.43}$$

is defined via its components $\mathcal{G}^{ijkl} := 48^{-1}\sqrt{h}\left(h^{ik}h^{jl} + h^{il}h^{jk} - 2h^{ij}h^{kl}\right)$. Note that the unconventional prefactor 48^{-1} and our choice of units are tailored to the application of the Misner variables. The DeWitt metric $\mathrm{d}\mathcal{S}^2$ constitutes a metric on the configuration space $\mathcal{M}$. We can then write the action as

$$\mathcal{S}_{\mathrm{EH}} = \int \mathrm{d}t \ N \left[2\mathcal{G}^{ijkl}K_{ij}K_{kl} + \sqrt{h} \ {}^{(3)}R/12 \right] \ , \tag{2.44}$$

The total Hamiltonian of the system, obtained via the Dirac-Bergmann algorithm, can be written as

$$H = N\mathcal{H} + N^i\mathcal{H}_i \ . \tag{2.45}$$

Where the Hamiltonian and momentum constraints are given by

$$\begin{aligned} \mathcal{H} &= \frac{1}{2}\mathcal{G}_{ijkl}p^{ij}p^{kl} - \sqrt{h}\,{}^{(3)}R/12 \simeq 0 \ , \\ \mathcal{H}_i &= 2C^j_{il}h_{jk}p^{kl} \simeq 0, \end{aligned} \tag{2.46}$$

respectively. Here $\mathcal{G}_{ijkl} := \frac{12}{\sqrt{h}}\left(h_{ik}h_{jl} + h_{il}h_{jk} - h_{ij}h_{kl}\right)$ are the components of the inverse DeWitt metric and $p^{ij} = 2\mathcal{G}^{ijkl}K_{kl}$ denote the ADM momenta, that is, the momenta canonically conjugate to the configuration space variables h_{ij}. The notation "$\simeq 0$" means that the constraints weakly vanish in the Dirac sense.

We perform now the diagonal/off-diagonal decomposition of the metric according to equation (2.19) and pick the parametrization (2.22) for the diagonalizing matrix $\mathbf{S}$. Let us first take care of the kinetic term in the action. It is advantageous to define a generalized "angular velocity" ω^k via

$$\mathbf{S}^{-1}\dot{\mathbf{S}} = \left\{ \left(S^{-1}\right)_i{}^k \dot{S}_k{}^j \right\} =: \omega^k \boldsymbol{\kappa}_k \ . \tag{2.47}$$

The "angular velocity vector" can be expanded as $\omega^i =: W^i{}_j\dot{\theta}^j$, where $W^i{}_j$ are the coordinate components of the left invariant co-frame $\{\hat{\sigma}^i\}$ on $T^*\hat{G}$ defined in (2.24). A calculation then yields

$$\dot{h}_{ij} = S_i{}^k S_j{}^l \dot{\bar{h}}_{kl} + 2S_{(i|}{}^k\omega^l[\kappa_l]^n{}_k(S^{-1})_n{}^m h_{m|j)} \ . \tag{2.48}$$

The Lagrangian in the quasi-Gaussian gauge $N^i = 0$ then takes the form

$$L = N\mathrm{e}^{3\alpha}\left[\frac{-\dot{\alpha}^2 + \dot{\beta}_+^2 + \dot{\beta}_-^2 + I_{ij}\omega^i\omega^j}{2N^2} + {}^{(3)}R/12\right] \ , \tag{2.49}$$

where the "moment of inertia" tensor is given by

$$I_{ij} = \frac{1}{3}[\boldsymbol{\kappa}_i]^k{}_l\left(\delta^l_m\delta^n_k + \bar{h}_{km}\bar{h}^{ln}\right)[\boldsymbol{\kappa}_j]^m{}_n \ . \tag{2.50}$$

Note that the "moment of inertia" tensor is symmetric and completely independent of the scale factor α and the generalized angles θ^i, that is, it only depends on the anisotropy factors $\beta_\pm$. For the types VI_0, VIII and IX in particular we obtain via the diagonalization procedure presented in section 2.1.3 that

$$\{I_{ij}\} = \mathrm{diag}\,(I_1, I_2, I_3)\ , \quad \text{where} \quad I_1 = \frac{1}{3}\left(\hat{n}_2 \mathrm{e}^{\sqrt{3}\beta_- - 3\beta_+} - \hat{n}_3 \mathrm{e}^{-\sqrt{3}\beta_- + 3\beta_+}\right)^2\ ,$$
$$I_2 = \frac{1}{3}\left(\hat{n}_3 \mathrm{e}^{\sqrt{3}\beta_- + 3\beta_+} - \hat{n}_1 \mathrm{e}^{-\sqrt{3}\beta_- - 3\beta_+}\right)^2 \quad \text{and} \quad I_3 = \frac{1}{3}\left(\hat{n}_1 \mathrm{e}^{-2\sqrt{3}\beta_-} - \hat{n}_2 \mathrm{e}^{2\sqrt{3}\beta_-}\right)^2\ . \tag{2.51}$$

The momenta canonically conjugate to the Misner variables are given by

$$p_\alpha = \frac{\mathrm{e}^{3\alpha}\dot{\alpha}}{N} \quad \text{and} \quad p_\pm = \frac{\mathrm{e}^{3\alpha}\dot{\beta}_\pm}{N}\ , \tag{2.52}$$

while the momenta conjugate to the generalized angles read

$$p_i := \frac{\partial L}{\partial \dot{\theta}^i} = \frac{\mathrm{e}^{3\alpha}}{N} I_{jk}\omega^j W^k{}_i \tag{2.53}$$

in the gauge $N^i = 0$. For convenience we define the angular momentum like variables

$$\ell_i := \frac{\mathrm{e}^{3\alpha}}{N} I_{ij}\omega^j = \left(W^{-1}\right)_i{}^j p_j\ . \tag{2.54}$$

By making use of the Poisson brackets of the canonical variables $(\theta^i,\, p_i)$ and equation (2.28) one can show that the angular momenta obey the Poisson bracket algebra

$$\{\ell_i, \ell_j\} = \hat{C}^k_{ij}\ell_k\ . \tag{2.55}$$

We are now in the position to express all constraints in terms of the variables α, $\beta_\pm$, θ_i and their momenta. For the Hamiltonian constraint one obtains

$$\mathcal{H} = \frac{\mathrm{e}^{-3\alpha}}{2}\left(-p_\alpha^2 + p_+^2 + p_-^2 + (I^{-1})^{ij}\ell_i\ell_j - \frac{\mathrm{e}^{6\alpha}}{6}{}^{(3)}\!R\right) \simeq 0\ , \tag{2.56}$$

where $(I^{-1})^{ij}$ denotes the inverse of the moment of inertia tensor, that is, $(I^{-1})^{ik}I_{kj} = \delta^i_j$. Moreover, we find from this expression that DeWitt metric is brought into the form

$$\mathrm{d}\mathcal{S}^2 = \mathrm{e}^{3\alpha}\left(-\mathrm{d}\alpha^2 + \mathrm{d}\beta_+^2 + \mathrm{d}\beta_-^2 + I_{ij}\hat{\sigma}^i \otimes \hat{\sigma}^j\right)\ , \tag{2.57}$$

where $\{\mathrm{d}\alpha, \mathrm{d}\beta_+, \mathrm{d}\beta_-\}$ is a basis of $T^*\mathrm{Diag}(3,\mathbb{R})^+$ and $\{\hat{\sigma}^i\}$ is the basis of $T^*\hat{G}$ defined by equation (2.24). The momentum constraints are found to become

$$\mathcal{H}_i = \frac{1}{2}(S^{-1})_i{}^k \rho_k{}^j \ell_j\ , \tag{2.58}$$

where ${\rho_j}^k$ was defined in (2.38). Thus the number of the non trivially satisfied linearly independent momentum constraints is given by the rank of the matrix $\{{\rho_i}^j\}$. The rank of $\{{\rho_i}^j\}$ is equal to the dimension of the inner automorphism subgroup and hence specific to each Bianchi model. Let us now turn to the discussion of the potential term $\sqrt{h}\ {}^{(3)}R$. Using the 2nd Cartan structure equation we obtain the curvature 2-form on Σ:

$$\begin{aligned} {}^{(3)}{\Omega^i}_j &= \mathrm{d}{\sigma^i}_j + {\sigma^i}_k \wedge {\sigma^k}_j = \frac{1}{2}{}^{(3)}{R^i}_{jkl}\sigma^k \wedge \sigma^l \ , \quad \text{with} \\ {}^{(3)}{R^i}_{jkl} &= -\Gamma^i_{jn}C^n_{kl} + \Gamma^i_{nk}\Gamma^n_{jl} - \Gamma^i_{nl}\Gamma^n_{jk} \ . \end{aligned} \tag{2.59}$$

The Ricci scalar on Σ for the Bianchi class A models can then be written as

$${}^{(3)}R = \frac{1}{2h}\left(h_{ij}h_{kl} - 2h_{ik}h_{jl}\right)n^{ij}n^{kl} \ = -\frac{1}{24\sqrt{h}}\,\mathcal{G}_{ijkl}n^{ij}n^{kl} \ . \tag{2.60}$$

At this stage we can see another advantage of choosing $\mathbf{S} \in \hat{G} \subseteq S\mathrm{Aut}_{\mathbf{e}}(\mathfrak{g})$ as the diagonalizing matrix. Namely that we can replace the metric h_{ij} in the expression (2.60) by the diagonalized metric $\bar{h}_{ij}$ and all dependence on the generalized angles θ^i drops out. Consequently the curvature potential of the Bianchi class A models can be expressed solely in terms of the Misner variables:

$$\begin{aligned} -\frac{\mathrm{e}^{6\alpha}}{12}{}^{(3)}R = \frac{\mathrm{e}^{4\alpha}}{24}\Big[&\left(n^{(1)}\right)^2 \mathrm{e}^{4\beta_+ + 4\sqrt{3}\beta_-} + \left(n^{(2)}\right)^2 \mathrm{e}^{4\beta_+ - 4\sqrt{3}\beta_-} + \left(n^{(3)}\right)^2 \mathrm{e}^{-8\beta_+} \\ &-2n^{(2)}n^{(3)}\mathrm{e}^{-2\beta_+ - 2\sqrt{3}\beta_-} - 2n^{(3)}n^{(1)}\mathrm{e}^{-2\beta_+ + 2\sqrt{3}\beta_-} - 2n^{(1)}n^{(2)}\mathrm{e}^{4\beta_+}\Big] \ . \end{aligned} \tag{2.61}$$

Note that the curvature potential is non-negative for all class A models except for type IX. The potential can be understood as a self-interaction term which couples the gravitational field h_{ij} to itself. For the Bianchi type I case we have ${}^{(3)}R = 0$. In this sense the type I model can be viewed as a free model, that is, a system without any self-interaction.

Remark on the Hamiltonian formulation of the Bianchi class B models

The procedure of reducing the symmetry at the level of the action as outlined in the previous section 2.1.3 at the example of the Bianchi class A is to be understood as a heuristic procedure to obtain a Lagrangian/Hamiltonian formulation for the dynamics of a symmetry reduced model. After performing the procedure it should in principle be checked if the equations of motion obtained from the Lagrangian/Hamiltonian are the correct ones, that is, if they coincide with the equations of motion that are obtained by plugging the ansatz directly into the Einstein field equations. It is well known that the procedure works well for the

Bianchi class A models [31] and also in the case of spherical symmetry (see e.g. [10] and the references therein). However, the procedure leads to an erroneous result in the case of the Bianchi class B models. To be more precise the resulting Hamiltonian formulation does not yield the correct Einstein field equations. This is indicated by the fact that the constraints one obtains by naively applying the procedure are not preserved in time. In order to obtain the correct equations of motion from the flawed Hamiltonian formulation one can add an ad hoc forcing term to the Hamiltonian equations of motion (see e.g. [31]). It might, nevertheless, be possible to find a valid Hamiltonian description of the dynamics. This has, for example been achieved in [37] for the Bianchi type V model.

The question under which circumstances a symmetry reduction can be carried at the level of the action out can also be investigated with mathematical rigor (see the Engelbert Schücking in [29]).

On the automorphism group

So far we have seen that the special automorphism group $\mathrm{SAut}_{\mathbf{e}}(\mathfrak{g})$ plays an important role for the dynamical description of the Bianchi models. As in the full theory of general relativity the system of secondary constraints $\mathcal{H}$ and $\mathcal{H}_i$ for the vacuum Bianchi class A models is first class, that is, the constraints are preserved in time. This is equivalent to the statement that the constraint algebra closes:

$$\{\mathcal{H},\mathcal{H}_i\} = 0 \quad \text{and} \quad \{\mathcal{H}_i,\mathcal{H}_j\} = \mathcal{C}^k_{ij}\mathcal{H}_k \ , \tag{2.62}$$

where the structure coefficients $\mathcal{C}^k_{ij}$ of the momentum constraint algebra are specific to each Bianchi model and they satisfy the equation

$$\mathcal{C}^n_{ij}\rho_n{}^k = \rho_i{}^l\rho_j{}^m\hat{\mathcal{C}}^n_{lm} \ . \tag{2.63}$$

Consequently the $\mathcal{H}_i$ can be identified with the generators of a subgroup of $\hat{G} \subseteq \mathrm{Aut}_{\mathbf{e}}(\mathfrak{g})$. More precisely, these are the generators of the inner automorphism subgroup $\boldsymbol{k}_i = C^k_{ij}\mathbf{e}^j{}_k$ defined in equation (2.32).

As we have already pointed out before for Bianchi types VIII and IX the inner automorphism sub group coincides with the automorphism group. For all other types, however, this is not true since there are outer automorphisms in addition. Let us denote the matrix representation of the outer automorphism algebra by

$$\boldsymbol{E}_i = E^k_{ij}\mathbf{e}^j{}_k \ . \tag{2.64}$$

The phase space representation of the generators then reads

$$\mathcal{E}_i = E^k_{ij} h_{kl} p^{jl} \tag{2.65}$$

As it is shown in [35], the Poisson brackets of $\mathcal{E}_i$ with the constraints weakly vanishes in the Dirac sense. Consequently the generators $\mathcal{E}_i$ imply the existence of certain constants of motion, which are specific to each vacuum Bianchi model. We can now conclude this section.[6]

Conclusion. *The special automorphism group $SAut(\mathfrak{g})$ is the symmetry group of the equations of motion, satisfied by the metric h_{ij}, in the absence of matter sources.*

All scalar combinations constructed from the metric h_{ij} and the structure constants C^i_{jk} are scalars on $\mathcal{M}$ which are invariant under the action of the special automorphism group. Possible combinations are for example

$$C^i_{jk} C^j_{il} h^{lk} \ , \quad C^i_{jk} C^l_{nm} h_{il} h^{lk} h^{kn} \quad \text{and so on.} \tag{2.66}$$

Since curvature invariants on the spatial hypersurfaces $({}^{(3)}R,\ {}^{(3)}R^{ij}\,{}^{(3)}R_{ij}\ ,\ \ldots)$ are linear combinations of such terms they are invariant under the action of the special automorphism group as well. The authors of [37] have used these facts to construct a set of independent variables, invariant under the action of the special automorphism group. Note that such a construction is only possible because we performed the symmetry reduction to minisuperspace. In the full theory such a construction is impossible.

Homegeneity preserving diffeomorphisms

So far we have discussed the symmetries (automorphisms) of the Bianchi models from a dynamical point of view. The purpose of this section is to link the previous discussion to a spacetime point of view. More precisely the special automorphisms can be linked to coordinate transformations which manifestly preserve the spatial homogeneity of the line element. This fact was first noted by Ashtekar and Samuel [32]. We will use the paper [37] as a guideline.

In the following we suppose that spacetime manifold M is parametrized by a time coordinate t and spatial coordinates $\{x^{\hat{i}}\} =: \boldsymbol{x}$ and that the spacetime metric is in the ADM form, that is

$$\mathrm{d}s^2 = -N^2 \mathrm{d}t^2 + h_{ij} \left(N^i \mathrm{d}t + \boldsymbol{\sigma}^i\right) \otimes \left(N^j \mathrm{d}t + \boldsymbol{\sigma}^j\right) . \tag{2.67}$$

[6] The following conclusion was first provided by Jantzen in [30].

The spatial coframe can be expanded according to

$$\boldsymbol{\sigma}^i(\boldsymbol{x}) = \sigma^i{}_{\hat{i}}(\boldsymbol{x})\,\mathrm{d}x^{\hat{i}} \ . \tag{2.68}$$

A *homogeneity preserving diffeomorphism* is a coordinate transformation

$$\{t, x^{\hat{i}}\} \mapsto \{\tilde{t}, \tilde{x}^{\hat{i}}\} \ , \tag{2.69}$$

which leaves the ADM metric (2.18) form invariant. That means the transformed line element takes the form

$$\mathrm{d}s^2 = -\widetilde{N}^2\mathrm{d}\tilde{t}^2 + \widetilde{h}_{ij}\left(\widetilde{N}^i\mathrm{d}\tilde{t} + \tilde{\boldsymbol{\sigma}}^i\right) \otimes \left(\widetilde{N}^j\mathrm{d}\tilde{t} + \tilde{\boldsymbol{\sigma}}^j\right) . \tag{2.70}$$

where $\widetilde{N}$, $\widetilde{N}^i$ and $\widetilde{h}_{ij}$ are functions of $\tilde{t}$ only and $\tilde{\boldsymbol{\sigma}}^i = \sigma^i{}_{\hat{i}}(\tilde{\boldsymbol{x}})\,\mathrm{d}\tilde{x}^{\hat{i}}$.

First, let us consider a transformation of the time variable

$$t \mapsto \tilde{t}(t) \ . \tag{2.71}$$

The coefficients of the spatial metric transform as

$$h_{ij}(t) \mapsto h_{ij}(t(\tilde{t})) =: \tilde{h}_{ij}(\tilde{t}) \tag{2.72}$$

while the lapse and shift functions transform as

$$N(t) \mapsto N(t(\tilde{t}))\frac{\partial t}{\partial \tilde{t}} = \widetilde{N}(\tilde{t}) \quad \text{and} \quad N^i(t) \mapsto N^i(t(\tilde{t}))\frac{\partial t}{\partial \tilde{t}} = \widetilde{N}^i(\tilde{t}) \ . \tag{2.73}$$

Hence (2.71) is a homogeneity preserving diffeomorphism. More interesting are transformations of the spatial coordinates

$$\{t, x^{\hat{i}}\} \mapsto \{\tilde{t}(t), \tilde{x}^{\hat{i}}(t, \boldsymbol{x})\} \ , \tag{2.74}$$

where $\tilde{t}(t) = t$. One then obtains that

$$\boldsymbol{\sigma}^i(\boldsymbol{x}) = \sigma^i{}_{\hat{j}}(\boldsymbol{x})\left[\frac{\partial x^{\hat{j}}}{\partial \tilde{t}}\mathrm{d}\tilde{t} + \frac{\partial x^{\hat{j}}}{\partial \tilde{x}^{\hat{i}}}\mathrm{d}\tilde{x}^{\hat{i}}\right] \ . \tag{2.75}$$

Since both $\sigma^i{}_{\hat{i}}(\boldsymbol{x})$ and $\sigma^i{}_{\hat{i}}(\tilde{\boldsymbol{x}})$ are invertible there exists a non-singular matrix $L^i{}_j\left(\tilde{t}, \tilde{\boldsymbol{x}}\right)$ and a triplet $\Delta N^i(\tilde{t}, \tilde{\boldsymbol{x}})$, such that

$$\begin{aligned} \sigma^i{}_{\hat{i}}\left(\tilde{\boldsymbol{x}}\right) \frac{\partial x^{\hat{i}}}{\partial \tilde{x}^{\hat{k}}} &= L^i{}_j\left(\tilde{t}, \tilde{\boldsymbol{x}}\right) \sigma^j{}_{\hat{k}}\left(\boldsymbol{x}\right) \ , \\ \sigma^i{}_{\hat{i}}\left(\tilde{\boldsymbol{x}}\right) \frac{\partial x^{\hat{i}}}{\partial \tilde{t}} &= \Delta N^i(\tilde{t}, \tilde{\boldsymbol{x}}) \ . \end{aligned} \tag{2.76}$$

For the coordinate transformation to be homogeneity preserving $L^i{}_j(\tilde{t}, \tilde{\boldsymbol{x}})$ and $\Delta N^i(\tilde{t}, \tilde{\boldsymbol{x}})$ must be independent of the spatial coordinates $\tilde{\boldsymbol{x}}$. The resulting line element is then indeed of the form (2.70) with

$$\widetilde{N} = N \ , \quad \widetilde{h}_{ij} = h_{kl} L^k{}_i L^l{}_j \ , \quad \text{and} \quad \widetilde{N}^i = \left(L^{-1}\right)^i{}_j \left(N^j + \Delta N^j\right) \tag{2.77}$$

and therefore manifestly spatially homogeneous. The equations (2.76) is to be regarded as a set of first order partial differential equations for the inverse coordinate transformation $\{\tilde{t}, \tilde{x}\} \mapsto x^{\hat{i}}(\tilde{t}, \tilde{x})$. The local existence of solutions is guaranteed by the Frobenius theorem (see appendix A.2) provided that the necessary and sufficient conditions are satisfied. One finds [37] that these conditions can be brought into the form

$$\begin{aligned} L^i{}_l C^l_{jk} &= C^i_{nl} L^n{}_j L^l{}_k \ , \\ \Delta N^k C^i_{kl} L^l{}_j &= \frac{1}{2} \dot{L}^i{}_j \ . \end{aligned} \tag{2.78}$$

The solutions $\{L^i{}_j, \Delta N^i\}$ to (2.78) have the property that they form a group under the composition law

$$\begin{aligned} (L_3)^i{}_j &= (L_1)^i{}_k (L_2)^k{}_j \\ (\Delta N_3)^i &= (\Delta N_1)^i + (L_1)^i{}_j (\Delta N_2)^j \ . \end{aligned} \tag{2.79}$$

where $\{L_1, \Delta N_1\}$ and $\{L_2, \Delta N_2\}$ are two consecutive transformations of the form (2.77). Note that there are particular solutions of the form $L^i{}_j(\tilde{t}) = L^i{}_j = const.$ with $\{L^i{}_j\} \in \mathrm{SAut}(\mathfrak{g})$ and $\Delta N^i = 0$. These solutions can be trivially identified with the special automorphism group. In general however the group formed by the solutions to (2.78) is larger than the special automorphism group. The particular solutions $\{L^i{}_j\} \in \mathrm{SAut}(\mathfrak{g})$ and $\Delta N^i = 0$ can be regarded as the remaining gauge degrees of freedom after having fixed the lapse and shift.

Furthermore, there are solutions with $\Delta N^k(\tilde{t})$ being arbitrary. To see that we note that the matrix $2\{\Delta N^k(\tilde{t}) C^i_{kj}\} = 2\Delta N^i(\tilde{t}) \boldsymbol{k}_i$ is by definition a path in the Lie algebra of the inner automorphism group. Having that in mind we can conclude that a further particular solution to (2.78) is provided by the time ordered exponential[7]

$$\{L^i{}_j\,(\tilde{t})\} = \mathcal{T}\exp\left(2\int_{\tilde{t}_0}^{\tilde{t}} \mathrm{d}t\ \Delta N^k\,(t)\,\boldsymbol{k}_k\right) \in I\mathrm{Aut}_e(\mathfrak{g})\ , \tag{2.80}$$

where $\Delta N^i(\tilde{t})$ is arbitrary. In fact the time ordered exponential is the unique solution to the initial value problem

$$\Delta N^k C^i_{kl} L^l{}_j = \frac{1}{2}\dot{L}^i{}_j\ , \quad L^i{}_j(\tilde{t}_0) = \delta^i_j\ . \tag{2.81}$$

Because of the group structure of the solution space we conclude that the most general solution to (2.78) can be obtained via the composition of (2.80) and a constant special automorphism.

One can show that if $\{N, N^i, h_{ij}\}$ and $\{\widetilde{N}, \widetilde{N}^i, \widetilde{h}_{ij}\}$ are related by (2.77) and $L^i{}_j$ and ΔN^i solve (2.78) then $\mathcal{S}_{\mathrm{EH}}[\widetilde{N}, \widetilde{N}^i, \widetilde{h}_{ij}] = \mathcal{S}_{\mathrm{EH}}[N, N^i, h_{ij}]$. Hence, as one would expect, the vacuum action (2.44) is invariant under the transformation. It follows now that if $\{N, N^i, h_{ij}\}$ is a solution to equations of motion then $\{\widetilde{N}, \widetilde{N}^i, \widetilde{h}_{ij}\}$ is a solution as well. We are now in the position to conclude this section.

Conclusion. *Two solutions* $\{N, N^i, h_{ij}\}$ *and* $\{\widetilde{N}, \widetilde{N}^i, \widetilde{h}_{ij}\}$ *which are related via* (2.77) *such that* $L^i{}_j$ *and* ΔN^i *satsify* (2.78) *are also related via a homogeneity preserving diffeomorphism.*

The general solution to the equations (2.78) for several Bianchi models can be found in [37]. For a mathematically more rigorous treatment see [33]. The latter reference, however, employs a stronger definition of homogeneity preserving diffeomorphism, which leads to slightly different results (only constant automorphism are homogeneity preserving diffeomorphisms).

Remark on the curvature of the class A minisuperspaces

We compute the Ricci scalar of the Riemannian space $(\mathcal{M}, \mathrm{d}\mathcal{S}^2)$ with the DeWitt metric given by (2.43). The result is $\mathcal{R} = -\frac{45}{\sqrt{h}} = -45\mathrm{e}^{-3\alpha}$. After performing a conformal transformation of the DeWitt metric according to $\mathrm{d}\mathcal{S}^2 \mapsto \mathrm{d}\widetilde{\mathcal{S}}^2 = \mathrm{e}^{-3\alpha}\mathrm{d}\mathcal{S}^2$ we obtain that $\widetilde{\mathcal{R}} = -90$. Consequently the unconstrained minisuperspace of the vacuum Bianchi models is conformal to a space of constant negative scalar curvature. The unconstrained minisuperspace is

[7] The time ordered exponential can be formally defined via

$$\mathcal{T}\exp\left(\int_0^t \mathrm{d}t'\boldsymbol{a}(t')\right) := \sum_{n=0}^{\infty}\int_0^t\int_0^{t'_n}\int_0^{t'_{n-1}}\cdots\int_0^{t'_2}\boldsymbol{a}(t'_n)\boldsymbol{a}(t'_{n-1})\ldots\boldsymbol{a}(t'_1)\mathrm{d}t'_1\ldots\mathrm{d}t'_{n-1}\mathrm{d}t'_n\ .$$

not conformally flat which follows from computing the Weyl squared scalar $\widetilde{\mathcal{W}}^2 = 1890$ corresponding to the metric $\mathrm{d}\widetilde{\mathcal{S}}^2$.

2.1.4 Singularities in general relativity and relativistic cosmology

In this section we provide the definition and classification of singularities. It is sufficient for our purposes to have a rather loose discussion. For an overview of precise definitions, theorems and classifications of singularities in Einstein's theory see for example the review article by Senovilla [52].

Geodesic incompletess

A spacetime is called *geodesically incomplete* or singular if there exists a geodesic that cannot be extended past some affine parameter. Penrose and Hawking [3] have shown that, under the assumption of general energy conditions, solutions to the Einstein field equation necessarily admit incomplete geodesics. Such results have become known as singularity theorems. These prove the fact that singularities are not a mere artifact of a certain symmetry reduction but rather a generic feature of Einstein's theory of gravity. However, while these theorems provide information about the existence of singularities they do not tell us anything about the nature of such singularities.

We have to distinguish between curvature singularities and conical singularities. Further distinction should be made between spacelike and timelike singularities. Since we are only dealing with spatially homogeneous cosmological models in this thesis we will restrict our attention to spacelike singularities.

Curvature singularities

A curvature singularity (or curvature pathology) is a point or a collection of points in spacetime at which certain curvature scalars diverge. This definition is quite arbitrary since in principle one can construct infinitely many curvature scalars on a (pseudo-)Riemannian manifold. The precise definition of a curvature singularity is an open issue known as the *curvature pathology definition problem.* Furthermore, the relation between the blowing up of curvature invariants and geodesic incompleteness is an ongoing debate. In particular there exist solutions to the Einstein field equations which admit incomplete geodesics while no curvature pathology occurs [52]. It will be sufficient in the context of this thesis to call a point in spacetime a *curvature singularity* if the Kretschmann scalar $R^{\mu\nu\lambda\sigma}R_{\mu\nu\lambda\sigma}$ diverges at this point. As it is well known, the Kretschmann scalar can be decomposed as

$$R^{\mu\nu\lambda\sigma}R_{\mu\nu\lambda\sigma} = C^{\mu\nu\lambda\sigma}C_{\mu\nu\lambda\sigma} + 2\left(R_{\mu\nu}R^{\mu\nu} - \frac{1}{6}R^2\right) \tag{2.82}$$

where $C^{\mu}{}_{\nu\lambda\sigma}$ is the Weyl squared tensor. The decomposition allows for further distinctions [53]. We call a curvature singularity

- Weyl or conformal singularity if $C^{\mu\nu\lambda\sigma}C_{\mu\nu\lambda\sigma}$ diverges.
- Ricci singularity if $R_{\mu\nu}R^{\mu\nu} - \frac{1}{6}R^2$ diverges.

While Ricci singularities are related to unbounded matter densities via the Einstein field equations, Weyl singularities are related to gravitational field divergences in the vacuum. The Oppenheimer-Snyder model [54] describes the homogeneous and spherically symmetric gravitational collapse of a cloud of dust particles and provides a particular example: the interior of the dust sphere, described by a dust filled closed Friedmann universe, collapses into a Ricci singularity, while the exterior, described by a vacuum Kantowski-Sachs model, collapses into a Weyl singularity. Note also that a singularity can be both Ricci and Weyl at the same time. This situation can occur for example in the case of matter filled spatially homogeneous but anisotropic cosmological models. Further distinctions in the characterization of curvature singularities were given by Barrow and Hervik [55]. The authors also provide asymptotic expressions of the Weyl squared scalar for the Bianchi models filled with ideal fluids in the vicinity of the singularity.

We also remark that the scalar

$$l_c := \frac{1}{|R^{\mu\nu\lambda\sigma}R_{\mu\nu\lambda\sigma}|^{\frac{1}{4}}} \tag{2.83}$$

defines a natural *curvature length scale*. Thus l_c might be compared against the Planck length to provide an indicator for the setting in of Quantum Gravity effects.

The strength of singularities

The idea behind a classification of the strength of a singularities (see e.g. [56]) is as follows: Loosely speaking, a singularity is called *strong* if the tidal forces are strong enough to destroy any extended object (e.g. a string) that comes close to the singularity. A singularity is called *weak* if it is in principle traversable by an object which is rigid enough. More precise definitions, based on considerations of the geodesic deviation equation, were given by Tipler [57] and Królak [58]. Let u^{μ} and τ be the four velocity and proper time along a timelike geodesic respectively. Suppose the geodesic hits the singularity when $\tau = \tau_*$. The singularity is called strong

- according to Krolak if one of the integrals $\int_0^\tau \mathrm{d}\tau' R^\mu{}_{\alpha\nu\beta} u^\alpha u^\alpha$ diverges as $\tau \to \tau_*$.

- according to Tipler if one of the integrals $\int_0^\tau \mathrm{d}\tau' \int_0^{\tau'} \mathrm{d}\tau'' R^\mu{}_{\alpha\nu\beta} u^\alpha u^\alpha$ diverges as $\tau \to \tau_*$.

Otherwise the singularity is called weak. While Tipler's definition is usually regarded as being more physical, Królak's definition is easier to study in practice.

Singularities in spatially homogeneous models

We remark at this stage that all Bianchi class A models filled with matter fields that satisfy the usual energy conditions start their evolution in a spacelike singularity and expand for eternity. This is true for all Bianchi models except for the type IX model which recollapses and ends its evolution in a second singularity as proven by Lin and Wald [59]. Such a theorem also holds for the Kantowski-Sachs model [60]. In fact the so called *closed universe recollapse conjecture* (see e.g. [60]) states that all closed universes share this feature.

The asymptotic behavior of the Weyl squared scalar for spatially homogeneous models filled with (non-tilted) perfect fluids was studied by Barrow and Hervik [55]. If the usual energy conditions are satisfied and the expansion is anisotropic the Weyl squared scalar usually diverges when approaching the singularity. How fast it diverges depends on the equation of state parameter.

Classification in terms of the scale factor

The following classification scheme was designed for the application to Friedmann models filled with ideal fluids [25]. The classification, as given in the following, allows to distinguish between five types of singularities :

- Type 0 (Big Bang/Crunch): $a \to 0$, $\rho \to \infty$ and $p \to \infty$ in finite comoving time.

- Type I: $a \to \infty$, $\rho \to \infty$ and $p \to \infty$ in a finite comoving time. An example is given by the Big Rip singularity considered for example in [24].

- Type II (sudden singularity): a and ρ stay finite while $p \to \pm\infty$ in finite comoving time. Examples are the Big Brake and Big Démarrage considered in the references [27] and [26] respectively.

- Type III (finite scale factor singularity): $a \to a_* = const.$, $\rho \to \infty$ and $p \to \infty$ in finite comoving time. An example is the Big Freeze considered in [26].

- Type IV (Big Separation): a, ρ and p stay finite but the higher derivatives $\frac{\mathrm{d}^n}{\mathrm{d}t^n}a$ and $\frac{\mathrm{d}^{n-1}}{\mathrm{d}t^{n-1}}H$ for some $n \geq 3$ diverge in a finite comoving time t(H is the Hubble parameter).

- Type V (w-singularity): a, ρ and p stay finite but the equation of state parameter $w = p/\rho$ blows up in finite comoving time.

Here ρ and p are the energy density and the pressure of the perfect fluid coupled to the Friedmann model. According to the definition of Tipler only the Type 0 and I singularities are strong while according to Krolak also the Type III singularity is strong. The above classification scheme has been refined and enlarged (see e.g. [61] and the references therein). Since we can also define a scale factor for the more general spatially homogeneous but anisotropic models via $a^3 := \sqrt{h}$, we can borrow this classification and apply it (to some extend) to the case of spatially homogeneous cosmological models coupled to perfect fluids. Note, however, that not all matter fields (e.g. Yang-Mills fields) can be regarded as perfect fluids. Moreover, important singularities in vacuum solutions, for example the singularity of the Kasner solution, cannot be classified according to this scheme.

We should also remark that $a \to 0$ is not a sufficient criterion for the existence of a physical singularity. The Taub-NUT-M solution (see e.g. [45]) is a special case of the vacuum Bianchi type IX model. Here in fact $a \to 0$ is a coordinate singularity known as the Misner interface, which represents a Killing horizon at which one of the spacelike Killing vector fields becomes lightlike. The solution can be analytically extended. The solution on the other side of the Misner interface, however, possesses 2 spacelike and 1 timelike Killing vector fields. The singularity is thus a coordinate artifact similar to the Schwarzschild horizon in the Schwarzschild coordinates.

VTD and AVDT

If the dynamics of cosmological model is completely determined by the kinetic term in the Einstein-Hilbert action we call the dynamics velocity term dominated (VTD). The Kasner solution provides the prototype of a VTD spacetime. If such a behavior is recovered approximately in the dynamical regime close to the singularity the approach to the singularity is called asymptotically velocity term dominated (AVTD). This behavior can for example be found for the Bianchi II vacuum solution where the influence of the curvature potential on the spacetime dynamics is negligible asymptotically close to the singularity. Another example is given by the Bianchi I model filled with an ideal fluid which we shall consider later in

3.1.3. In this case "matter doesn't matter" in the regime close to the singularity (this is true except for the isotropic solution). In the Bianchi IX model the three curvature term (2.61) forms a trapping potential and influences the dynamics of the universe all the way down to the singularity. Therefore the singularity of the Bianchi IX model provides a prototypical example which is not AVTD. For more details see [64].

The BKL conjecture

The question whether singularities are a generic feature of Einstein's theory was also interesting to Landau. In fact he considered the singularity problem to be one of the main problems in physics at that time [65]. His idea was to expand the general solution of Einstein's field equations in the vicinity of a generic spacelike singularity. This analysis was carried out by the members of his group, Belinski, Khalatnikov and Lifshitz (BKL) [66]. The heuristic analysis of BKL then suggested that points in space decouple and the dynamics of a small enough region then turn out to be effectively the same as those of the (non-diagonal) Bianchi IX or Bianchi VIII universe. The dynamics of of these models in the vicinity of the singularity are characterized by an infinite number of oscillations which give rise to a chaotic character of the solutions. The BKL conjecture states that this behavior is a generic feature of solutions to Einsteins field equations in the vicinity of a spacelike singularity. Progress towards improving the mathematical rigor of the conjecture has been made by the authors of [48]. Additionally numerical studies giving support to the conjecture have been performed in [67] and in the context of gravitational collapse in [68]. The BKL conjecture has also been studied within the context of the Gowdy spacetimes [69]. The results of [70] indicate that the conjecture is indeed true within these models. For a recent overview of the BKL conjecture see [49]. See also [64] for an overview of numerical results.

2.1.5 A generalized setup for the dynamics of spatially homogeneous models

In this section we introduce a general setup which will serve as a starting point for quantization. Recall that we did not discuss the inclusion of matter fields in section 2.1.3. The case of ideal fluids was discussed by Jantzen [31]. For a canonical treatment of ideal fluids one might employ the formalism developed by Schutz [71, 72] and for the particular case of dust the one by Brown and Kuchař [73]. The setup we will introduce should be general enough to cover the coupling of matter fields such as scalar fields and Yang-Mills fields to spatially homogeneous cosmological models. Most importantly it should emulate the main features of the minisuperspace models obtained via the symmetry reduction of general relativity to spatially homogeneous spacetimes. The setup that we will introduce in the following has the virtue of offering a quite general view on the dynamics of minisuperspace models and on the geometry of minisuperspace. It has, however, a major disadvantage: while the spatially homogeneous cosmological models admit a dynamical and a spacetime point of view, the model considered here offers only a dynamical point of view. Although the following setup is more general than the homogeneous cosmological model, we will nevertheless use the terminology that is common in the context of (quantum) cosmology.

We assume a d-dimensional minisuperspace $\mathcal{M}$ parametrized by the variables $\{q_0, \ldots, q_{d-1}\}$ with an action of the form

$$S = \int \mathrm{d}t\ L = \int \mathrm{d}t \left[\frac{1}{2N} \mathcal{G}_{AB} \left(\dot{q}^A - N^i A_i{}^A \right) \left(\dot{q}^B - N^j A_j{}^B \right) - N\mathcal{V} \right] , \tag{2.84}$$

where $N =: N^0$ and N^i are Lagrange multipliers and the index i runs from 1 to $d_{\mathrm{mc}} < d$ (for cosmological models usually $d_{\mathrm{mc}} \leq 3$). The vectors $\boldsymbol{A}_i = A_i{}^A(\mathbf{q})\partial_A$ are assumed to be linearly independent in all points $\mathbf{q} \in \mathcal{M}$. The (generalized) DeWitt metric[8] is defined via

$$\mathrm{d}\mathcal{S}^2 := \mathcal{G}_{AB} \mathrm{d}q^A \otimes \mathrm{d}q^B \ . \tag{2.85}$$

The DeWitt metric constitutes a metric on minisuperspace. In general it has a Lorentzian signature $(-, +, \ldots, +)$. This signals the presence of a lightcone structure in $\mathcal{M}$. The function $\mathcal{V} : \mathcal{M} \to \mathbb{R}$ is the minisuperspace potential, which is determined by the spatial three-curvature and the matter potentials. We adopt the terminology of Misner [42, 43] and Ryan [45] and refer to the configuration $\mathbf{q} = \{q^A\} \ \in \mathcal{M}$ of the universe as the *universe point.*

[8]Often one calls the metric on the gravitational part of $\mathcal{M}$ the DeWitt metric. In this thesis, we will call the metric on $\mathcal{M} = \mathcal{M}_{\mathrm{grav}} \times \mathcal{M}_{\mathrm{matter}}$ the DeWitt metric.

Note that the coupling of phantom fields [24] changes the signature of the DeWitt metric. The volume element on minisuperspace is given by

$$\star 1 = \sqrt{|\mathcal{G}|}\, \mathrm{d}q_0 \wedge \mathrm{d}q_1 \wedge \ldots \wedge \mathrm{d}q_{d-1} \ , \tag{2.86}$$

where $\mathcal{G}$ is the determinant of the DeWitt metric, that is, $\mathcal{G} := \det\left(\{\mathcal{G}_{AB}\}\right)$.

In the following we want to go over to the Hamiltonian formulation via the Dirac-Bergmann algorithm. We will use thereby to the terminology of Sundermeyer [74]. Note that the first step of the algorithm has already been performed by identifying the lapse and shift functions as non–dynamical variables.

The DeWitt metric and the vector fields ${A_i}^A$ both appear in the Legendre transform

$$\left(q^A, \dot{q}^A\right) \mapsto \left(q^A, p_A = \frac{1}{N}\mathcal{G}_{AB}\left[\dot{q}^B - N^i {A_i}^B\right]\right) \ . \tag{2.87}$$

The Legendre transform provides a linear map from the velocity phase space $T\mathcal{M}$ to the momentum phase space $T^*\mathcal{M}$. Performing the Legendre transform at the level of the action we obtain

$$S = \int \mathrm{d}t \left(\dot{q}^A p_A - N^0 \mathcal{H}_0 - N^i \mathcal{H}_i + \lambda^0 P_0 + \lambda^i P_i\right) \ . \tag{2.88}$$

The variables Λ^0 and Λ^i are Lagrange multipliers, which ensure that the momenta conjugate to N^0 and N^i weakly vanish, that is, $P_0 \simeq 0$ and $P_i \simeq 0$. These are the so called primary constraints, which are usually not written explicitly and we will also omit these terms from now on. The Hamiltonian constraint takes the form

$$\mathcal{H}_0 = \frac{1}{2}\mathcal{G}^{AB} p_A p_B + \mathcal{V} \simeq 0 \ , \tag{2.89}$$

This equation provides some important information about the dynamics. It tells us if the momentum $\mathbf{p} = \{p_A\}$ is "timelike", "spacelike" or "lightlike" as determined by the sign of the potential. This already allows us to make some simple qualitative statements about the behavior of the solutions. For example, the trajectory of a recollapsing universe has to turn "spacelike" in a region around the turning point. Consequently, if $\mathcal{V} \geq 0$ for all $\mathbf{q} \in \mathcal{M}$, the trajectory of the universe point will be "timelike" or "lightlike" and a recollapse is impossible. In addition we assume in (2.84) the presence of d_{mc} momentum constraints, which are linear in the momenta. They have the form

$$\mathcal{H}_i = {A_i}^A p_A \simeq 0 \ . \tag{2.90}$$

We collect the constraints into a single vector by introducing the notation $\mathcal{H}_\mu = \{\mathcal{H}_0, \mathcal{H}_i\}$, where $\mu = 0, 1, \dots, d_{\mathrm{mc}}$.

In order to emulate the dynamics of spatially homogeneous cosmological models we require the Dirac-Bergmann algorithm to stop at this point. Thus the secondary constraints $\mathcal{H}_\mu \simeq 0$ should be first class, that is, they should be preserved in time. This is equivalent to the requirement that the constraint algebra closes:

$$\{\mathcal{H}_\mu, \mathcal{H}_\nu\} = \mathcal{C}^\lambda_{\mu\nu}\mathcal{H}_\lambda \simeq 0 \ . \tag{2.91}$$

Note that the structure functions $\mathcal{C}^\lambda_{\mu\nu} = \mathcal{C}^\lambda_{\mu\nu}(\mathbf{q}, \mathbf{p})$ are functions of all the phase-space variables in general. The demand for closure of the constraint algebra will imply certain conditions on the DeWitt metric $\mathrm{d}\mathcal{S}^2$, the potential $\mathcal{V}$ and most importantly the vector fields $\boldsymbol{A}_i$ which we will work out in the following. We readily find that

$$\{\mathcal{H}_i, \mathcal{H}_j\} = -\left[\boldsymbol{A}_i, \boldsymbol{A}_j\right]^A p_A = -\left(A_i{}^B \nabla_B A_j{}^A - A_j{}^B \nabla_B A_i{}^A\right) p_A \ , \tag{2.92}$$

where ∇ denotes the Levi-Civita connection compatible with $\mathrm{d}\mathcal{S}^2$. Hence the requirement (2.91) demands that the vector fields $\boldsymbol{A}_i$ form a closed Lie sub-algebra of vector fields, that is, $\mathcal{L}_{\boldsymbol{A}_i}\boldsymbol{A}_j = [\boldsymbol{A}_i, \boldsymbol{A}_j] = -\mathcal{C}^k_{ij}\boldsymbol{A}_k$. Following chapter 14 in the textbook [75], we can draw a clear geometrical picture of the situation. Because of the closure condition, the vector fields $\boldsymbol{A}_i$ define what is called an *integrable distribution*. This yields a foliation of the minisuperspace $\mathcal{M}$ into d_{mc}–dimensional sub-manifolds Σ.[9] These submanifolds are the so called *integral manifolds* of the vector fields $\boldsymbol{A}_i$, that is, their tangent space at any point $\boldsymbol{q}$ is spanned by the vectors $\boldsymbol{A}_i\,|_{\boldsymbol{q}}$. The integral manifolds are then also called the *leaves of the foliation*. For a cosmological minisuperspace model, the leaves are usually spacelike and, in the case of the vacuum Bianchi models, the leaves of the foliation can be identified with the inner automorphism group.

We can construct the components of the induced metric on the leaves via $\mathcal{G}_{ij} := A_i{}^A A_j{}^B \mathcal{G}_{AB}$. We define the dual of $\boldsymbol{A}_i$ as $\mathbf{B}^i = B_A{}^i \mathrm{d}q^A$, where $B_A{}^i := \mathcal{G}_{AB}\mathcal{G}^{ij}A_j{}^B$. By construction the duality relation $A_j{}^A B_A{}^i = \delta^i_j$ is satisfied. We can then write

$$\{\mathcal{H}_i, \mathcal{H}_j\} = -\left[\boldsymbol{A}_i, \boldsymbol{A}_j\right] \lrcorner \mathbf{B}^k \mathcal{H}_k = \mathcal{C}^k_{ij}\mathcal{H}_k \ . \tag{2.93}$$

Furthermore, the matrix

$$P_A{}^B := B_A{}^i A_i{}^B \tag{2.94}$$

[9] A d_{mc} – dimensional submanifold is also called submanifold of codimension $d - d_{\mathrm{mc}}$ in the mathematically inclined literature.

satisfies $P_A{}^C P_C{}^B = P_A{}^B$ and thus it acts as projection operator $T\mathcal{M} \to T\Sigma$ (and $T^*\mathcal{M} \to T^*\Sigma$). The projector $P_A{}^B$ maps the momenta into $\mathrm{span}\{\mathcal{H}_i\}$ and it is called the *tangential projection operator*. The *normal projection operator* can be defined as

$$\bar{P}_A{}^B := \delta_A^B - P_A{}^B \ . \tag{2.95}$$

The projector $\bar{P}_A{}^B$ is the *complement* of $P_A{}^B$, that is, $P_A{}^B \bar{P}_B{}^C = \bar{P}_A{}^B P_B{}^C = 0$. By construction the projectors are orthogonal, i.e.,

$$P^{AB} = P^{BA} \quad \text{and} \quad \bar{P}^{AB} = \bar{P}^{BA} \ . \tag{2.96}$$

The normal projector $\bar{P}_A{}^B$ provides a map $T\mathcal{M} \to \mathcal{N}(\Sigma)$ where $\mathcal{N}(\Sigma)$ is the so called *normal space*, which is the space of all vector fields in $\mathcal{N}(\Sigma)$ that are normal to the leaves Σ. For the traces of the projection operators, it holds that $P_A{}^A = d_{\mathrm{mc}}$ and $\bar{P}_A{}^A = d - d_{\mathrm{mc}}$. Furthermore, the projectors allow for a decomposition of the DeWitt metric into two parts according to

$$\mathcal{G}_{AB} = \bar{P}_A{}^C \bar{P}_B{}^D \mathcal{G}_{CD} + P_A{}^C P_B{}^D \mathcal{G}_{CD} \ . \tag{2.97}$$

Note that $P_A{}^C P_B{}^D \mathcal{G}_{CD} = B_A{}^i B_B{}^j \mathcal{G}_{ij}$ is the induced metric on the leaves. The decomposition of the inverse metric $\mathcal{G}^{AB}$ proceeds analogously.

Let us now consider the Poisson brackets $\{\mathcal{H}_0, \mathcal{H}_i\}$. By direct calculation, we find that

$$\begin{aligned} \{\mathcal{H}_0, \mathcal{H}_i\} &= \frac{1}{2}\left(\mathcal{L}_{\boldsymbol{A}_i} \mathrm{d}\mathcal{S}^2\right)^{AB} p_A p_B + \mathcal{L}_{\boldsymbol{A}_i} \mathcal{V} \\ &= -\nabla^{(A} A_i{}^{B)} p_A p_B + A_i{}^A \partial_A \mathcal{V} \ , \end{aligned} \tag{2.98}$$

where $(\mathcal{L}_{\boldsymbol{A}_i} \mathrm{d}\mathcal{S}^2)^{AB} = -2\nabla^{(A} A_i{}^{B)}$ is the Lie derivative of the (inverse) DeWitt metric with respect to the vector field $\boldsymbol{A}_i$. Our considerations so far lead us to impose the following conditions:

- The vector fields $\boldsymbol{A}_i$ define a distribution on $\mathcal{M}$.

- The DeWitt metric $\mathcal{G}_{AB}$, the potential $\mathcal{V}$ and the vector fields $\boldsymbol{A}_i$ satisfy

$$A_i{}^A \partial_A \mathcal{V} = 2\lambda_i \mathcal{V} \quad \text{and} \quad \left(\nabla^{(A} A_i{}^{B)} + \lambda_i \mathcal{G}^{AB}\right) \bar{P}_A{}^C \bar{P}_B{}^D = 0 \ , \tag{2.99}$$

  where λ_i is defined via

$$\lambda_i := -\frac{1}{d - d_{\mathrm{mc}}} \nabla^{(A} A_i{}^{B)} \bar{P}_A{}^C \bar{P}_B{}^D \mathcal{G}_{CD} \ . \tag{2.100}$$

From now on, we will always assume that these conditions are satisfied. Note that, as a particular case, $\boldsymbol{A}_i$ might be a conformal Killing vector field of both the metric and the potential. The conditions imply that the constraint algebra closes, that is, $\{\mathcal{H}_\mu, \mathcal{H}_\nu\} = \mathcal{C}^\lambda_{\mu\nu}\mathcal{H}_\lambda \simeq 0$, where the structure functions are given by

$$\begin{aligned}
\mathcal{C}^0_{0i} &= 2\lambda_i \ , \\
\mathcal{C}^j_{0i} &= -\left(\nabla^{(A} A_i{}^{B)} + \lambda_i \mathcal{G}^{AB}\right)\left(P_A{}^C + 2\bar{P}_A{}^C\right) p_C B_B{}^j \\
\mathcal{C}^k_{ij} &= -\left(A_i{}^A \nabla_A A_j{}^B - A_j{}^A \nabla_A A_i{}^B\right) B_B{}^k \ .
\end{aligned} \tag{2.101}$$

The calculation in this section shows that the conditions are both necessary and sufficient for the closure of the constraint algebra. Note that $\mathcal{C}^0_{0i}$ and $\mathcal{C}^k_{ij}$ are functions of only $\mathbf{q}$ while the $\mathcal{C}^j_{0i}$ are functions of $\mathbf{q}$ and $\mathbf{p}$.

Equations of motion: The evaluation of the Poisson brackets $\{q^A, H\}$ and $\{p_A, H\}$ gives $2 \times d$ equations of motion. In the momentum phase space, the equations of motion constitute the dynamical system

$$\begin{aligned}
\dot{q}^A =& N\mathcal{G}^{AB} p_B + N^i A_i{}^A \\
\dot{p}_A =& - N\mathcal{G}^{CD}\Gamma^B_{AC} p_B p_D - N\partial_A \mathcal{V} - N^i \partial_A A_i{}^B p_B \ .
\end{aligned} \tag{2.102}$$

The equations can now be solved after fixing the gauge N and N^i and setting up initial conditions $\{\mathbf{q}_{\text{in}}, \mathbf{p}_{\text{in}}\}$ obeying the constraints

$$\mathcal{H}_\mu(\mathbf{q}_{\text{in}}, \mathbf{p}_{\text{in}}) = 0 \ . \tag{2.103}$$

The time preservation of the constraints is implied by the closure of the constraint algebra. In configuration space, the equations of motion read

$$\begin{aligned}
(\partial_t - \partial_t \log N)\left(\dot{q}^A - N^i A_i{}^A\right) + \left(\Gamma^A_{BC}\dot{q}^B + N^i \mathcal{G}_{CD}\nabla^A A_i{}^D\right)\left(\dot{q}^C - N^i A_i{}^C\right)& \\
+ N\mathcal{G}^{AB}\partial_B \mathcal{V} = 0 \ ,&
\end{aligned} \tag{2.104}$$

where ∇_B is the Levi-Civita connection that is compatible with the DeWitt metric and Γ^A_{BC} are its coefficients. If we gauge $N^i = 0$ and assume that $N = N(\mathbf{q})$ we obtain

$$\left(\dot{q}^B \nabla_B - \partial_t \log N\right)\dot{q}^A + N\mathcal{G}^{AB}\partial_B \mathcal{V} = 0 \ . \tag{2.105}$$

Note that the equations of motion in configuration phase space are manifestly covariant. After choosing the gauge $N = 1$ we get

$$\ddot{q}^A + \Gamma^A_{BC}\dot{q}^B\dot{q}^C + \mathcal{G}^{AB}\partial_B\mathcal{V} = 0 \, , \tag{2.106}$$

This is of course the geodesic equation on $(\mathcal{M}, \mathrm{d}\mathcal{S}^2)$ for a parametrized curve with tangent vector $\dot{\mathbf{q}}$ plus a conservative force term. Note that the precise form of the solution curves $\boldsymbol{q}(t)$ depends on the gauge N^i.

Transformations of the constraint algebra: We consider the following transformation of the lapse and shift functions:

$$N \mapsto \widetilde{N} = \Omega^2 N \, , \tag{2.107}$$

$$N^i \mapsto \widetilde{N}^i = N^j L_j{}^i \, , \tag{2.108}$$

where $\Omega : \ \mathcal{M} \mapsto \mathbb{R}^+$ is sufficiently smooth and $\{L_j{}^i\} \in \mathrm{GL}(d_{\mathrm{mc}}, \mathbb{R})$.[10] The full Hamiltonian is invariant under this transformation, that is,

$$H = N^\mu \mathcal{H}_\mu \mapsto H = \widetilde{N}^\mu \widetilde{\mathcal{H}}_\mu \tag{2.109}$$

where the Hamiltonian and momentum constraints transform like

$$\mathcal{H}_0 \mapsto \widetilde{\mathcal{H}}_0 = \Omega^{-2}\mathcal{H}_0 = \frac{1}{2}\widetilde{\mathcal{G}}^{AB} p_A p_B + \widetilde{\mathcal{V}} \, , \tag{2.110}$$

$$\mathcal{H}_i \mapsto \widetilde{\mathcal{H}}_i = \widetilde{A}_i{}^A p_A \, , \tag{2.111}$$

with $\widetilde{\mathcal{G}}_{AB} = \Omega^2 \mathcal{G}_{AB}$, $\widetilde{\mathcal{V}} = \Omega^{-2}\mathcal{V}$ and $\widetilde{A}_i{}^A = L_i{}^j A_j{}^A$. In the context of Quantum Cosmology, we will refer to the transformation (2.107) as a conformal transformation. Furthermore, we introduce the obvious notation

$$\mathrm{d}\widetilde{\mathcal{S}}^2 = \Omega^2 \mathrm{d}\mathcal{S}^2 \, . \tag{2.112}$$

The transformation (2.108) can also be understood as a change of the basis on the leaves of the foliation. The full transformation made up of (2.107) and (2.108) induces a transformation of the structure functions according to

$$\{\widetilde{\mathcal{H}}_\mu, \widetilde{\mathcal{H}}_\nu\} = \widetilde{\mathcal{C}}^\lambda_{\mu\nu}\widetilde{\mathcal{H}}_\lambda \, . \tag{2.113}$$

[10]More generally, one could also consider transformations of the form $N^i \mapsto N^i + \Delta N^i$. We leave this investigation for future work.

The constraint algebra of the transformed system closes and the new structure functions are related to the old ones by

$$\begin{aligned}
\widetilde{\mathcal{C}}^0_{0i} &= L_i{}^j \left(\mathcal{C}^0_{0j} - 2A_j{}^A\partial_A \log\Omega\right) = 2\widetilde{\lambda}_i \ , \\
\widetilde{\mathcal{C}}^j_{0i} &= \Omega^{-2}\left[L_i{}^l\mathcal{C}^k_{0l} - \mathcal{G}^{AB}\left(\partial_A L_i{}^k\right)p_B\right]\left(L^{-1}\right)_k{}^j \ , \\
\widetilde{\mathcal{C}}^k_{ij} &= \left[L_i{}^l L_j{}^n \mathcal{C}^m_{ln} + L_j{}^l A_l{}^A\left(\partial_A L_i{}^m\right) - L_i{}^l A_l{}^A\left(\partial_A L_j{}^m\right)\right]\left(L^{-1}\right)_m{}^k \ .
\end{aligned} \tag{2.114}$$

Note that if we only consider rescalings of the lapse function then λ_i transforms similar to a Weyl vector field (see appendix B.3):

$$\lambda_i \mapsto \widetilde{\lambda}_i = \lambda_i - A_i{}^A\partial_A \log\Omega \ . \tag{2.115}$$

The transformation law suggests that we can interpret the one–form $\lambda_i\boldsymbol{B}^i$ as a Weyl one–form on the leaves of the foliation.

For completeness and later use, we remark that we can define the 2-form $\boldsymbol{\mathcal{F}} := \mathcal{F}_{ij}\boldsymbol{B}^i\wedge\boldsymbol{B}^j$, where

$$\mathcal{F}_{ij} := 2A_i{}^A A_j{}^B \nabla_{[A}\lambda_{B]} \quad \text{and} \quad \lambda_A := B_A{}^i\lambda_i \ . \tag{2.116}$$

Note that by definition $\bar{P}_A{}^B\lambda_B = 0$. The tensor $\boldsymbol{\mathcal{F}}$ is in certain aspects analogous to the Faraday 2-form in electrodynamics. Its most notable feature is its invariance under rescalings of the lapse. Moreover, it transforms covariantly under transformations of the shift functions. To be more precise, it transforms like $\mathcal{F}_{ij} \mapsto \widetilde{\mathcal{F}}_{ij} = L_i{}^k L_j{}^l \mathcal{F}_{kl}$ under the transformation (2.108). A certain simplification arises if $\boldsymbol{\mathcal{F}} = 0$. This is in particular true if all $\lambda_i = 0$ (or all $\widetilde{\lambda}_i = 0$ after a rescaling of the lapse) which is usually the case for spatially homogeneous cosmological models. If we, however, perform a rescaling of the lapse, which satisfies $A_i{}^A\partial_A\Omega \neq 0$, then $\widetilde{\lambda}_i = -A_i{}^A\partial_A\log\Omega$ is non-zero. The condition $\boldsymbol{\mathcal{F}} = 0$ seems to be important in the context of quantization. In fact, this condition is equivalent to the statement that the Weyl structure on the leaves is integrable, as we will show later in section 2.2.7.

In addition, we have encountered the objects

$$K_i^{AB} := \nabla^{(A}A_i{}^{B)} + \lambda_i\mathcal{G}^{AB} \tag{2.117}$$

in our calculations. We find that they transform as

$$K_i^{AB} \mapsto \widetilde{K}_i^{AB} = \Omega^{-2}K_i^{AB} \ , \tag{2.118}$$

when we rescale the lapse. This also implies that the scalars $K_i := \mathcal{G}_{AB}K_i^{AB}$ are invariant under rescalings of the lapse function. However, neither K_i^{AB} nor K_i transform covariantly under transformations of the shift. The K_i^{AB} transform as

$$K_i^{AB} \mapsto \widetilde{K}_i^{AB} = L_i{}^j K_j^{AB} + A_j{}^{(A}\partial^{B)} L_i{}^j \ . \tag{2.119}$$

Nevertheless, since $A_i{}^C \bar{P}_C{}^A = 0$ the object $K_i^{CD}\bar{P}_C{}^A\bar{P}_D{}^B$ transforms covariantly under transformations of the shift. Therefore, the condition $K_i^{CD}\bar{P}_C{}^A\bar{P}_D{}^B = 0$ has a covariant meaning. Furthermore, we remark that the structure functions $\mathcal{C}_{ij}^k$ can be rewritten as

$$\mathcal{C}_{ij}^k = 2A_{[i}{}^A A_{j]}{}^B \nabla_A B_B{}^k = 2A_i{}^A A_j{}^B \nabla_{[A} B_{B]}{}^k \ . \tag{2.120}$$

Our considerations so far might be important in the context of canonical quantization. The transformations (2.107) and (2.108) certainly leave the physics invariant. We will later demand that the same holds true for the quantized version of the system. We continue the discussion on the geometry of minisuperspace in section 2.2.7. But before closing this section let us have brief look at the notion of symmetries.

Symmetries: A phase-space function $f(\boldsymbol{q},\boldsymbol{p})$ is a constant of motion if it weakly commutes with all constraints

$$\{\mathcal{H}_\mu, f\} \simeq 0 \ . \tag{2.121}$$

We consider first functions of the form $f(\boldsymbol{q},\boldsymbol{p}) = \xi^A p_A$ with $\boldsymbol{\xi} = \xi^A\partial_A \in T\mathcal{M}$. The discussion proceeds analogously to the discussion of the momentum constraints. The condition (2.121) is satisfied if

- The vector field $\boldsymbol{\xi}$ satisfies $[\boldsymbol{\xi}, \boldsymbol{A}_i] \in \operatorname{span}\{\boldsymbol{A}_i\}$. In the mathematical literature on foliations, these vector fields are called *basic* or also *foliate*. The set of all basic vector fields forms a Lie algebra [76].

- $\xi^A\partial_A\mathcal{V} = 2\lambda_{\boldsymbol{\xi}}\mathcal{V}$ and $\left(\nabla^{(A}\xi^{B)} + \lambda_{\boldsymbol{\xi}}\mathcal{G}^{AB}\right)\bar{P}_A{}^C\bar{P}_B{}^D = 0$.

The scalar $\lambda_{\boldsymbol{\xi}}$ is completely analogous to the one defined in (2.100). Note that the above conditions are satisfied by the momentum constraints $\mathcal{H}_i$ as well (the associated constant of motion, however, is constrained to be zero). An important example of such a symmetry are the generators of the special automorphism group in the case of (vacuum) Bianchi models.

In full analogy to the vacuum Bianchi models, we introduce the following terminology: We refer to the group generated by all vector fields $\boldsymbol{\xi}$ which satisfy the above conditions as the *symmetry group of the system*. The subgroup generated by the vector fields $\boldsymbol{A}_i$ will be called the *inner symmetry group*. The group which is generated by all vector fields that are not in the span$\{\boldsymbol{A}_i\}$ will be called the *outer symmetry group*.

Let us next consider phase-space functions of the form $f(\boldsymbol{q}, \boldsymbol{p}) = X^{AB} p_B p_A$ with $\boldsymbol{X} = X^{AB} \partial_A \otimes \partial_B \in T\mathcal{M} \otimes T\mathcal{M}$ being a symmetric $\binom{2}{0}$–tensor field $X^{AB} = X^{BA}$. We compute the commutators with the secondary constraints as follows

$$
\begin{aligned}
\{f, \mathcal{H}_0\} &= 2p_A \left[\frac{1}{2} \nabla^{(A} X^{BC)} p_B p_C - X^{AB} \partial_B \mathcal{V} \right] \ , \\
\{f, \mathcal{H}_i\} &= \left(\mathcal{L}_{\boldsymbol{A}_i} \boldsymbol{X}\right)^{AB} p_A p_B \ .
\end{aligned}
\tag{2.122}
$$

We find that the condition (2.121) is satisfied if

- $(\mathcal{L}_{\boldsymbol{A}_i} \boldsymbol{X})^{AB} \bar{P}_A{}^C \bar{P}_B{}^D = 0$,
- $X^{AB} \partial_B \mathcal{V} = \lambda_{\boldsymbol{X}}{}^A \mathcal{V}$,
- $\left(\nabla^{(A} X^{BC)} + 2\lambda_{\boldsymbol{X}}{}^{(A} \mathcal{G}^{BC)}\right) \bar{P}_A{}^D \bar{P}_B{}^E \bar{P}_C{}^F = 0$.

The vector field $\lambda_{\boldsymbol{X}}{}^A \partial_A$ is the vector-field analogue of the scalar (2.100) and the last two conditions are in some sense equivalent to (2.99). As a particular sub-case, $\boldsymbol{X}$ might be a conformal Killing tensor field of the DeWitt metric and the potential. Another example is given by $\boldsymbol{X} = \boldsymbol{\xi} \otimes \boldsymbol{\xi}$ where $\boldsymbol{\xi}$ generates a symmetry. The reader can easily convince herself/himself that this tensor satisfies all requirements.

2.1.6 Hamilton-Jacobi formalism

The Hamilton-Jacobi formalism might be considered as the formulation of classical mechanics which is closest to quantum mechanics. In fact, it was Schrödinger's actual starting point for deriving his famous wave equation [77]. In this sense the current section will serve as a preparation for quantization, which is to be understood in this thesis as a procedure that tries to reverse the eikonal approximation. More precisely, the Wheeler-DeWitt equation and the quantum momentum constraints should be constructed such that the Hamilton-Jacobi equation is recovered in the semi-classical limit. We write now the action in the form

$$
S_0[\mathbf{q}, \mathbf{p}, \mathbf{q}_{\text{in}}, \mathbf{p}_{\text{in}}] = \int_\gamma \mathrm{d}t \left[\dot{q}^A p_A - N^\mu \mathcal{H}_\mu \right] \ , \tag{2.123}
$$

where γ is a path with starting point $\mathbf{q}_{\text{in}}$, $\mathbf{p}_{\text{in}}$ and end point $\mathbf{q} \in \mathcal{M}$, $\mathbf{p} \in T^*_{\mathbf{q}}\mathcal{M}$. The physical path is the one that minimizes the action. The Hamiltonian and momentum constraint vanish for physical trajectories. On-shell, the action therefore becomes

$$S_0[\mathbf{q},\mathbf{p},\mathbf{q}_{\mathrm{in}},\mathbf{p}_{\mathrm{in}}]\doteq\int_\gamma \mathrm{d}\tau \ := \int_\gamma \left(\partial_A S_0\right)\mathrm{d}q^A = \int_\gamma p_A \mathrm{d}q^A \ . \tag{2.124}$$

The 1-form $\mathrm{d}\tau$ is the differential of the so called WKB time. It can now be shown that (on-shell) S_0 satisfies the Hamilton-Jacobi equations

$$\begin{aligned}\mathcal{H}_0\left(\mathbf{q},\mathbf{p}=\partial_A S_0 \mathrm{d}q^A\right) &= \frac{1}{2}\mathcal{G}^{AB}(\partial_A S_0)(\partial_B S_0)+\mathcal{V}=0 \ , \\ \mathcal{H}_i\left(\mathbf{q},\mathbf{p}=\partial_A S_0 \mathrm{d}q^A\right) &= A_i{}^A\partial_A S_0 = 0 \ ,\end{aligned} \tag{2.125}$$

where initial conditions are to be given on some suitable hypersurface $\Sigma\subset\mathcal{M}$. The initial momenta $\partial_A S_0|_\Sigma$ are then also subject to the constraints $\mathcal{H}_\mu\left(q_A,\partial_A S_0\right)|_\Sigma=0$. Note that after solving the equations S_0 provides a scalar field on some submanifold of $\mathcal{M}$. Moreover, if S_0 is a solution to the Hamilton-Jacobi equations then $-S_0$ is also a solution. By switching to the Hamilton-Jacobi formalism, we shift the problem of solving equations of motion to the problem of solving one non-linear first order partial differential equation for the so called Hamilton-Jacobi action. Moreover, the formalism so far is completely independent of the gauge N^μ. After solving the Hamilton-Jacobi equation, we obtain the physical momenta $p_A=\partial_A S_0$ by construction. The momentum constraints $A_i{}^A\partial_A S_0 = A_i{}^A p_A = 0$ imply that S_0 is constant on the leaves of the foliation spanned by the vector fields $\boldsymbol{A}_i$.

Note also that the Hamilton-Jacobi equations (2.125) are completely independent of any external time parameter. We can, however, define a time vector field by

$$\partial_\tau := \frac{\partial}{\partial\tau} := \mathcal{G}^{AB}(\partial_B S_0)\partial_A \in T\mathcal{M} \ . \tag{2.126}$$

The momentum constraints $A_i{}^A\partial_A S_0=0$ ensure that S_0 does not change in the direction $\boldsymbol{A}_i$ which implies that ∂_τ does not have components proportional to the vectors $\boldsymbol{A}_i$; in formulas:

$$P^A{}_B(\partial_\tau)^B = 0 \ . \tag{2.127}$$

Furthermore, we obtain the Lie bracket

$$[\partial_\tau,\boldsymbol{A}_i] = -2\lambda_i\partial_\tau + 2(\partial_A S_0)\nabla^{(A}A_i{}^{B)}B_B{}^j\boldsymbol{A}_j \ . \tag{2.128}$$

This implies that the algebra formed by $\{\partial_\tau, A_i\}$ closes.[11] If we want to obtain the physical

[11] This might be important in the context of semi-classical Quantum Cosmology since ∂_τ appears on the left hand side of the functional Schrödinger equation [10, 78].

trajectories in $\mathcal{M}$ we have to solve the equation

$$\frac{1}{N}\dot{\mathbf{q}} = \frac{\partial}{\partial\tau} + n^i \boldsymbol{A}_i \ , \tag{2.129}$$

which requires to fix a gauge N and $n^i := \frac{N^i}{N}$. The solution $\mathbf{q}(t)$ is then an integral curve of the vector field $N\left(\frac{\partial}{\partial\tau} + n^i \boldsymbol{A}_i\right)$. We note that the flow of this vector field depends on the gauge n^i. We conclude that while different gauges for N only yield different parametrizations of the solution curves, different gauges n^i, that is, different foliations, certainly yield different trajectories in $\mathcal{M}$. A relation between WKB time τ and the coordinate time t can be obtained from the equation

$$\mathrm{d}\tau := \mathrm{d}S_0 = p_A \mathrm{d}q^A = \mathcal{G}_{AB}\left(\frac{\dot{q}^A}{N} - n^i A_i{}^A\right)\dot{q}^B \mathrm{d}t \ . \tag{2.130}$$

Let us now turn to a discussion of symmetries at the level of the Hamilton-Jacobi formulation. Let $f(\boldsymbol{q},\boldsymbol{p}) = \xi^A p_A$ be a symmetry of the system as discussed in section 2.1.5 of this thesis. We denote the flow generated by the vector $\boldsymbol{\xi}$ by

$$\begin{aligned} \Phi_{\boldsymbol{\xi}} : \ & \mathcal{M} \times \mathbb{R} \to \mathcal{M} \\ & (\boldsymbol{q}, T) \mapsto \Phi^T_{\boldsymbol{\xi}}(\boldsymbol{q}) = \exp\left(T\boldsymbol{\xi}\right)\boldsymbol{q} \ . \end{aligned} \tag{2.131}$$

Furthermore, we define

$$\widetilde{S}^T(\boldsymbol{q}) := S\left(\Phi^T_{\boldsymbol{\xi}}(\boldsymbol{q})\right) \ . \tag{2.132}$$

One can now show the following:

If $\boldsymbol{\xi}$ generates a symmetry and S solves the Hamilton-Jacobi equations (2.125) *then $\tilde{S}^T$ is a solution as well.*

It is sufficient to prove the infinitesimal version of this statement. We first expand $\tilde{S}^T$ around $T = 0$. Using the fact that S solves (2.125) and that ξ generates a symmetry one can show that

$$\frac{1}{2}G^{AB}(\partial_A\tilde{S})(\partial_B\tilde{S}) + \mathcal{V} = \mathcal{O}(T^2) \quad \text{and} \quad A_i{}^A\partial_A\widetilde{S} = \mathcal{O}(T^2) \ . \tag{2.133}$$

The terms linear in T vanish identically and hence we can conclude the proof. Recall that the subalgebra of vector fields $\{\boldsymbol{A}_i\}$ generate symmetries as well. The momentum constraints $A_i{}^A\partial_A S = 0$, however, ensure that $\tilde{S}(\Phi(\boldsymbol{q})) = S(\boldsymbol{q})$ if the flow Φ was generated by this subalgebra.

Recall that an important example of the symmetries in this discussion are the automorphisms in the case of the vacuum Bianchi models. In that case $\boldsymbol{\xi}$ could be taken as a generator of a constant special automorphism, that is, for a fixed T the flow is given by $\Phi^T_\xi(h_{ij}) = h_{kl}L^k{}_iL^l{}_j$, where $\{L^i{}_j\}$ is a constant element of $S\mathrm{Aut}(\mathfrak{g})$.

The Van Vleck factor

An important feature of any quantum theory of gravity should be that it contains the classical theory in some specific limits. In the Wheeler-DeWitt approach, one of the steps that leads to the recovery a classical limit usually involves the WKB approximation (see [10] or section of this 2.2.3 thesis). In the semi-classical limit, the wave functions are then of the form

$$\Psi \approx \sqrt{D}\mathrm{e}^{\mathrm{i}S} \tag{2.134}$$

where S is a solution to the Hamilton-Jacobi equation and D is the so called van Vleck factor (mostly referred to as van Vleck determinant). The following considerations might therefore be considered a first step into the realm of Quantum Cosmology.

Suppose that we have a solution S to the Hamilton-Jacobi equation (2.125). In the following, we want to derive a notion of a momentum flux density D in $\mathcal{M}$ for the given solution S . We define the momentum flux

$$J^A := D\mathcal{G}^{AB}\partial_B S_0 \tag{2.135}$$

and demand that it is conserved, that is,

$$\nabla_A J^A = 0\ . \tag{2.136}$$

The conservation equation yields a linear transport equation for D which reads

$$\partial_\tau D = -(\Box S)D \tag{2.137}$$

We remark that the definition (2.135) and the conservation law (2.136) correspond in some sense to Fick's first and second law, respectively.

We can set up initial conditions for D at some point $\mathbf{q}_{\mathrm{in}} \in \mathcal{M}$ and then evolve it along the streamlines γ of the momentum flux by

$$D(\mathbf{q}) = D(\mathbf{q}_{\mathrm{in}})\exp\left(-\int_\gamma \mathrm{d}\tau\,\Box S\right)\ . \tag{2.138}$$

Note that the choice of the initial condition $D(\mathbf{q}_{\mathrm{in}}) > 0$ corresponds to some choice of a reference density.

Furthermore, note that the definition of D depends on the metric $\mathrm{d}\mathcal{S}^2$ and therefore on the choice of the gauge N. More precisely, the van Vleck factor transforms as

$$D \mapsto \widetilde{D} = \Omega^{2-d} D \tag{2.139}$$

under a rescaling of the lapse function (2.107). We might say that D transforms in a conformally covariant way. This implies that the flux

$$\boldsymbol{J} = D \star \mathrm{d}\tau \ , \tag{2.140}$$

on the other hand, is invariant under rescalings of the lapse function. Note that the Hodge star operator depends on the metric $\mathrm{d}\mathcal{S}^2$ and therefore it is not invariant under rescalings of the lapse. We denote the Hodge dual associated to the rescaled metric $\mathrm{d}\widetilde{\mathcal{S}}^2$ by $\widetilde{\star}$. The transformation law for the Hodge star under conformal transformations can be found in the appendix (B.5).

Recall that in the minisuperspace models the momentum constraints act as diffeomorphism inducing generators in the phase space $T^*\mathcal{M}$. We might want to demand that D is as well invariant under the action of the inner symmetries, that is, $\mathcal{L}_{\boldsymbol{A}_i} D = A_i{}^A \partial_A D = 0$. This equation is however not invariant under rescalings of the lapse. We therefore impose the equation

$$\left[A_i{}^A \partial_A + (d-2)\lambda_i \right] D = 0 \tag{2.141}$$

instead. Existence of solutions to the system of equations (2.137) and (2.141) follows from the fact that the algebra $\{\partial_\tau, \boldsymbol{A}_i\}$ closes and by application of the Frobenius theorem if the additional condition $\boldsymbol{\mathcal{F}} = 0$ is satisfied.

It was already noticed by Hawking and Page [79] that the van Vleck factor is intimately connected to the coordinate time t. Suppose now that we have solved the Hamilton-Jacobi equation and we obtained S_0 and $p_A = \partial_A S_0$. After fixing the gauge N and N_i, we are able to obtain the trajectories $q^A(t)$ in terms of the coordinate time t by solving

$$\dot{q}^A = N \mathcal{G}^{AB} p_B + N^i A_i{}^A \ . \tag{2.142}$$

Using (2.130), we find that

$$\star D = N \mathrm{d}t \wedge \boldsymbol{J} \ . \tag{2.143}$$

Recall that the current $\boldsymbol{J}$ is conserved and invariant under rescalings of the lapse. The line element $N\mathrm{d}t$ is the infinitesimal time interval which corresponds to the infinitesimal coordinate time interval in the spacetime metric when N is set equal to 1. Under rescalings of the lapse $\star D$ transforms as $\star D \mapsto \widetilde{\star}\widetilde{D} = \Omega^2 \star D$.

2.2 Quantum Cosmology

2.2.1 The Wheeler-DeWitt equation in minisuperspace

In the following, we consider again a general d-dimensional minisuperspace $\mathcal{M}$ as described in section 2.1.5. The task of canonical quantization is now to “reverse the eikonal approximation”. Quantization is performed heuristically á la Dirac with the variables q^A as configuration space variables. Recall that q^A can contain both the three metric components h_{ij} and matter degrees of freedom. The process gives rise to the Wheeler-DeWitt equation which is usually a hyperbolic partial differential equation that resembles the form of a Klein-Gordon equation. Instead of sharp trajectories in minisuperspace, one now obtains wave packets as solutions to the Wheeler-DeWitt equation. It is then expected that it is possible to construct wave packets which are roughly peaked over the classical trajectories in certain regions of $\mathcal{M}$. We replace now the constraints $\mathcal{H}_\mu \simeq 0$ by their quantum versions $\hat{\mathcal{H}}_\mu \Psi = 0$. The momenta are thereby substituted according to the quantization rule $p_A \mapsto -\mathrm{i}\hbar\partial_A$. Following this procedure, we obtain the minisuperspace Wheeler-DeWitt equation and the quantum versions of the momentum constraints

$$\begin{aligned} \hat{\mathcal{H}}\Psi = 0 \ , \quad \text{where} \quad \hat{\mathcal{H}} &= -\frac{\hbar^2}{2} \text{ “ } \mathcal{G}^{AB}\partial_A\partial_B \text{ ” } + \mathcal{V} \\ \hat{\mathcal{H}}_i\Psi = 0 \ , \quad \text{where} \quad \hat{\mathcal{H}}_i &= -\mathrm{i}\hbar \text{ “ } {A_i}^A\partial_A \text{ ” } . \end{aligned} \tag{2.144}$$

The Wheeler-DeWitt approach to Quantum Cosmology comes with all of conceptual problems mentioned in the introduction 1.1. We will not specify in which vector space wave functions are supposed to live in. There are several questions in this regard which remain unanswered. For example: Should wave packets be real or complex valued? It has sometimes been argued that wave functions should be real based on the fact that the Wheeler-DeWitt equation contains only real quantities. Moreover, it is not clear if and how boundary conditions are to be imposed on the wave function. We will shortly comment on this issue in section 2.2.6. The notation “ . ” in (2.144) indicates that the factor ordering is left open. To be more precise, it can make an immense difference if we, for example, write $\mathcal{G}^{AB}\partial_A\partial_B\Psi$ or $\partial_A\left(\mathcal{G}^{AB}\partial_B\Psi\right)$ in the Wheeler-DeWitt equation. The factor ordering problem, or more precisely, the problem of how to construct the quantization map $\mathcal{H}_\mu \mapsto \hat{\mathcal{H}}_\mu$ constitutes a major open problem in

Quantum Cosmology. Indeed, we should pay close attention to this issue because, as we will see in the following, the factor ordering has a strong influence on the discussion of singularity avoidance.

It is beyond the scope of this thesis to cover all facets of Quantum Cosmology in the Wheeler-DeWitt framework. For additional aspects and different perspectives, see in particular [10, 78, 80, 81] and the references therein.

2.2.2 The conformally covariant Wheeler-DeWitt equation

For the sake of simplicity, we start the discussion with the case when there are no momentum constraints, that is, the momentum constraints are either trivially satisfied or the classical dynamics were reduced in such a way that only the Hamiltonian constraint remains.

The invariance of the classical theory under rescalings of the lapse function motivates us to use the conformal factor ordering, that is, we choose the quantization map

$$\mathcal{G}^{AB} p_A p_B \mapsto -\left(\Box - \xi_d \mathcal{R}\right) \ , \tag{2.145}$$

where $\xi_d = \frac{d-2}{4(d-1)}$ and we have set $\hbar = 1$. The operator $\Box - \xi_d \mathcal{R}$ is the conformal Laplace-Beltrami operator (or Yamabe operator) with $\Box := \frac{1}{\sqrt{-\mathcal{G}}} \partial_A \left(\sqrt{-\mathcal{G}} \mathcal{G}^{AB} \partial_B\right)$ being the Laplace-Beltrami operator and $\mathcal{R}$ being the Ricci scalar on the Riemannian manifold $(\mathcal{M}, \mathrm{d}\mathcal{S}^2)$. The choice of the Laplace-Beltrami factor ordering renders the Wheeler-DeWitt equation invariant under coordinate transformations in minisuperspace, that is, the quantum theory does not depend on the choice of the minisuperspace coordinates. Note that this symmetry is already present at the classical level and it seems natural to regain it at the quantum level. The general covariance on $\mathcal{M}$ is not spoiled by adding a term proportional to $\mathcal{R}$. In $d = 2$ the Laplace-Beltrami and the conformal factor ordering coincide. In addition to the general covariance in minisuperspace the conformal factor ordering renders the kinetic term in the Wheeler-DeWitt equation covariant under conformal transformations of the minisuperspace DeWitt metric and a conformal rescaling of the wave function

$$\mathcal{G}_{AB} \mapsto \widetilde{\mathcal{G}}_{AB} := \Omega^2 \mathcal{G}_{AB} \quad \text{and} \quad \Psi \mapsto \widetilde{\Psi} := \Omega^{-\frac{d-2}{2}} \Psi \ . \tag{2.146}$$

where $\Omega : \ \mathcal{M} \to \mathbb{R}_+$. An object $\boldsymbol{\mathcal{T}}$ (e.g. a tensor or tensor density) that transforms as $\boldsymbol{\mathcal{T}} \to \widetilde{\boldsymbol{\mathcal{T}}} = \Omega^{w(\boldsymbol{\mathcal{T}})} \boldsymbol{\mathcal{T}}$ under conformal rescaling of the metric is now said to be conformally covariant with *conformal weight* $w(\boldsymbol{\mathcal{T}})$. In particular, we say that $\boldsymbol{\mathcal{T}}$ is conformally invariant if $w(\boldsymbol{\mathcal{T}}) = 0$. By definition $w(\mathrm{d}\mathcal{S}^2) = 2$ and $w(\Psi) = -(d-2)/2$. The square root of the determinant of the DeWitt metric transforms as $\sqrt{-\mathcal{G}} \mapsto \sqrt{-\widetilde{\mathcal{G}}} = \Omega^d\sqrt{-\mathcal{G}}$. The volume element on minisuperspace has therefore conformal weight $w(\star 1) = d$. Recall that a conformal rescaling of the DeWitt metric can be induced by a rescaling of the lapse function

$$N \mapsto \widetilde{N} = \Omega^2 N \ . \tag{2.147}$$

This induces a transformation of the Hamiltonian constraint into

$$\mathcal{H} \mapsto \widetilde{\mathcal{H}} = \frac{1}{2}\widetilde{\mathcal{G}}^{ij} p_i p_j + \widetilde{\mathcal{V}} \ , \tag{2.148}$$

where $\widetilde{\mathcal{V}} = \Omega^{-2}\mathcal{V}$. Consequently the minisuperspace potential is to be regarded as a scalar with conformal weight $w(\mathcal{V}) = -2$. The transformation law for the conformal Laplace-Beltrami operator is

$$\begin{aligned} &\Box - \xi_d\mathcal{R} = \Omega^{2-2p}\left(\widetilde{\Box} - \xi_d\widetilde{\mathcal{R}}\right)\Omega^{2p} \ , \quad \text{where} \\ &\widetilde{\mathcal{R}} = \Omega^{-2}\left[\mathcal{R} - 2(d-1)\frac{\Box\Omega}{\Omega} - (d-1)(d-4)\mathcal{G}^{AB}\frac{\partial_A\Omega\partial_B\Omega}{\Omega^2}\right] \ . \end{aligned} \tag{2.149}$$

Because of this transformation law, the conformal Laplace-Beltrami operator maps scalars with conformal weight $-\frac{d-2}{2}$ into scalars with conformal weight $-\frac{d-2}{2} - 2$ and we say that the operator carries the *conformal bi-weight*

$$w(\Box - \xi_d\mathcal{R}) = (w(\Psi) - 2, w(\Psi)) = \left(-\frac{d-2}{2} - 2, -\frac{d-2}{2}\right) \ . \tag{2.150}$$

The Wheeler-DeWitt equation then transforms as

$$\hat{\mathcal{H}}\Psi = \left(-\frac{1}{2}\left[\Box - \xi_d\mathcal{R}\right] + \mathcal{V}\right)\Psi = \left(-\frac{1}{2}\Omega^{2-2p}\left[\widetilde{\Box} - \xi_d\widetilde{\mathcal{R}}\right] + \Omega^{-2p}\mathcal{V}\right)\widetilde{\Psi} = \Omega^{2-2p}\ \hat{\widetilde{\mathcal{H}}}\widetilde{\Psi} \ . \tag{2.151}$$

Note that $\hat{\widetilde{\mathcal{H}}}\widetilde{\Psi} = 0$ is just the Wheeler-DeWitt equation obtained when applying the quantization procedure to the transformed Hamiltonian constraint $\widetilde{\mathcal{H}} = 0$. We conclude also that if Ψ is a solution to $\hat{\mathcal{H}}\Psi = 0$ then $\widetilde{\Psi}$ solves $\hat{\widetilde{\mathcal{H}}}\widetilde{\Psi} = 0$. In this sense, the conformal factor ordering renders the Wheeler-DeWitt equation truly independent of the choice of the lapse function N. The conformal covariance of the quantum formalism might therefore be regarded as a direct consequence of the time reparametrization invariance at the classical level. Furthermore, these considerations motivate us to regard the minisuperspace $\mathcal{M}$ as a *conformal manifold*, that is, a manifold equipped with a conformal equivalence class of metrics

$$\left[\mathrm{d}\mathcal{S}^2\right] := \left\{\Omega^2 \mathrm{d}\mathcal{S}^2 \mid \Omega : \mathcal{M} \to \mathbb{R}_+\right\} \ . \tag{2.152}$$

From now on, we shall call this equivalence class the (conformal) DeWitt metric. Based on this discussion, we should also think of the wave function as an equivalence class of pairs $[\mathrm{d}\mathcal{S}^2, \Psi]$.

Some issues regarding the conformal factor ordering were already discussed by Misner in [17] with the following conclusion: "*The choice of Δ_c rather than Δ, or some other second order operator, ... , is a decision on a quantum 'factor ordering' problem. In the mini examples we have so far considered the criterion of conformal invariance led to this decision, but further decisions to be resolved on some other basis will no doubt arise in more complex examples.*"

It seems that such a situation arises, in particular, when momentum constraints are present. In the next sections, we will only consider the cases with no additional constraint except for the Hamiltonian constraint $\mathcal{H}_0 \simeq 0$. The quantum implementation of the momentum constraints appears to be highly non-trivial and will be discussed at the end of this chapter in section 2.2.7.

Klein-Gordon current

The Wheeler-DeWitt equation is usually a hyperbolic Klein-Gordon type differential equation. If we allow for complex wave functions Ψ, we can consider the Klein-Gordon current

$$\begin{aligned} \boldsymbol{J}[\Psi_1, \Psi_2] &:= \frac{1}{2\mathrm{i}} \star (\Psi_1^* \mathrm{d}\Psi_2 - \Psi_2 \mathrm{d}\Psi_1^*) = J_A[\Psi_1, \Psi_2] \star \mathrm{d}q^A \ , \qquad \text{where} \\ J_A[\Psi_1, \Psi_2] &= \frac{1}{2\mathrm{i}} \ \Psi_1^* \overleftrightarrow{\partial}_A \Psi_2 \ := \frac{1}{2\mathrm{i}} \left[\Psi_1^*(\partial_A \Psi_2) - (\partial_A \Psi_1^*)\Psi_2\right]. \end{aligned} \tag{2.153}$$

The current is conserved in the sense that $\mathrm{d}\boldsymbol{J}[\Psi_1, \Psi_2] = 0$ if Ψ_1 and Ψ_2 are both solutions of the Wheeler-DeWitt equation. The current has the following properties:

- $\boldsymbol{J}[\Psi_1, \Psi_2] = -\boldsymbol{J}[\Psi_2^*, \Psi_1^*] = \boldsymbol{J}[\Psi_1, \Psi_2]^*$. Therefore the current is real.
- It is bi-linear: $\boldsymbol{J}[\Psi_1 + \Psi_2, \Psi_3] = \boldsymbol{J}[\Psi_1, \Psi_3] + \boldsymbol{J}[\Psi_2, \Psi_3]$ and $\boldsymbol{J}[\Psi_1, c\Psi_2] = c\boldsymbol{J}[\Psi_1, \Psi_2] = \boldsymbol{J}[c^*\Psi_1, \Psi_2]$.
- $J_A[\Psi_1, \Psi_2]$ has conformal weight $2 - d$. This implies that $\sqrt{-\mathcal{G}}\mathcal{G}^{AB}\Psi_1^* \overleftrightarrow{\partial}_B \Psi_2$ has conformal weight 0 and hence most importantly $w(\boldsymbol{J}) = 0$.

As we will see, the current $\boldsymbol{J}[\Psi, \Psi]$ can be interpreted as a quantum version of the classical flux $D \star \mathrm{d}\tau$, which is conserved along classical trajectories by construction of the van Vleck determinant.

2.2.3 The WKB-approximation and the semi-classical limit

As a starting point, we take the action $S = S_0 + S_\Phi$, where S_0 is the minisuperspace action and S_Φ is an action of matter field perturbations. This gives the full Hamiltonian

$$N\mathcal{H} = N(\mathcal{H}_0 + \mathcal{H}_\Phi) = 0 \tag{2.154}$$

where $N\mathcal{H}_0$ is the minisuperspace Hamiltonian and $N\mathcal{H}_\Phi$ is the Hamiltonian for the perturbations. We now quantize to obtain the Wheeler-DeWitt equation $\hat{\mathcal{H}}\Psi = (\hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_\Phi)\Psi = 0$ where

$$\hat{\mathcal{H}}_0 = -\frac{1}{2m_p^2}\left(\Box - \xi_d \mathcal{R}\right) + m_p^2 \mathcal{V} \ , \tag{2.155}$$

with $\Box_c := \Box - \xi_d \ {}_{\mathcal{G}}\mathcal{R}$ being the conformal Laplace-Beltrami operator. In order to perform the approximation, we have reinserted the Planck mass m_p in this section.[12] The Planck mass serves as a large parameter with respect to which the semiclassical expansion will be performed. In order to proceed we do a Born-Oppenheimer + WKB type ansatz:

$$\Psi(\mathbf{q}, \Phi] = \mathrm{e}^{\mathrm{i}m_p^2 S_0}\mathrm{e}^{\mathrm{i}S_1}\chi\left(\mathbf{q}, \Phi\right] + \mathcal{O}\left(m_p^{-2}\right) \ , \tag{2.156}$$

where m_p^2 serves as a large expansion parameter (ignoring the fact that m_p^2 has a dimension). We already anticipate here that $\chi\left(\mathbf{q}, \Phi\right]$ will be identified with the wave functional of the scalar field perturbations in the gravitational background. This is fully in the spirit of the Born-Oppenheimer approximation. We also assume in this section that we are always in the regions of $\mathcal{M}$ where the WKB-approximation is valid. After inserting the ansatz in the Wheeler-DeWitt equation one obtains at the two lowest orders:

$$\mathcal{O}\left(m_p^2\right) \ : \ \frac{1}{2}\mathcal{G}^{AB}(\partial_A S_0)(\partial_B S_0) + \mathcal{V}(\mathbf{q}) = 0 \ , \tag{2.157}$$

$$\mathcal{O}\left(m_p^0\right) \ : \ \left[-\mathrm{i}\ \mathcal{G}^{AB}(\partial_A S_0)\partial_B + \hat{\mathcal{H}}_\Phi\right]\chi = \left[\frac{\mathrm{i}}{2}\Box S_0 - \mathcal{G}^{AB}(\partial_A S_0)(\partial_B S_1)\right]\chi \ . \tag{2.158}$$

The first equation is just the Hamilton-Jacobi equation for the classical action S_0. By using the principle of constructive interference, it is then argued that one can construct wave

[12] More precisely, m_p is a parameter which is of the order of the Planck mass.

packets which are peaked over a classical configuration space trajectory [78].

It is reasonable to regard S_0 as a conformally invariant scalar, that is, $w(S_0) = 0$. The Hamilton-Jacobi equation (2.157) is then form invariant under conformal transformations. We now take care of equation (2.158). Note that no traces of $\mathcal{R}$ are to be found at this order. The Ricci scalar will first appear at the next order $\mathcal{O}(m_p^{-2})$. Recall, however, that Ψ is supposed to have conformal weight $w(\Psi)$. For consistency, all orders of the approximation should carry the same conformal weight. This now raises the question which term on the right hand side of (2.156) carries this conformal weight. It appears to be convenient to assume that it is fully contained in the term $\exp(\mathrm{i}S_1) = \exp(\mathrm{iRe}S_1 - \mathrm{Im}S_1)$. This means that $\mathrm{Im}S_1$ should transform as

$$\mathrm{Im}S_1 \mapsto \mathrm{Im}\widetilde{S}_1 = \mathrm{Im}S_1 - w(\Psi)\log\Omega\ . \tag{2.159}$$

Furthermore, it is convenient to introduce the WKB time τ by

$$\frac{\partial}{\partial\tau} := \mathcal{G}^{AB}(\partial_A S_0)\partial_B\ . \tag{2.160}$$

The vector $\frac{\partial}{\partial\tau}$ is orthogonal to the congruences of constant S_0 and tangential to the classical trajectories. The WKB time transforms under a conformal transformation as

$$\frac{\partial}{\partial\tau} \mapsto \frac{\partial}{\partial\widetilde{\tau}} = \Omega^{-2}\,\frac{\partial}{\partial\tau}\ , \tag{2.161}$$

i.e. $\frac{\partial}{\partial\tau}$ has conformal weight -2 while $\mathrm{d}\tau = (\partial_A S_0)\,\mathrm{d}q^A$ has conformal weight 0. With the definition of $\frac{\partial}{\partial\tau}$, equation (2.158) simplifies to

$$\left[-\mathrm{i}\frac{\partial}{\partial\tau} + \hat{\mathcal{H}}_\Phi\right]\chi = \left[\frac{\mathrm{i}}{2}\Box S_0 - \frac{\partial S_1}{\partial\tau}\right]\chi\ . \tag{2.162}$$

We now formally define a scalar product for the perturbations by

$$\langle\chi_1,\chi_2\rangle_{\mathbf{q}} = \int \mathcal{D}\Phi\ \chi_1^*\left(\mathbf{q},\Phi\right]\chi_2\left(\mathbf{q},\Phi\right]\ . \tag{2.163}$$

Having solved (2.157) and plugging the result in (2.158) we are left with too many unknown functions. In order to proceed, two assumptions have to be made:

- $\frac{\partial}{\partial\tau}\langle\chi,\chi\rangle_{\mathbf{q}} = 0$. This condition is obviously conformally invariant when we assign to χ the conformal weight 0.

- $\hat{\mathcal{H}}_\Phi$ is self-adjount with respect to the scalar product.

We now choose χ to be normalized, that is, $\langle\chi,\chi\rangle_{\mathbf{q}} = 1$, and take the scalar product of equation (2.158) with χ. The real and imaginary part of the resulting equation have to cancel independently. The imaginary part gives

$$\frac{\partial \mathrm{Im} S_1}{\partial \tau} = \frac{1}{2}\Box S_0 \tag{2.164}$$

while the real part gives

$$\mathrm{i}\frac{\partial \chi}{\partial \tau} = \left[\hat{\mathcal{H}}_\Phi + \frac{\partial \mathrm{Re} S_1}{\partial \tau}\right]\chi \ . \tag{2.165}$$

There is no condition left for fixing $\mathrm{Re}S_1$. It can, however, be transformed away. After redefining $\bar{\chi} = \mathrm{e}^{\mathrm{iRe}S_1}\chi$, we obtain now the functional Schrödinger equation for the scalar perturbations on a classical gravitational background

$$\mathrm{i}\frac{\partial}{\partial \tau}\bar{\chi} = \hat{\mathcal{H}}_\Phi \bar{\chi} \ . \tag{2.166}$$

Recall the transformation law for the Hamiltonian constraint. We deduce that for consistency we require that $\tilde{\hat{\mathcal{H}}}_\Phi \chi = \Omega^2 \hat{\mathcal{H}}_\Phi \chi$. The functional Schrödinger equation is then conformally covariant. Let us now discuss equation (2.164). After defining $D := \exp\left(-2\ \mathrm{Im}S_1\right)$, the equation becomes

$$\frac{\partial}{\partial \tau} D = -(\Box S_0) D \ . \tag{2.167}$$

This is now just the classical evolution equation for the van Vleck factor. The van Vleck factor has weight $w(D) = 2w(\Psi)$ and the defining equation (2.167) is conformally covariant.

Let us close this section by recapitulating. The solution to the Wheeler-DeWitt equation in the first order WKB + Born-Oppenheimer type approximation is given by

$$\Psi = \sqrt{D}\ \mathrm{e}^{\mathrm{i}m_p^2 S_0}\bar{\chi} + \mathcal{O}(m_p^{-2}) \ , \tag{2.168}$$

with S_0 being the classical Hamilton-Jacobi action and $\bar{\chi}$ being the wave functional for the scalar perturbations obeying the functional Schrödinger equation. D is the van Vleck factor, which carries all of the conformal weight of the wave function. The validity of the WKB approximation implies a strong correlation between position and momenta by $p_i = \frac{\partial S_0}{\partial q_i}$. In this sense we have recovered aspects of classical cosmology plus quantum field theory on the cosmological background. Note, however, that it is a widespread belief (see e.g. [78]) that the validity of the WKB-approximation on its own is not sufficient to ensure the emergence of classical physics. It is often argued that decoherence plays a crucial role in recovering classical gravity from the quantum theory [20, 21].

Let us also have a brief look at the Klein-Gordon current in the WKB approximation.

For simplicity we will disregard the matter perturbations (formally by setting $\chi = 1$) from now on. For the WKB mode functions $\Psi = \sqrt{D}\,\mathrm{e}^{\mathrm{i}m_p^2 S_0 + \mathcal{O}(m_p^{-2})}$ we obtain $|\Psi| = \sqrt{D} + \mathcal{O}(m_p^{-2})$ and

$$m_p^{-2} J^A[\Psi, \Psi]\partial_A = D\frac{\partial}{\partial\tau} + \mathcal{O}(m_p^{-2}) \tag{2.169}$$

In this sense the conformally invariant $(d-1)$-form $\boldsymbol{J}$ can be regarded as a quantum version of the classical conserved current $D\star\mathrm{d}\tau$. Recall that at the classical level this current did not depend on the gauge N. For a general wave packet Ψ we might thus be tempted to define the smeared out version of the WKB-time by

$$\frac{\partial}{\partial\tau[\Psi]} := \frac{J^A[\Psi, \Psi]}{(m_p|\Psi|)^2}\partial_A \ . \tag{2.170}$$

Note the intriguing property $\frac{\partial}{\partial\tau[\Psi^*]} = -\frac{\partial}{\partial\tau[\Psi]}$. We will not consider this object any further in this thesis. It would, however, be interesting to study the integral curves of $\frac{\partial}{\partial\tau[\Psi]}$ since one might think of them as quantum corrected trajectories.

2.2.4 Interpretation of the wave function of the universe

A Hilbert space structure would be desirable as it provides a straightforward probability interpretation. It is, however, an open question if a Hilbert space is needed at all in Quantum Gravity.

Klein-Gordon scalar product

A “natural” scalar product in minisuperspace is given by the Klein-Gordon scalar product. In order to construct it we foliate minisuperspace into “spacelike” hypersurfaces Σ_α of constant scale factor α. We define the scalar product on such hypersurfaces to be

$$(\Psi_1, \Psi_2)_{\mathrm{KG}} := \int\limits_{\Sigma_\alpha} \boldsymbol{J}\,[\Psi_1, \Psi_2] = \mathrm{i}\int\limits_{\Sigma_\alpha} (\partial_\alpha \lrcorner \star 1)\ \mathcal{G}^{\alpha i}\Psi_1^* \overleftrightarrow{\partial}_i \Psi_2 \ , \tag{2.171}$$

where $\boldsymbol{J}$ is the Klein-Gordon current. As can now be shown, this scalar product is invariant under coordinate transformations and deformations of the hypersurfaces Σ_α. Furthermore, the scalar product is invariant under conformal transformations of the DeWitt metric and conserved in “time”

$$\partial_\alpha\,(\Psi_1, \Psi_2)_{\mathrm{KG}} = 0 \ , \tag{2.172}$$

for $\Psi_{1/2}$ being solutions to the Wheeler-DeWitt equation. We have the usual problems that come with the Klein-Gordon scalar product. Firstly, $(.,.)_{\mathrm{KG}}$ is not positive definite.

We therefore have the problem of interpreting positive and negative "frequency" solutions. Furthermore, it is in general impossible to clearly separate positive and negative frequency modes [82]. Consequently the scalar product does not provide a clear probability interpretation. Recall that in the context of relativistic quantum theory this issue with the Klein-Gordon equation was resolved via second quantization. The Wheeler-DeWitt formalism, however, is already a second quantized theory. Performing now a second quantization would therefore actually correspond to a third quantization. This leads to some sort of multiverse picture [83] and we will not follow this path in this thesis.

The second problem with the use of the Klein-Gordon scalar product is, that it relies on the interpretation of the scale factor a as being a "time" variable. In some of the models (e.g. Kantowski-Sachs, Bianchi IX) physically reasonable solutions to the Wheeler-DeWitt equation satisfy $(\Psi, \Psi)_{\mathrm{KG}} = 0$. This should always be the case for recollapsing models as can be seen as follows: Physical reasonable wave packets are expected to be peaked over the classical trajectory. Hence we also expect that Ψ or any other physically relevant quantity constructed from Ψ approaches 0 as $a \to \infty$. From the conservation law $\partial_\alpha (\Psi, \Psi)_{\mathrm{KG}} = 0$ it follows then that $(\Psi, \Psi)_{\mathrm{KG}} = 0$ for all $\alpha \in \mathbb{R}$. In this sense the interpretation of the scale factor $a = \mathrm{e}^\alpha$ being a suitable "time" variable breaks down for recollapsing models.

We can conclude that the Klein-Gordon scalar product is in general not suitable for application in Quantum Cosmology. This does, however, not imply that the Klein-Gordon current is useless for our purposes. This point of view was also advocated by Vilenkin [84], who used it in particular for the formulation of boundary conditions.

Hawking-Page formula

Hawking apparently disregarded the usage of the Klein-Gordon current as a route to probability interpretation. One reason for this might be that wave packets which obey the Hartle-Hawking no-boundary condition are real and hence their Klein-Gordon current is identically zero. Instead Hawking and Page [79] assign to each WKB mode the momentum current

$$J_A = D \partial_A S_0 \ , \tag{2.173}$$

which coincides with the Klein-Gordon current of the WKB modes $\Psi = \sqrt{D} \mathrm{e}^{\mathrm{i} S_0}$. The probability $P(A)$ of finding the configuration of the universe in the region A in minisuperspace $\mathcal{M}$ is then taken to be

$$P(A) \propto \int_A \star |\Psi|^2 \ . \tag{2.174}$$

Now let $B \subset \mathcal{M}$ be a thin pencil that is drawn out by classical trajectories. In the region of minisuperspace where the WKB approximation is valid the contribution of B to the probability is given by

$$P(A \cap B) \propto \int_{A\cap B} \star|\Psi|^2 \approx \int_{A\cap B} \star D = F(B) \int N \mathrm{d}t \tag{2.175}$$

where we have used the relation (2.130) and defined the flux

$$F(B) := \int_{\Sigma_\tau \cap B} \boldsymbol{J} = \int_{\Sigma_\tau \cap B} J_A \star \mathrm{d}q^A \ . \tag{2.176}$$

The flux is independent of the choice of hypersurface $\Sigma_\tau \subset \mathcal{M}$. The contribution of B to $P(A)$ is therefore proportional to the coordinate-time that the classical solutions filling out the pencil B spend in the region A.

Note that in defining the probability $P(A)$ we have to pick out a gauge, by which we mean a representation of the DeWitt metric and a corresponding wave function. Under a conformal transformation $\sqrt{-\mathcal{G}}|\Psi|^2 \to \Omega^2\sqrt{-\mathcal{G}}|\Psi|^2$ and hence $\star|\Psi|^2$ is not conformally invariant, in other words

$$w(\star|\Psi|^2) = 2 \ . \tag{2.177}$$

This is nevertheless consistent and reflects the fact that $\mathrm{d}t$ depends of course on the gauge N. Hawking and Page [79] for example pick for their calculations the representation in which $\mathrm{d}t$ becomes the differential of the comoving time. Recall that the current $\boldsymbol{J}$ has weight $w(\boldsymbol{J}) = 0$ and thus $F(B)$ is conformally invariant.

In general $P(\mathcal{M})$ will not be finite. The Hawking-Page probability P might then only be useful for computing conditional probabilities, i.e. one is restricted to ask the right question. One possible question (extensively discussed in the lecture notes [78, 81]) is the probability for sufficient inflation for a given "initial" state of the wave function.

It is not clear if one can assign meaning to the Hawking-Page probability outside of the region in minisuperspace where the semi-classical approximation is valid.

2.2.5 Singularity avoidance

If we had a Hilbert space at hand we would also have a clear probability interpretation and hence a clear notion of singularity avoidance. This is, however, so far not the case and we have to rely on criteria that we can make us of without these notions.

The most prominent criterion for singularity avoidance is the DeWitt criterion also called the DeWitt boundary condition: *A singularity is said to be avoided if* $\Psi \to 0$ *in the vicinity* *of the classical singularity.* However, our discussion above shows up problems with this criterion. Since different representations of the wave function are related by $\widetilde{\Psi} = \Omega^{\frac{2-d}{2}}\Psi$ this criterion is not conformally invariant. When $d > 2$ it is in general not true that $\Psi \to 0$ is equivalent to $\widetilde{\Psi} \to 0$. Moreover, there does not seem to be a privileged representative of the wave function for the imposition of this criterion.

If we decided stick to the Hawking-Page probability interpretation we would use the following definition: *A singularity is said to be avoided if* $\star|\Psi|^2 \to 0$ *in the vicinity of the classical singularity.* But since $\star|\Psi|^2$ is not conformally invariant this criterion suffers from the same problem as the DeWitt criterion.

The following two criteria satisfy the demand to be invariant under both coordinate transformations and conformal transformations:

Criterion 1. *A singularity is said to be avoided if* $\boldsymbol{J}[\Psi, \Psi] \to 0$ *in the vicinity of the classical singularity.*

The problem with this criterion is that $\boldsymbol{J}[\Psi, \Psi] \equiv 0$ if Ψ is real. We remark that a similar criterion based, however, on the Schrödinger current was used in [85].

Criterion 2. *A singularity is said to be avoided if* $\star\,|\Psi|^{\frac{2d}{d-2}} \to 0$ *in the vicinity of the classical singularity.*

Note that $|\Psi|^{\frac{2d}{d-2}} \to |\Psi|^2$ as $d \to \infty$. Unlike criterion 1 the second criterion does not seem to suffer from any problems. The only issue that appears is that there is no clear physical interpretation of the quantity $\star\,|\Psi|^{\frac{2d}{d-2}}$.

Is it a problem, that the criteria 1 and 2 are formulated by using densities instead of usual scalars/tensors? We can for example compare the situation with the case of the non-relativistic wave function of a particle in a Coulomb potential in 3–dimensional Euclidean space. Here the wave function $\Psi(r, \vartheta, \varphi)$ and the square of its absolute value do not vanish value at $r = 0$. The probability density $\star|\Psi(r, \vartheta, \varphi)|^2 = |\Psi(r, \vartheta, \varphi)|^2 r^2 \sin(\vartheta) \mathrm{d}r \wedge \mathrm{d}\vartheta \wedge \mathrm{d}\varphi$, however, vanishes and implies a zero probability of the particle being at the singular point $r = 0$. This comparison suggests that the criteria should indeed be formulated in terms of densities.

Another criterion first proposed by Dąbrowski and Kiefer [24] states:

Criterion 3. *A wave packet is said to avoid the singularity if the wave packet spreads in the vicinity of the classical singularity.*

A spreading of the wave packets indicates the breakdown of the eikonal approximation and therefore the classical limit. The singularity theorems by Hawking and Penrose do then no longer apply. In the examples we consider in this work we shall see that wave packets spread close to the initial singularity if the dimension d of minisuperspace is larger than 2. The spreading can be linked to a decrease of the amplitude of Ψ which might lead to an avoidance of the singularity by both criteria 1 and 2. In particular the examples we consider later on give the impression that there is a correlation between the criteria 1 and 3.

Singularity avoidance in other approaches to Quantum Cosmology

Let us give a short overview over the status of singularity avoidance in other approaches to Quantum Cosmology.

Loop Quantum Cosmology (LQC) is the symmetry reduced minisuperspace version of Loop Quantum Gravity (LQG) [86]. It is often found in LQC that singularities are avoided by replacing them with a bounce. These results are mostly based on the effective quantum corrected equations of motion arising from LQC (see e.g. [87]). More rigorous results at the level of the full LQC equations are only known in the context of the isotropic models [88, 89]. The situation in LQC, however, seems to be anything but settled [13]. Other results [90] that take perturbations into account, for example, indicate that instead of a bounce a transition into an Euclidean regime takes place (similar to Hartle's and Hawking's no-boundary proposal).

In the Bohmian approach to Quantum Cosmology [91] the wave function of the Universe Ψ is interpreted as a pilot wave. This interpretation is universal in the sense that it can be applied to any approach to Quantum Cosmology. In the case of the Wheeler-DeWitt equation it can be applied as follows: The wave function is written as $\Psi = |\Psi|\mathrm{e}^{iS}$, with S being a real valued phase (in general this is not the Hamilton-Jacobi function). In addition to the Wheeler-DeWitt equation a guidance equation is postulated:

$$\dot{q}^A = \mathcal{G}^{AB}\partial_B S \ . \tag{2.178}$$

The momentum conjugate to q^A is then defined via $p_A = \mathcal{G}_{AB}\dot{q}^B = \partial_A S$.[13] It follows now from the Wheeler-DeWitt equation that the Bohmian dynamics are described by the quantum corrected Hamiltonian constraint

$$\mathcal{H}_\mathcal{Q} = \frac{1}{2}\mathcal{G}^{AB}p_A p_B + \mathcal{V} + \mathcal{Q} = 0 \ , \tag{2.179}$$

where $\mathcal{Q} = -\frac{1}{2}|\Psi|^{-1}(\Box - \xi\mathcal{R})|\Psi|$ is called the quantum potential. The quantum potential is

[13] We remark that this momentum coincides with the smeared out version of the WKB time $\frac{\partial}{\partial\tau[\Psi^*]}$ that we defined in .

thought of as a quantum correction to the classical potential. The presence of $\mathcal{Q}$ can lead to a bouncing scenario for the Bohmian trajectory $q^A(t)$. This feature is, however, not generic and it depends strongly on the choice of the wave packet Ψ.

Singularity avoidance was also studied in the context of gravitational collapse models. Quantization was performed for a reduced system describing the spherically symmetric collapse of a thin null dust shell [92]. This approach lead to a Schrödinger equation. As a direct consequence of the demand for a unitary time evolution of the quantum state it was found that the singularity was replaced by a bounce. Similar results were obtained for the marginally–bound Lemaître-Tolman-Bondi model [93], where the decoupling of the single dust shells allows to treat the dynamics of each single dust shell like a minisuperspace model. These results are also directly transferable to the Oppenheimer-Snyder model [94]. Bounces which lead to a Black hole to white hole transitions and to an accompanying avoidance of the singularity are also believed to occur in LQG. [95] offers a review on quantum bounces in the context of gravitational collapse.

Another approach to Quantum Cosmology is provided by the so-called *affine coherent state quantization*. This approach was for example employed in [96] and [97] where it was shown that it indeed leads to singularity avoidance in the case of the Bianchi IX model.

The authors of [85] studied the resolution of Big Bang type singularities in FLRW models filled with dust. To this end they used a criterion which is similar to the criterion 1 (vanishing of KG current) in this thesis, based, however, on the Schrödinger probability current. It was found that the singularity can be avoided for certain classes of factor orderings. The resolution of the singularity can be understood to be caused by a repulsive potential that is generated by a particular class of factor orderings.

We remark that in some of the above mentioned approaches it is often made use of the fact that matter acts as a clock. After quantization one can then obtain a Schrödinger type equation. This has the advantage that a clear probability interpretation emerges. One has, however, to deal with a multiple choice problem, that is, the choice of a clock is not unique and different choices lead to in-equivalent quantum theories [98].

The paper [99] employs a relational approach to quantization. This approach allows for the construction of a Hilbert space as well. By applying such a quantization to the Bianchi I model the author of [99] showed that the probability to reach the singularity was zero for a specific wave packet. The singularity is here replaced by a bounce as well.

The framework used in [100] yields effective quantum corrected dynamics based on a certain moment decomposition of the quantum state of the universe. It has been applied to the Bianchi I model. The results obtained there indeed indicate that the singularity is avoided.

2.2.6 Boundary conditions

Boundary conditions appear to be an important ingredient for Quantum Cosmology. The most prominent boundary conditions in this context are the no-boundary proposal of Hartle and Hawking [101] and the “tunneling” proposal of Vilenkin (see e.g. [102, 103] and the references in [103]). One of the scopes of these proposals is to specify a unique wave function of the universe. In the case of a Friedmann universe with a minimally coupled inflaton field, the two proposals select two different wave functions [78]. In this sense the two proposals lead to different predictions.

The boundary conditions stand of course in some relation to our discussion of singularity avoidance. The Hartle-Hawking proposal for example assumes in some sense from the outset that the singularity is avoided. Instead of hitting the singularity the universe enters a Euclidean regime in which time disappears due to a signature change in the metric. The proposal by Vilenkin states in a sense the opposite to our first criterion for singularity avoidance which demands that $\boldsymbol{J}[\Psi, \Psi] \to 0$ at the singular boundary of minisuperspace. Vilenkin's proposal in contrast demands that the Klein-Gordon current carries flux out at the singular boundaries.

Of some relevance in this thesis is the Hawking-Page boundary condition proposed in [79]. It requires that the wave function Ψ goes to zero in classically forbidden regions. The condition is often helpful to select physically reasonable wave functions out of the full solution space of the Wheeler-DeWitt equation. This is for example the case for a closed Friedmann model with a minimally coupled massless scalar field [10, 104]. In this example, the application of the Hawking-Page boundary condition leads to a matching of the expanding and recollapsing branches of wave packets. In this sense, the boundary condition selects solutions which are peaked over the entire classical trajectories instead of just one particular branch.

The demand for conformal covariance in this thesis poses issues for the Hawking-Page boundary conditions. This was indeed no problem in [10, 104], where the minisuperspace was 2–dimensional. In this case it made sense to impose boundary conditions on Ψ since the wave functions themselves are conformally invariant. In higher dimensional minisuperspaces, however, wave functions carry a non-vanishing conformal weight. The question then arises how to impose boundary conditions in a conformally invariant manner. A similar problem arises of course for Vilenkin's proposal when formulated in terms of the Klein-Gordon current 1-form $J_A \mathrm{d}q^A = \star^{-1}\boldsymbol{J}$ because it carries conformal weight $w(J_A \mathrm{d}q^A) = d-2$. The most naive way out of this would be of course to formulate boundary conditions in terms of conformally invariant quantities, that is for example, the Klein-Gordon current $\boldsymbol{J}[\Psi,\Psi]$ or the density $\star\,|\Psi|^{\frac{2d}{d-2}}$. In the case of the Klein-Gordon current, we encounter the usual issue that the criterion is not applicable in the case of real wave packets.

We will not attempt to give a full answer to the question of boundary conditions in this thesis. The models discussed in chapter 3 might nevertheless provide some hints on how boundary conditions are to be implemented in a conformally covariant framework.

2.2.7 Momentum constraints and conformal ordering

The ambitious goal of this section is to devise a generic quantization prescription for the full constrained system introduced in section 2.1.5 including the momentum constraints. The hope is then to finally apply the prescription to homogeneous cosmological models with and without additional matter degrees of freedom.

We saw that the conformal structure and the fact that Ψ carries a conformal weight is well compatible with the semi-classical approximation. Therefore we shall accept that the conformal structure is a fundamental pillar of Quantum Cosmology (at least for this section and the remaining parts of this thesis).

Another important aspect of the quantum theory is the Dirac consistency of the algebra of quantum operators [10]. What is the mathematical relation between the Dirac consistency and the existence of non-trivial solutions to the system of partial differential equations composed of the quantum constraint equations $\hat{\mathcal{H}}_\mu\Psi = 0$? Unfortunately we can only provide a partial answer to this question. For that purpose, ignore the momentum constraints for a moment. The global existence of solutions to the Wheeler-DeWitt equation might then simply follow by using the theorem in appendix A.1. Now ignore the Wheeler-DeWitt equation and only consider the system composed of the momentum constraints $\hat{\mathcal{H}}_i\Psi = 0$. Local existence results for this system might then be provided by the Frobenius theorem ((see Appendix A)). As a prerequisite the theorem requires the algebra of the operators $\hat{\mathcal{H}}_i$ to close. Is the closure of the full operator algebra $\hat{\mathcal{H}}_\mu$ a necessary condition for the existence of solutions? This question is unfortunately beyond the scope of this thesis. We will, nevertheless, assume that Dirac consistency is a fundamental ingredient for Quantum Cosmology and use it as a guiding principle in this section.

Before discussing the canonical quantization of the constraint system $\mathcal{H}_\mu = 0$, let us have a short interlude on the geometry of minisuperspace. In the following, we assume that the reader is familiar with the basics of Weylian geometry (see appendix B.3).

Interlude on the geometry of minisuperspace

The projection operators allow for a decomposition of the DeWitt metric according to

$$\mathrm{d}\mathcal{S}^2 = \bar{\mathcal{G}}_{AB}\mathrm{d}q^A \otimes \mathrm{d}q^B + \mathrm{d}\mathcal{S}^2 \mid_\Sigma \ . \tag{2.180}$$

The tensor $\bar{\mathcal{G}}_{AB}\mathrm{d}q^A\mathrm{d}q^B = \bar{P}_A{}^C\bar{P}_B{}^D\mathcal{G}_{CD}$ is called the *transverse metric* [76]. It constitutes a metric on the normal bundle. The induced metric on the leaves of the foliation Σ is given by

$$\mathrm{d}\mathcal{S}^2 \mid_\Sigma = \mathcal{G}_{ij}B^i \otimes B^j \ , \tag{2.181}$$

where the components of the induced metric are

$$\mathcal{G}_{ij} = A_i{}^A A_j{}^B \mathcal{G}_{AB} \tag{2.182}$$

in the (in general anholonomic) basis $\{\boldsymbol{A}_i\}$. The components of the inverse of the induced metric can be written as

$$\mathcal{G}^{ij} = \mathcal{G}^{AB}B_A{}^i B_B{}^j \ . \tag{2.183}$$

The components of the Levi-Civita connection on the leaves of the foliation are then given by

$$\Gamma^i_{kl} = \frac{1}{2}\mathcal{G}^{im}\left(A_l{}^A\partial_A\mathcal{G}_{mk} + A_k{}^A\partial_A\mathcal{G}_{ml} - A_m{}^A\partial_A\mathcal{G}_{kl}\right) + \frac{1}{2}\mathcal{C}^i_{kl} - \mathcal{G}^{kj}\mathcal{C}^m_{j(k}\mathcal{G}_{l)m} \ . \tag{2.184}$$

We shall simply denote the Levi-Civita connection on the leaves by ∇_i. We can then, for example, write

$$\mathcal{F}_{ij} = \nabla_i\lambda_j - \nabla_j\lambda_i \ . \tag{2.185}$$

Recall that this tensor was shortly studied in section 2.1.5. Under a conformal transformation, λ_i transforms as

$$\lambda_i \mapsto \widetilde{\lambda}_i = \lambda_i - A_i{}^A\partial_A \log\Omega, \tag{2.186}$$

in accordance to the transformation law of λ_i under rescalings of the lapse in the classical setup. The Weyl one-form λ_i allows us to construct a *conformal connection* on the leaves according to appendix B.3. The coefficients of the conformal connection are conformally invariant by construction . This construction allows us to differentiate conformally covariant tensors in a conformally covariant manner by introducing the so called scale covariant derivative $\mathcal{D}_i$ on the leaves of the foliation. We are now in the position to construct an intrinsic conformal geometry (say conformally covariant curvature tensors) on the leaves according to B.3.

Let us now turn to the *extrinsic curvature* of the leaves. For the definition of the extrinsic curvature tensor, we require a set of orthonormal vectors which are normal to the leaves of the foliation.[14] We denote these vectors by $\boldsymbol{e}_{\bar{i}} = e_{\bar{i}}{}^{A}\partial_A$, where $\bar{i}$ runs from 1 to $d - d_{\mathrm{mc}}$. The normalization condition demands that $\mathrm{d}\mathcal{S}^2\left(\boldsymbol{e}_{\bar{i}}, \boldsymbol{e}_{\bar{j}}\right) = \eta_{\bar{i}\bar{j}}$ where $\eta_{\bar{i}\bar{j}}$ is diagonal with eigenvalues ± 1. If the leaves of the foliation are spacelike then $\eta_{\bar{i}\bar{j}}$ has a Lorentzian signature. Note that normal vectors have by definition a conformal weight of $w(\boldsymbol{e}_{\bar{i}}) = -1$. Hence, their normalization is preserved under conformal transformations. We denote the orthonormal covectors dual to $\boldsymbol{e}_{\bar{i}}$ by $\boldsymbol{\vartheta}^{\bar{i}} = \vartheta_A{}^{\bar{i}}\mathrm{d}q^A$. The components are defined by $\vartheta_A{}^{\bar{i}} := \mathcal{G}_{AB}\eta^{\bar{i}\bar{j}}e_{\bar{j}}{}^{B}$. They satisfy the duality relation $\boldsymbol{e}_{\bar{i}} \lrcorner \boldsymbol{\vartheta}^{\bar{j}} = \delta_{\bar{i}}^{\bar{j}}$ and $\vartheta_A{}^{\bar{i}}e_{\bar{i}}{}^{B} = \bar{P}_A{}^{B}$. The conformal weight of the covectors is $w(\boldsymbol{\vartheta}^{\bar{i}}) = 1$. This renders the duality relation $\boldsymbol{e}_{\bar{i}} \lrcorner \boldsymbol{\vartheta}^{\bar{j}} = \delta_{\bar{i}}^{\bar{j}}$ conformally invariant.[15] The components of the extrinsic curvature tensor (see e.g. [105]) can then be obtained by using the *Weingarten equation*

$$\mathcal{K}^A{}_{ij} = A_{(i}{}^{B}A_{j)}{}^{C}\left(\nabla_B\vartheta_C{}^{\bar{i}}\right)e_{\bar{i}}{}^{A} \ . \tag{2.188}$$

For convenience we rewrite this equation as

$$\mathcal{K}^A{}_{ij} = -\left(A_{(i|}{}^{B}\nabla_B A_{|j)}{}^{C}\right)\bar{P}_C{}^{A} \ . \tag{2.189}$$

The extrinsic curvature tensor has the following properties:

- It satisfies $P^A{}_B\mathcal{K}^B{}_{ij} = 0$.
- It is symmetric in the last two indices, that is, $\mathcal{K}^A{}_{ij} = \mathcal{K}^A{}_{ji}$.
- Under a conformal transformation the extrinsic curvature tensor transforms as

$$\mathcal{K}^A{}_{ij} \mapsto \widetilde{\mathcal{K}}^A{}_{ij} = \mathcal{K}^A{}_{ij} + \mathcal{G}_{ij}\bar{P}^{AB}\partial_B \log\Omega \ . \tag{2.190}$$

The *mean curvature* vector is defined by tracing over the intrinsic indices of the extrinsic curvature tensor, that is,

$$\mathcal{K}^A := \mathcal{G}^{ij}\mathcal{K}^A{}_{ij} \ . \tag{2.191}$$

[14] An orthonormal set of vectors normal to the leaves can be constructed via the Gram-Schmidt process.

[15] We remark that with these definitions the metric tensor can be decomposed into

$$\mathrm{d}\mathcal{S}^2 = \eta_{\bar{i}\bar{j}}\boldsymbol{\vartheta}^{\bar{i}} \otimes \boldsymbol{\vartheta}^{\bar{j}} + \mathcal{G}_{ij}\boldsymbol{B}^i \otimes \boldsymbol{B}^j \ . \tag{2.187}$$

Under a conformal transformation it transforms as

$$\mathcal{K}^A \mapsto \widetilde{\mathcal{K}}^A = \Omega^{-2}\left(\mathcal{K}^A + d_{\mathrm{mc}}\bar{P}^{AB}\partial_B \log\Omega\right) \ . \tag{2.192}$$

This is indeed remarkable since this implies that

$$\boldsymbol{\varphi} := \left(\lambda_A - \frac{1}{d_{\mathrm{mc}}}\mathcal{K}_A\right) \mathrm{d}q^A \tag{2.193}$$

transforms like a Weyl one-form on $\mathcal{M}$. Furthermore, we note that the trace-free part of the extrinsic curvature,

$$\text{trace-free part of } \mathcal{K}^A{}_{ij} = \mathcal{K}^A{}_{ij} - \frac{1}{d_{\mathrm{mc}}}\mathcal{K}^A\mathcal{G}_{ij} \ , \tag{2.194}$$

is conformally invariant. Consequently, the tensor

$$\mathcal{T}_{AB} := \mathcal{K}_A{}^{ij}\mathcal{K}_{Bij} - \frac{1}{d_{\mathrm{mc}}}\mathcal{K}_A\mathcal{K}_B = \mathcal{G}^{ik}\mathcal{G}^{jl}(\text{tracefree part of } \mathcal{K}_{Aij})(\text{tracefree part of } \mathcal{K}_{Bkl}) \tag{2.195}$$

is conformally invariant as well. This further implies that the curvature scalar

$$\mathcal{T} := \mathcal{G}^{AB}\mathcal{T}_{AB} \tag{2.196}$$

is conformally covariant with $w(\mathcal{T}) = -2$.

If we project the Riemann tensor on $\mathcal{M}$ onto the leaves Σ, it splits according to the *Gauss equation* (see e.g. [105]) into

$$P_A{}^E P_B{}^F P_C{}^G P_D{}^H \mathcal{R}_{EFGH} = {}^{(\Sigma)}\mathcal{R}_{ABCD} - \mathcal{G}^{EF}\left(\mathcal{K}_{EAB}\mathcal{K}_{FCD} - \mathcal{K}_{EAD}\mathcal{K}_{FBC}\right) \ , \tag{2.197}$$

where ${}^{(\Sigma)}\mathcal{R}_{ABCD}$ is the induced Riemann tensor on the leaves of the foliation Σ.

Let us also consider again the condition $\left(\mathcal{L}_{\boldsymbol{A}_i}\mathcal{G}^{AB} - 2\lambda_i\mathcal{G}^{AB}\right)\bar{P}_A{}^C\bar{P}_B{}^D = 0$ which we imposed on the classical system in 2.1.5. As we will show in the following, this condition is, in fact, equivalent to the statement

$$\mathcal{L}_{\boldsymbol{A}_i}\bar{\mathcal{G}}_{AB} = -2\lambda_i\bar{\mathcal{G}}_{AB} \ . \tag{2.198}$$

Thus, $\boldsymbol{A}_i$ is a conformal Killing vector field with respect to the transverse metric $\bar{\mathcal{G}}_{AB}$.[16] Recall that equation (2.198) is canonical in the sense that it is independent of the choice

[16] If $\lambda_i = 0$, the transverse metric would be called bundle-like [76]. Equation (2.198) appears to be a conformally covariant generalization of this notion.

of basis $\{\boldsymbol{A}_i\}$ on $T\Sigma$. To show the equivalence of $\left(\mathcal{L}_{\boldsymbol{A}_i}\mathcal{G}^{AB} - 2\lambda_i\mathcal{G}^{AB}\right)\bar{P}_A{}^C\bar{P}_B{}^D = 0$ and $\mathcal{L}_{\boldsymbol{A}_i}\bar{\mathcal{G}}_{AB} = -2\lambda_i\bar{\mathcal{G}}_{AB}$, we need to show that $\mathcal{L}_{\boldsymbol{A}_i}\bar{\mathcal{G}}_{AB} = \bar{P}_A{}^C\bar{P}_B{}^D\mathcal{L}_{\boldsymbol{A}_i}\mathcal{G}_{CD}$. First, we note that $\mathcal{L}_{\boldsymbol{A}_i}P_A{}^B = -\mathcal{L}_{\boldsymbol{A}_i}\bar{P}_A{}^B$. Furthermore, it follows by direct calculation that

$$\mathcal{L}_{\boldsymbol{A}_i}P_A{}^B = \left(\mathcal{L}_{\boldsymbol{A}_i}B_A{}^j\right)A_j{}^B - B_A{}^j\mathcal{C}^k_{ij}A_k{}^B \ . \tag{2.199}$$

Hence, $\left(\mathcal{L}_{\boldsymbol{A}_i}P_A{}^C\right)\bar{P}_C{}^A = -\left(\mathcal{L}_{\boldsymbol{A}_i}\bar{P}_A{}^C\right)\bar{P}_C{}^A = 0$. As a direct consequence of this and the properties of the projection operators, it now also follows that $\mathcal{L}_{\boldsymbol{A}_i}\bar{P}_A{}^B = \left(\mathcal{L}_{\boldsymbol{A}_i}\bar{P}_A{}^C\right)P_C{}^B$. If we now apply the Leibniz rule, we get $\mathcal{L}_{\boldsymbol{A}_i}\bar{\mathcal{G}}_{AB} = \mathcal{L}_{\boldsymbol{A}_i}\left(\bar{P}_B{}^D\bar{P}^C_A\mathcal{G}_{CD}\right) = \bar{P}_A{}^C\bar{P}_B{}^D\mathcal{L}_{\boldsymbol{A}_i}\mathcal{G}_{CD}$.

The form of the quantum constraints

We are looking for an operator implementation of the Hamiltonian constraint $\hat{\mathcal{H}}_0$ and the momentum constraints $\hat{\mathcal{H}}_i$. We desire to implement the following properties:

1. All quantum constraint equations should be invariant under coordinate transformations in minisuperspace $\mathcal{M}$. This also means that the quantum theory should not depend on the choice of the basis on the leaves of the foliation. Hence, the quantum constraint equations should transform covariantly under a transformation of the basis on the tangent space to the leaves of the foliation,

$$\boldsymbol{A}_i \mapsto \widetilde{\boldsymbol{A}}_i = L_i{}^j\boldsymbol{A}_j \quad \text{where} \quad \{L_i{}^j\} : \mathcal{M} \to \mathrm{GL}(d_{\mathrm{mc}}, \mathbb{R}) \ . \tag{2.200}$$

   Note that this requirement can in some sense be viewed as an implementation of the invariance under transformations of the shift functions.

2. The operators are conformally covariant, when acting on wave functions of weight $w(\Psi)$. In particular, this means that they should have the conformal bi-weights

$$w(\hat{\mathcal{H}}_0) = (2 + w(\Psi), w(\Psi)) \quad \text{and} \quad w(\hat{\mathcal{H}}_i) = (w(\Psi), w(\Psi)) \ . \tag{2.201}$$

3. The quantum constraint algebra is Dirac consistent, that is,

$$\left[\hat{\mathcal{H}}_\mu, \hat{\mathcal{H}}_\nu\right]\Psi = \mathrm{i}\,\hat{\mathcal{C}}^\lambda_{\mu\nu}\left(\hat{\mathcal{H}}_\lambda\Psi\right) \ . \tag{2.202}$$

   The precise form of the structure operators $\hat{\mathcal{C}}^\lambda_{\mu\nu}$ has to be determined from the constraint operators. It might in addition be desirable that the quantum algebra is isomorphic to the classical algebra.

4. The quantum system should have a reasonable semi-classical limit.

We remark that a similar plan to ours was followed by the authors of [35] in the specific case of the vacuum Bianchi class A models. It was, indeed, found that the quantum algebra is isomorphic to the classical one. The authors, however, employed a different quantization procedure which requires a certain kind of reduction before quantization. We will try to follow a different route here.

One of the main conclusion we can draw from the discussion in section 2.1.5 and the interlude in this section is that the minisuperspace $\mathcal{M}$ comes equipped with a rich structure. Firstly, there is the conformal metric $[\mathrm{d}\mathcal{S}^2]$. Secondly, we have a foliation of $\mathcal{M}$ into the integral manifolds of the vector fields $\boldsymbol{A}_i$. Moreover, the integral manifolds are equipped with the Weyl one-form $\boldsymbol{\lambda}$, which together with the conformal metric, allows to construct a conformal connection on the integral manifolds. We have also learned that we can in principle combine $\boldsymbol{\lambda}$ with the mean curvature on the leaves $\mathcal{K}_A$ to obtain a Weyl structure on the whole minisuperspace manifold $\mathcal{M}$. This fact allows for the construction of several conformally covariant tensors and operators. Thus we have opened the door for numerous possibilities of constructing factor orderings which at least satisfy the requirements 1 and 2. The critical points, however, are the requirements 3 and 4. The hope is that these criteria finally select a factor ordering or at least constrain the possibilities. Moreover, it should be tested how the factor ordering performs when it is applied to the homogeneous cosmological models (with and without additional matter degrees of freedom).

Let $w(\Psi)$ be arbitrary for the moment. The question "What is the conformal weight of Ψ?" will be regarded as part of the factor ordering problem. We first deal with the quantum momentum constraints, which we implement as follows:

$$\hat{\mathcal{H}}_i\Psi = -\mathrm{i}\left(A_i{}^A\partial_A + w(\Psi)\lambda_i\right)\Psi = 0 \tag{2.203}$$

The operator $\left(A_i{}^A\partial_A + w(\Psi)\lambda_i\right)$ is the scale covariant derivative $\mathcal{D}_i$ acting on scalar fields of conformal weight $w(\Psi)$. Note that the operators $\hat{\mathcal{H}}_i$ have the required bi-weight via construction. Note also that via the chosen ordering $\hat{\mathcal{H}}_i$ satisfies requirement 2. We compute the commutator of the momentum constraints as follows

$$\left[\hat{\mathcal{H}}_i, \hat{\mathcal{H}}_j\right]\Psi = \left(\mathrm{i}\mathcal{C}^k_{ij}\hat{\mathcal{H}}_k + w(\Psi)\mathcal{F}_{ij}\right)\Psi\ . \tag{2.204}$$

Hence the requirement for Dirac consistency demands that either $\mathcal{F}_{ij} = 0$ or $w(\Psi) = 0$. The former is usually satisfied by the vacuum Bianchi models since we can find a representation in which all $\lambda_i = 0$. In particular $\boldsymbol{\lambda} = \lambda_i\boldsymbol{B}^i$ is closed. Note that the condition $\mathcal{F}_{ij} = 0$

is equivalent to the statement that the Weyl structure is integrable on each leave of the foliation. We will from now on always assume that $\mathcal{F}_{ij} = 0$. The Poincaré lemma then implies that λ is locally exact. Hence, we can locally always transform λ away via a conformal transformation.[17]

Let us now turn to the most critical point: The commutators between the momentum constraint operators and the quantum Hamiltonian constraint operator. Let us first elaborate on what we would expect if the algebra closes. We would wish to find that

$$\left[\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_i\right] \Psi = \mathrm{i}\hat{\mathcal{C}}^{\mu}_{0i} \left(\hat{\mathcal{H}}_\mu \Psi\right) = \mathrm{i}2\lambda_i \hat{\mathcal{H}}_0 \Psi + \mathrm{i}\,\hat{\mathcal{C}}^{j}_{0i} \left(\hat{\mathcal{H}}_i \Psi\right) \ . \tag{2.205}$$

We note that the operators $\left[\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_i\right] - 2\mathrm{i}\lambda_i \hat{\mathcal{H}}_0$ are conformally covariant with conformal bi-weight $(w(\Psi) - 2, w(\Psi))$. We can therefore conclude that the $\hat{\mathcal{C}}^{j}_{0i}$ are first order differential operators with conformal bi-weight $w(\hat{\mathcal{C}}^{j}_{0i}) = (w(\Psi) - 2, w(\Psi))$. This is in accordance with equations (2.101) and (2.114) and thus resembles the transformation rules of the classical constraint algebra. Consequently, we can write

$$\hat{\mathcal{C}}^{j}_{0i} = -\mathrm{i}\left(Z_i^{jA}\partial_A + z_i^j\right) \ , \tag{2.206}$$

where we require that the vector fields Z_i^{jA} are conformally covariant with $w(Z_i^{jA}) = -2$ while the scalars z_i^j have to transform according to $z_i^j \mapsto \widetilde{z}_i^j = \Omega^{-2}\left[z_i^j - w(\Psi) Z_i^{jA}\partial_A \log(\Omega)\right]$. We note that the divergence of a conformally covariant vector field transforms as

$$\nabla_A v^A \mapsto \widetilde{\nabla}_A \widetilde{v}^A = \Omega^{w(v)}\left(\nabla_A v^A + [d + w(v)]v^A \partial_A \log\Omega\right) \ . \tag{2.207}$$

We can therefore write z_i^j as

$$z_i^j = -\frac{w(\Psi)}{d-2}\nabla_A Z_i^{jA} + \text{a conformally covariant scalar with conformal weight -2}\ . \tag{2.208}$$

The ansatz (2.206) yields

$$\begin{aligned} &\mathrm{i}\hat{\mathcal{C}}^{j}_{0i}\left(\hat{\mathcal{H}}_j \Psi\right) = \\ &-\mathrm{i}\left[Z_i^{jA} A_j{}^B \nabla_A \partial_B + \left(\left[Z_i^{jA}\nabla_A + z_i^j\right] A_j{}^B + w(\Psi)\lambda_j Z_i^{jB}\right)\partial_B + w(\Psi)\left(Z_i^{jA}\partial_A + z_i^j\right)\lambda_j\right]\Psi \ . \end{aligned} \tag{2.209}$$

[17] A closed one form on Σ is globally exact if the first Betti number of Σ vanishes [106]. This would mean that the Weyl structure on the leaves is trivial. In particular, this allows us to find a conformal representation in which $\boldsymbol{\lambda} = 0$ and hence $\mathcal{C}^0_{0i} = 0$ holds globally on Σ.

Given an operator implementation of the Hamiltonian constraint $\hat{\mathcal{H}}_0$, our strategy for checking the Dirac consistency is as follows: we compute the commutator $\left[\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_i\right]$ and compare it to equation (2.209) we got from the ansatz (2.206). In particular, we obtain three equations: one by comparing terms in front of the second derivative operator operator $\nabla_A \partial_B$, a second one from terms in front of ∂_A and a third one from the remaining scalar part of the equation. It will be possible to solve the first equation for the vector fields Z_j^{iA}. The second equation can be split into two equations by employing the projection operators ${P_A}^B$ and ${\bar{P}_A}^B$. One equation then yields the scalars z_j^i. The other equation is a consistency condition.

These results should then be plugged into the third equation, which will finally yield a second consistency condition. Consequently, we expect the appearance of two consistency conditions. For the calculation, it is beneficial to keep in mind that these conditions should transform covariantly with respect to conformal transformations and the transformations (2.200). The first consistency condition is (symbolically) of the form $\text{Tensor}_i^B {\bar{P}_B}^A = 0$, while the second condition is of the form $\text{Tensor}_i = 0$.

Naive conformal ordering

The most naive way to implement the Hamiltonian constraint is to simply use the conformal ordering discussed 2.2.2. Let us now check if the conformally ordered Hamiltonian constraint operator, that is,

$$\hat{\mathcal{H}}_0 = -\frac{1}{2}\left(\Box - \xi_d \mathcal{R}\right) + \mathcal{V} \quad \text{and} \quad w(\Psi) = \frac{2-d}{2} \;, \tag{2.210}$$

satisfies our requirements. The requirements 1 and 2 are certainly satisfied. What remains is to check the Dirac consistency. The computation is rather lengthy and therefore transferred to the appendix C.1. We collect the results in the following.

Conclusion. *The quantum system of equations*

$$\begin{aligned} \hat{\mathcal{H}}_0 \Psi &= \left[-\frac{1}{2}\left(\Box - \xi_d \mathcal{R}\right) + \mathcal{V}\right] \Psi = 0 \;, \\ \hat{\mathcal{H}}_i \Psi &= -\mathrm{i}\left({A_i}^A \partial_A + w(\Psi)\lambda_i\right) \Psi = 0 \;, \end{aligned} \tag{2.211}$$

where $w(\Psi) = (2-d)/2$, is Dirac consistent if the three conditions

$$
\begin{aligned}
&1.)\quad \text{The Weyl structure on the leaves is integrable, that is } \mathcal{F}_{ij} = 2\nabla_{[i}\lambda_{j]} = 0 \ , \\
&2.)\quad \left[2\nabla_A\left(K_i^{D[A}P_D{}^{B]}\right) + 2w(\Psi)K_i^{BA}\lambda_A + \frac{1}{2}\nabla^B K_i\right]\bar{P}_B{}^C = 0 \ , \\
&3.)\quad w(\Psi)\left(Z_i^{jA}\partial_A + z_i^j\right)\lambda_j = -\frac{w(\psi)}{2}\Box\lambda_i - \xi_d\left(A_i{}^A\partial_A - \lambda_i\right)\mathcal{R} \ ,
\end{aligned}
\tag{2.212}
$$

are satisfied. The structure operators $\hat{\mathcal{C}}^\mu_{\nu\lambda}$ are then given by

$$
\begin{aligned}
&\hat{\mathcal{C}}^0_{0i} = \mathcal{C}^0_{0i} = 2\lambda_i \ , \\
&\hat{\mathcal{C}}^j_{0i} = -\mathrm{i}\left(Z_i^{jA}\partial_A + z_i^j\right) \ , \\
&\text{where } Z_i^{jA} = -K_i^{CD}B_D{}^j\left(P_C{}^A + 2\bar{P}_C{}^A\right) \\
&\text{and } z_i^j = \frac{1}{2}\nabla_A Z_i^{jA} + \frac{1}{2}(\nabla^A K_i)B_A{}^j - \left[\frac{1}{2}\nabla_A(K_i^{jk}A_k{}^A) - w(\Psi)K_i^{jk}\lambda_k\right] + Z_i^{kA}A_k{}^B\nabla_{[A}B_{B]}{}^j \\
&\hat{\mathcal{C}}^k_{ij} = -\left(A_i{}^A\nabla_A A_j{}^B - A_j{}^A\nabla_A A_i{}^B\right)B_B{}^k \ .
\end{aligned}
\tag{2.213}
$$

Remarks: All three conditions (2.212) are of course conformally covariant and they transform covariantly under the transformation $\boldsymbol{A}_i \mapsto \widetilde{\boldsymbol{A}}_i = L_i{}^j\boldsymbol{A}_j$. Unfortunately, we were not able to present these conditions in a more transparent form. Recall that $K_i^{AB} := \nabla^{(A}A_i{}^{B)} + \lambda_i\mathcal{G}^{AB}$.

Certain simplifications arise if we choose a representation $\mathrm{d}\mathcal{S}^2 \in [\mathrm{d}\mathcal{S}^2]$ in which all $\lambda_i = 0$ (recall that this representation exists if $\mathcal{F}_{ij} = 0$). In this gauge, the consistency conditions become

$$
\begin{aligned}
\nabla_A\left(\nabla^{(D}A_i{}^{[A)}P_D{}^{B]} + \frac{1}{4}\mathcal{G}^{AB}\nabla_D A_i{}^D\right)\bar{P}_B{}^C = 0 \ , \\
\xi_d A_i{}^A\partial_A\mathcal{R} = 0 \ .
\end{aligned}
\tag{2.214}
$$

At least the lower condition can now be easily interpreted geometrically. It is satisfied if $d = 2$ and/or $\mathcal{R}$ is constant on the leaves of the foliation.

In chapter 3, we will encounter certain problems with the naive ordering. In particular, it generates undesired terms in the case of the Bianchi IX model discussed in section 3.4.4. Due to the presence of theses terms the WKB approximation loses its validity in regions where we would expect it to be valid. In this sense the naive ordering violates the forth requirement. The ordering is certainly one of the simplest factor orderings that we can construct. So far, we we did not make much use of the rich geometrical structure of the minisuperspace in the construction of the ordering. In case there are no additional structures (e.g. momentum constraints or symmetries), the conformal ordering appears, however, to be the only option which has the chance to meet all four requirements.

Modified conformal ordering

Let us now consider another valid factor ordering. We make use of the fact that the DeWitt metric splits into

$$\mathrm{d}\mathcal{S}^2 = \bar{\mathcal{G}}_{AB}\mathrm{d}q^A \otimes \mathrm{d}q^B + \mathcal{G}_{ij}\boldsymbol{B}^i \otimes \boldsymbol{B}^j \ , \tag{2.215}$$

where $\bar{\mathcal{G}}_{AB} = \bar{P}_A{}^C \bar{P}_B{}^D \mathcal{G}_{AB}$ and $\mathcal{G}_{ij} = A_i{}^A A_j{}^B \mathcal{G}_{AB}$. We can then construct the following Wheeler-DeWitt equation

$$\hat{\mathcal{H}}_0\Psi = \left[-\frac{1}{2}\left(\bar{\Box} - \xi_{d-d_{\mathrm{mc}}}\bar{\mathcal{R}} + \mathcal{D}^2\right) + \mathcal{V}\right]\Psi = 0 \ . \tag{2.216}$$

We denote by $\bar{\nabla}$ the transverse Levi-Civita connection compatible with $\bar{\mathcal{G}}_{AB}\mathrm{d}q^A \otimes \mathrm{d}q^B$ and $\bar{\Box} = \bar{G}^{AB}\bar{\nabla}_A\bar{\nabla}_B = \bar{G}^{\bar{i}\bar{j}}\bar{\nabla}_{\bar{i}}\bar{\nabla}_{\bar{j}}$ is the transverse Laplacian operator. $\bar{\mathcal{R}}$ is the transverse Ricci scalar constructed from the transverse metric $\bar{\mathcal{G}}_{AB}\mathrm{d}q^A \otimes \mathrm{d}q^B$. The operator $\mathcal{D}^2$ is the conformal Laplacian (see B.3) on the leaves of the foliation. That is,

$$\mathcal{D}^2\Psi = \mathcal{G}^{ij}\mathcal{D}_i\mathcal{D}_j\Psi = \mathcal{G}^{ij}\mathcal{D}_i\left[\left(A_j{}^B\partial_B + w(\Psi)\lambda_j\right)\Psi\right] \ . \tag{2.217}$$

Setting now

$$w(\Psi) = \frac{2-(d-d_{\mathrm{mc}})}{2} \ , \tag{2.218}$$

renders the Wheeler-DeWitt equation conformally covariant. Imposing the momentum constraints $\hat{\mathcal{H}}_i\Psi = 0$ implies that the Wheeler-DeWitt equation reduces to

$$\hat{\mathcal{H}}_0^{(r)}\Psi := \left[-\frac{1}{2}\left(\bar{\Box} - \xi_{d-d_{\mathrm{mc}}}\bar{\mathcal{R}}\right) + \mathcal{V}\right]\Psi = 0 \ . \tag{2.219}$$

We call $\hat{\mathcal{H}}_0^{(r)}\Psi = 0$ the reduced Wheeler-DeWitt equation. The full Wheeler-DeWitt equation in the modified ordering (2.216) can then be written as

$$\left(\hat{\mathcal{H}}_0^{(r)} - \frac{1}{2}\mathcal{D}^2\right)\Psi = 0 \ . \tag{2.220}$$

Let us now consider the Dirac consistency of the factor ordering. We use the notation employed in appendix B.3, that is, we denote for example the conformal curvature tensor on the leaves of the foliation by $\mathcal{R}^i{}_{jkl}$ and so on. As a first step, we consider the commutator $[\mathcal{D}^2, \hat{\mathcal{H}}_k]$. Note that $[\mathcal{D}^2, \hat{\mathcal{H}}_k]\Psi$ is not conformally covariant. This is because $\hat{\mathcal{H}}_k$ has conformal bi-weight $w(\hat{\mathcal{H}}_k) = (w(\Psi), w(\Psi))$. But $w(\mathcal{D}^2) = (w(\Psi) - 2, w(\Psi))$. The term $\hat{\mathcal{H}}_k\left(\mathcal{D}^2\Psi\right)$ in the commutator is therefore not conformally covariant. However, the term

$$\left([\mathcal{D}^2, \hat{\mathcal{H}}_k] - 2\mathrm{i}\lambda_k \mathcal{D}^2\right)\Psi \tag{2.221}$$

is conformally covariant with weight -2. After using that $\mathcal{F}_{ij} = 0$, we obtain

$$[\mathcal{D}^2, \hat{\mathcal{H}}_k]\Psi = 2\mathrm{i}\lambda_k \mathcal{D}^2\Psi + \mathrm{i}\,\mathcal{D}^j\left(\mathcal{C}^i_{kj}\hat{\mathcal{H}}_i\ \Psi\right) + \mathrm{i}\,\mathcal{C}^i_{kj}\mathcal{D}^j\left(\hat{\mathcal{H}}_i\ \Psi\right) + \mathrm{i}\,\mathcal{R}_k{}^i\hat{\mathcal{H}}_i\Psi\ . \tag{2.222}$$

We can already conclude that if the system is Dirac consistent then $\hat{\mathcal{C}}^0_{0i} = \mathcal{C}^0_{0i} = 2\lambda_i$, as expected. Let us next turn our attention to the commutator $[\hat{\mathcal{H}}^{(r)}_0, \hat{\mathcal{H}}_k]$. The term

$$\left([\hat{\mathcal{H}}^{(r)}_0, \hat{\mathcal{H}}_k] - 2\mathrm{i}\lambda_k \mathcal{H}^r_0\right)\Psi \tag{2.223}$$

is conformally covariant with conformal weight -2. We conclude that we require that

$$\left([\hat{\mathcal{H}}^{(r)}_0, \hat{\mathcal{H}}_k] - 2\mathrm{i}\lambda_k \mathcal{H}^{(r)}_0\right)\Psi = \mathrm{i}\left(\hat{\mathcal{C}}^i_{0k} - \mathcal{R}_k{}^i\right)\hat{\mathcal{H}}_i\Psi - \mathrm{i}\,\mathcal{D}^j\left(\mathcal{C}^i_{kj}\hat{\mathcal{H}}_i\ \Psi\right) - \mathrm{i}\,\mathcal{C}^i_{kj}\mathcal{D}^j\left(\hat{\mathcal{H}}_i\ \Psi\right)\ . \tag{2.224}$$

The right hand side of this equation is weakly 0. Note that in the particular case when $\left([\hat{\mathcal{H}}^{(r)}_0, \hat{\mathcal{H}}_k] - 2\mathrm{i}\lambda_k \mathcal{H}^{(r)}_0\right)\Psi = 0$ the system is automatically Dirac consistent. This knowledge appears to be sufficient for any applications in the context of the Bianchi models. We remark, however, that the condition $\left([\hat{\mathcal{H}}^{(r)}_0, \hat{\mathcal{H}}_k] - 2\mathrm{i}\lambda_k \mathcal{H}^{(r)}_0\right)\Psi = 0$ is certainly a sufficient but not a necessary condition. This cannot be the case because the condition does not transform covariantly under transformations of the shift functions. One might acquire some deeper geometrical insights into the modified ordering by identifying the relevant terms inside the commutator $[\hat{\mathcal{H}}^{(r)}_0, \hat{\mathcal{H}}_k]$. We leave this issue for future studies.

Example: A simple toy model

We consider a simple 3–dimensional toy model, which is constructed to have similar features as the Bianchi models. The minisuperspace manifold is chosen to be $\mathcal{M} = \mathbb{R}\times\mathbb{R}\times S^1$ and we parametrize it via the variables $T, z \in \mathbb{R}$ and $\varphi \in [0, 2\pi]$. The DeWitt metric is defined by

$$\mathrm{d}\mathcal{S}^2 = -\mathrm{d}T^2 + \mathrm{d}z^2 + b^2(z)\mathrm{d}\varphi^2\ . \tag{2.225}$$

The function $b(z)$ should be sufficiently smooth and non zero but can be arbitrary apart from that. In addition, we introduce one momentum constraint defined by

$$\boldsymbol{A}_1 = \partial_\varphi\ . \tag{2.226}$$

The minisuperspace potential is chosen to be $\mathcal{V} = 0$. The constraints are then given by

$$\mathcal{H}_0 = \frac{1}{2}\left(-p_T^2 + p_z^2 + \frac{p_\varphi^2}{b^2(z)}\right) \simeq 0 \quad \text{and} \quad \mathcal{H}_1 = p_\varphi \simeq 0 \; . \tag{2.227}$$

We find that $\{\mathcal{H}_0, \mathcal{H}_1\} = 2\lambda_1 = 0$ and hence the constraint algebra closes. Moreover,

$$\{\mathcal{H}_0, p_z\} = -\frac{b'}{b^3} p_\varphi^2 \simeq 0 \quad \text{and} \quad \{\mathcal{H}_1, p_z\} = 0 \; , \tag{2.228}$$

that is the vector p_z is a constant of motion.

Let us now turn to the quantization of the system. Since $d = 3$ the conformal weight of the wave function is $w(\Psi) = 1/2$. We first consider the naive conformal ordering. The Ricci scalar of the model is given by

$$\mathcal{R} = -2b''(z)/b(z) \; . \tag{2.229}$$

Consequently, the quantum system of equations is given by

$$\begin{aligned} \hat{\mathcal{H}}_0\Psi &= \frac{1}{2}\left[\partial_T^2 - \partial_z^2 - \frac{b'(z)}{b(z)} - \frac{1}{b^2(z)}\partial_\varphi^2 - \frac{1}{4}\frac{b''(z)}{b(z)}\right]\Psi = 0 \; , \\ \hat{\mathcal{H}}_1\Psi &= -\mathrm{i}\partial_\varphi \Psi = 0 \; , \end{aligned} \tag{2.230}$$

The quantum constraint algebra is clearly Dirac consistent. The constraint $\hat{\mathcal{H}}_1\Psi = 0$ simply tells us that $\Psi = \Psi(T, z)$ is independent of φ and can be easily implemented. The "Wheeler-DeWitt equation" then becomes

$$\left[\partial_T^2 - \partial_z^2 - \frac{b'(z)}{b(z)} - \frac{1}{4}\frac{b''(z)}{b(z)}\right]\Psi = 0 \; . \tag{2.231}$$

The naive factor ordering has generated an undesired potential term $\mathcal{U}(z) := -\frac{b'(z)}{b(z)} - \frac{1}{4}\frac{b''(z)}{b(z)}$. While in the classical model the phase space function $f = p_z$ was a constant of motion, that is $\{f, \mathcal{H}_\mu\} \simeq 0$, the operator version $\hat{f} = -\mathrm{i}\partial_z$ satisfies $[\hat{f}, \hat{\mathcal{H}}_1]\Psi = 0$, but

$$[\hat{f}, \hat{\mathcal{H}}_0]\Psi = \mathrm{i}\left(\frac{b'}{b^3}\partial_\varphi^2 - \partial_z \mathcal{U}\right)\Psi \; . \tag{2.232}$$

Thus $\hat{f}$ is only a good quantum number if $\partial_z \mathcal{U} = 0$. We conclude that the naive conformal factor leads to a Dirac consistent quantum system. The quantization procedure spoiled, however, a symmetry that was present at the classical level.

Let us now consider the modified conformal ordering. Since $d - d_{\mathrm{mc}} = 2$ the wave function has now conformal weight $w(\Psi) = 0$. Furthermore, the transverse metric is (conformally) flat and the quantum system of equations now takes the much simpler form

$$\begin{aligned} \hat{\mathcal{H}}_0\Psi &= \frac{1}{2}\left[\partial_T^2 - \partial_z^2 - \frac{1}{b^2(z)}\partial_\varphi^2\right]\Psi = 0 \ , \\ \hat{\mathcal{H}}_1\Psi &= -\mathrm{i}\partial_\varphi\Psi = 0 \ . \end{aligned} \tag{2.233}$$

After implementing the constraint $\hat{\mathcal{H}}_1\Psi = 0$, the Wheeler-DeWitt equation simply becomes

$$\hat{\mathcal{H}}_0^{(r)}\Psi = \frac{1}{2}\left[\partial_T^2 - \partial_z^2\right]\Psi = 0 \ . \tag{2.234}$$

From the fact that $[\hat{\mathcal{H}}_0^{(r)}\,,\,\hat{\mathcal{H}}_1]\Psi = 0$ we conclude that the quantum system is Dirac consistent. Moreover, $\hat{f} = -\mathrm{i}\partial_z$ is now a good quantum number. In this aspect, the modified ordering performs better than the naive one in the example under consideration.

Concluding remarks

In the 3–dimensional toy model we just considered the application of the modified ordering preserved the symmetries of the classical model. The preservation of symmetries is an important issue in Quantum Cosmology. Recall that outer automorphism are symmetries of the Bianchi models which also generate homogeneity preserving diffeomorphisms. We can conclude that the quantization procedure should preserve these symmetries. Otherwise it would spoil the diffeomorphism invariance. The outer automorphism subgroup is generalized in our setup by the notion of the outer symmetry group. We recap from section 2.1.5: if $\boldsymbol{\xi} = \xi^A\partial_A$ is a generator of outer symmetries, then $f = \xi^A p_A$ is a classical constant of motion. We might then define an operator version of f as follows:

$$\hat{f}\Psi := -\mathrm{i}\left(\xi^A\partial_A + w(\Psi)\lambda_\xi\right)\Psi \ . \tag{2.235}$$

By construction the operator is conformally covariant with bi-weight $w(\hat{f}) = (w(\Psi), w(\Psi))$. The symmetry is preserved after quantization if $\hat{f}$ weakly commutes with all quantum constraints. That means that we can find a wave functions ψ_f such that

$$\hat{\mathcal{H}}_\mu\psi_f = 0 \quad \text{and} \quad \hat{f}\psi_f = f\psi_f \ , \tag{2.236}$$

where $f \in \mathbb{R}$ is a good quantum number that corresponds to the classical constant of motion. The following questions remain open in this thesis:

- What are the conditions such that symmetries are preserved after quantization?

- Can one design a quantization prescription which enforces the preservation of symmetries?

Regarding the last question: recall from section 2.1.5 that generators of outer symmetries are also foliate vector fields. If the algebra of all symmetries closes (this must in general not be the case) then the generators of symmetries define a distribution. This can be used for a construction analogous to the modified factor ordering (but with a higher dimensional distribution).

We remark that we did not exploit the vast possibilities of constructing factor orderings which meet at least the requirements 1 and 2. In particular the mean curvature $\mathcal{K}_A$ facilitates us to construct an infinite amount of alternatives to the ones already mentioned by making use of the Weyl vector defined by (2.193). Moreover, we might add any scalar with conformal weight -2 to the Hamiltonian constraint operator without spoiling the conformal covariance. Examples for such a tensors are the one defined by (2.196) and the conformal curvature scalar constructed in the appendix B.3.

Chapter 3

Models

3.1 Bianchi I

The Bianchi I universe might be regarded as the simplest anistropic cosmological model. It describes the temporal evolution of homogeneous three spaces admitting the isomotry group $\mathbb{R}^3$ of spatial translations. Its structure constants are all identically zero, $C^i_{jk} = 0$. Hence the special automorphism group is $S\mathrm{Aut}(\mathfrak{g}) = SL(3, \mathbb{R})$ and all automorphisms are outer automorphism. Consequently all momentum constraints are trivially satisfied in the vacuum case.

For simplicity we will first focus on the diagonal Bianchi I model in this section. Note that this section has overlap with our publication [T3].

3.1.1 Metric and action for the diagonal model

The diagonal Bianchi I metric is given by

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + a_x^2\mathrm{d}x^2 + a_y^2\mathrm{d}y^2 + a_z^2\mathrm{d}z^2 \ , \tag{3.1}$$

where a_i can be interpreted as directional scale factors. The relation to the Misner variables is given by the following relations

$$a = \sqrt[3]{a_x a_y a_z} = \mathrm{e}^{\alpha} \ , \quad a_x/a = \mathrm{e}^{\beta_+ + \sqrt{3}\beta_-} \ , \quad a_y/a = \mathrm{e}^{\beta_+ - \sqrt{3}\beta_-} \ , \quad a_z/a = \mathrm{e}^{-2\beta_+} \ . \tag{3.2}$$

If we set the factor $\frac{3}{4\pi G}\int \mathrm{d}^3x = 1$ the action becomes

$$S = \frac{1}{2}\int \mathrm{d}t \left[-\frac{a\dot{a}^2}{N} + \frac{a^3}{N}\left(\dot{\beta}_+^2 + \dot{\beta}_-^2\right)\right] = \frac{1}{2}\int \mathrm{d}t \ \frac{\mathrm{e}^{3\alpha}}{N}\left(-\dot{\alpha}^2 + \dot{\beta}_+^2 + \dot{\beta}_-^2\right) \ . \tag{3.3}$$

The Lagrangian has exactly the same form as the Lagrangian of a flat Friedmann universe with two minimally coupled homogeneous massless scalar fields. Note that under the rescaling $a \to c\, a$, where $c \in \mathbb{R}$, the Lagrangian transforms as $L \to c^3 L$. Consequently $a \to ca$ maps solutions into solutions. If matter is added to the system, this symmetry will be broken in most cases. The gravitational Hamiltonian as obtained from the above action reads

$$H = \frac{N e^{-3\alpha}}{2} \left(-p_\alpha^2 + p_+^2 + p_-^2 \right) = N\mathcal{H} \ . \tag{3.4}$$

In configuration space the Hamiltonian constraint equation is given by

$$-\dot{\alpha}^2 + \dot{\beta}_+^2 + \dot{\beta}_-^2 = 0 \ . \tag{3.5}$$

3.1.2 Kasner solution

Note that β_+ and β_- are cyclic; this implies that

$$p_+ = \frac{e^{3\alpha}}{N} \dot{\beta}_+ = constant \quad \text{and} \quad p_- = \frac{e^{3\alpha}}{N} \dot{\beta}_- = constant. \tag{3.6}$$

A translation in the anisotropy factors is an outer automorphism. It is related to a homogeneity preserving diffeomorphism that corresponds to a constant rescaling of the coordinates. For example the translation $(\beta_+, \beta_-) \mapsto (\beta_+ + c/2, \beta_- + c/(2\sqrt{3}))$ corresponds to the rescaling $(x, y, z) \mapsto (e^c x, y, z)$. The symmetries are still present if we add matter fields that do not couple directly to the anisotropy factors, for example scalar fields or ideal fluids.

Time dependence in comoving gauge

When we plug the constants of motion (3.6) into the Hamiltonian constraint (3.5) we obtain

$$\dot{a}^2 = \frac{N^2}{a^4} \left(p_+^2 + p_-^2 \right) \ . \tag{3.7}$$

In the comoving gauge $N = 1$ and if $p_+^2 + p_-^2 \neq 0$ this is solved by

$$a(t) = \sqrt[3]{\sqrt{p_+^2 + p_-^2}\,(t - t_0)} \ , \quad \beta_\pm(t) = \frac{p_\pm}{3\sqrt{p_+^2 + p_-^2}} \ln(t - t_0) + C_\pm \ . \tag{3.8}$$

For the case $p_+ = 0 = p_-$ the solution is just the Minkowski space. In the literature the Kasner metric is often given in the form

$$ds^2 = -dt^2 + t^{2p_x} dx^2 + t^{2p_y} dy^2 + t^{2p_z} dz^2 \ , \tag{3.9}$$

where the relation between the momenta is given by

$$p_x = \frac{1}{3}\left(1 + \frac{p_+ + \sqrt{3}p_-}{\sqrt{p_+^2 + p_-^2}}\right) \ , \quad p_y = \frac{1}{3}\left(1 + \frac{p_+ - \sqrt{3}p_-}{\sqrt{p_+^2 + p_-^2}}\right) \ ,$$
$$p_z = \frac{1}{3}\left(1 - \frac{2p_+}{\sqrt{p_+^2 + p_-^2}}\right) \ . \tag{3.10}$$

As it can be easily verified the momenta satisfy

$$p_x^2 + p_y^2 + p_z^2 = 1 \quad \text{and} \quad p_x + p_y + p_z = 1 \ . \tag{3.11}$$

Note that the two equations define the intersection of a plane and a sphere (see figure 3.1). Therefore the momenta are constrained to lie on a circle, the so-called Kasner circle. If two of the p_i's are positive/negative, the other one must have the opposite sign. An isotropic expansion is therefore impossible without the coupling of any additional matter fields.

The Kasner circle can be parametrized by the single variable $u \in \mathbb{R}$ called the Lifshitz-Khalatnikov parameter. The parametrization reads

$$p_x = -\frac{u}{1 + u + u^2} \ , \quad p_y = \frac{1 + u}{1 + u + u^2} \ , \quad p_z = \frac{u(1 + u)}{1 + u + u^2} \ . \tag{3.12}$$

The nature of the singularity at $t \to 0$ depends on the value of the coefficients p_x, p_y, p_z. If one of them is equal to 1, the Kasner solution becomes the Milne universe which is diffeomorphic to slices of the Minkowski spacetime. The singularity is then only a coordinate singularity. For all other values, the singularity is physical, which is indicated by the divergence of the Kretschmann invariant $R_{\mu\nu\lambda\sigma}R^{\mu\nu\lambda\sigma}$. Since $R_{\mu\nu} = 0$, the curvature singularity is a pure Weyl singularity. If we use the u–parametrization of the Kasner circle, we find that

$$C_{\mu\nu\lambda\sigma}C^{\mu\nu\lambda\sigma} = \frac{16(1 + u)^2 u^2}{(1 + u + u^2)t^4} \ . \tag{3.13}$$

Note that the Weyl squared scalar satisfies $C_{\mu\nu\sigma\lambda}C^{\mu\nu\sigma\lambda} \geq 0$. It is identically zero for the values $u = -1, 0, -\infty, \infty$ which are the Milne universe. For all other values of u the scalar blows up as $t \to 0$.

Configuration space trajectory

When parametrized by the variables α, β_+ and β_-, the Kasner solutions follow straight lines in configuration space. This becomes clear by considering the form of the gravitational action (3.3) when we use the quasi-Gaussian gauge $N = \mathrm{e}^{3\alpha}$. The equations of motion will then

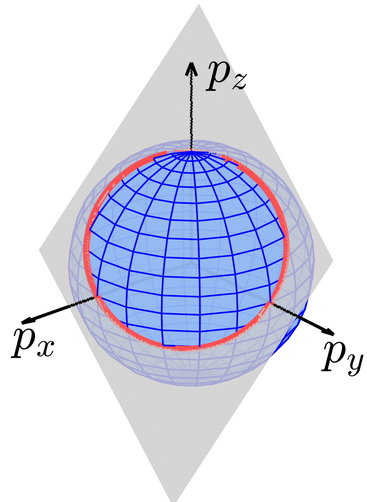


Figure 3.1: Intersection of the Kasner sphere and the Kasner plane. Allowed values of p_x, p_y and p_z lie on the red Kasner circle. The circle crosses the axes at the points $(1, 0, 0)$, $(0, 1, 0)$ and $(0, 0, 1)$. These points correspond to Milne universes (diffeomorphic to slices of the Minkowski spacetime).

reduce to those of a free relativistic particle in 2+1 dimensions. The Hamiltonian constraint (3.5) tells us that this particle is massless. Hence the solutions are just given by

$$\begin{aligned} \alpha(t) &= \pm\sqrt{p_+^2 + p_-^2}(t - t_0) \\ \beta_\pm(t) &= p_\pm(t - t_0) + C_\pm \ , \end{aligned} \tag{3.14}$$

where $C_\pm \in \mathbb{R}$ are arbitrary constants, which can be absorbed into the coordinates. When approaching the singularity , i.e. $t \to \mp\infty$, we have that

$$a = \mathrm{e}^\alpha \to 0 \quad \text{and} \quad \beta_\pm \ \to \begin{cases} \operatorname{sgn}(p_\pm)\ \infty & \text{if } p_\pm \neq 0 \\ C_\pm & \text{otherwise} \end{cases} . \tag{3.15}$$

It depends on the values of the momenta $p_\pm$ if the universe collapses into a line (cigarlike singularity or a plane (disclike singularity). If we set $p_- = 0$ for example we obtain a cylindrically symmetric sub case. The universe then collapses into a plane if $p_+ > 0$ and into a line if $p_+ < 0$.

Since the dynamics of the universe point resembles the dynamics of a free massless relativistic particle and there is no potential term in the action, the approach to the singularity is called velocity term dominated (VTD). The Bianchi I vacuum model is an important example since in many other homogeneous models it might turn out that in the vicinity of the initial singularity the curvature and matter potentials might become negligible as the three volume goes to zero. In this region the dynamics are well approximated by the dynamics of the Kasner model. In such a case the approach to the singularity is referred to as asymptotically velocity term dominated (AVTD).

Quantum Kasner solution

The DeWitt metric is conformally flat. A representative $\mathrm{d}\mathcal{S}^2 \in [\mathrm{d}\mathcal{S}^2]$ and the corresponding volume form are given by

$$\begin{aligned} \mathrm{d}\mathcal{S}^2 &= \mathrm{e}^{3\alpha}\left(-\mathrm{d}\alpha^2 + \mathrm{d}\beta_+^2 + \mathrm{d}\beta_-^2\right) \ , \\ \star 1 &= \mathrm{e}^{9\alpha/2}\mathrm{d}\alpha \wedge \mathrm{d}\beta_+ \wedge \mathrm{d}\beta_- \ . \end{aligned} \tag{3.16}$$

This representatives corresponds to the comoving gauge $N = 1$. After quantizing the constraint (3.4) we obtain the Wheeler-DeWitt equation

$$\hat{\mathcal{H}}\Psi = 0 \tag{3.17}$$

where the Hamiltonian constraint operator is given by

$$\hat{\mathcal{H}} = \frac{\hbar^2 \mathrm{e}^{-3\alpha}}{2}\left[\frac{\partial^2}{\partial\alpha^2} + 2f\frac{\partial}{\partial\alpha} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2} + \xi\mathcal{R}\mathrm{e}^{3\alpha}\right] \ . \tag{3.18}$$

The parameters f and ξ control the factor ordering which is partially left open for the moment. The Ricci scalar computed from the representative $\mathrm{d}\mathcal{S}^2$ reads

$$\mathcal{R} = \frac{9}{2}\mathrm{e}^{-3\alpha} \ . \tag{3.19}$$

For $f = \frac{3}{4}$, $\xi = 0$ one obtains the Laplace-Beltrami factor ordering. If we set $\xi = \xi_3 = 1/8$ instead , we obtain the conformal factor ordering. Note that independently of f and ξ the Hamiltonian constraint operator $\hat{\mathcal{H}}$ commutes with the momentum operators $\hat{p}_\pm = \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial\beta_\pm}$ and therefore their eigenvalues are good quantum numbers which we identify with the classical constants of motion $p_\pm$. We set $\hbar = 1$ in the following. After rescaling $\Psi =: \mathrm{e}^{-f\alpha}\ \widetilde{\Psi}$ the Wheeler-DeWitt equation simplifies to

$$\left[-\frac{\partial^2}{\partial\alpha^2} + \frac{\partial^2}{\partial{\beta_+}^2} + \frac{\partial^2}{\partial{\beta_-}^2} + f^2 - \frac{9}{2}\xi\right]\widetilde{\Psi} = 0 \ . \tag{3.20}$$

The equation is now just a Klein-Gordon equation with a "mass" $\sqrt{9\xi/2 - f^2}$. The "mass" vanishes for the conformal factor ordering while for the pure Laplace-Beltrami factor ordering it becomes imaginary. Solutions of the Wheeler-DeWitt equation in the Laplace-Beltrami factor ordering can therefore develop tachyonic behavior. Note that the "mass" squared term would be $\mathcal{O}(\hbar^2)$ if we re-insert the Planck constant. It is ad hoc not clear to us if the appearance of such "mass" squared terms is a feature or a failure in the quantum theory. We will regard it here as a failure and interpret the absence of the mass squared term as an argument in favor of the conformal factor ordering.

Wheeler-DeWitt equation in conformal factor ordering In the conformal factor ordering ($f = 3/4$ and $\xi = 1/8$) the Wheeler-DeWitt equation becomes the classical wave equation in $1+2$ dimensions

$$\left[\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2}\right]\widetilde{\Psi} = 0 \ , \tag{3.21}$$

The equation is now "massless" and the conformal factor ordering, hence, resolves the issues that appear when using for example the pure Laplace-Beltrami factor ordering. The transformation $\Psi \mapsto \widetilde{\Psi}$ we performed is to be understood as a conformal transformation. We now work in the representation in which the DeWitt metric is flat. This corresponds to the Taub gauge $N = \mathrm{e}^{3\alpha}$. The solutions can now be written as a mode expansion

$$\widetilde{\Psi}\left(\alpha,\beta_+,\beta_-\right) = \sum_{\sigma=\pm}\int\limits_{-\infty}^{\infty}\mathrm{d}p_+\int\limits_{-\infty}^{\infty}\mathrm{d}p_-\ \mathcal{A}_\sigma\left(p_+,p_-\right)\widetilde{\psi}^{\sigma}_{p_+,p_-}\left(\alpha,\beta_+,\beta_-\right)\ , \tag{3.22}$$

where the set of positive and negative frequency plane wave mode functions are given by

$$\widetilde{\psi}^{\pm}_{p_+,p_-}\left(\alpha,\beta_+,\beta_-\right) = \exp\left(\pm\mathrm{i}\sqrt{p_+^2+p_-^2}\ \alpha - \mathrm{i}p_+\beta_+ - \mathrm{i}p_-\beta_-\right)\ . \tag{3.23}$$

The amplitudes $\mathcal{A}_\pm$ are to be regarded as a distributions in momentum space. Note that a necessary condition for the existence of the integral in (3.22) is $\mathcal{A} \in \mathcal{L}_1\left(\mathbb{R}^2, \mathrm{d}p_+\mathrm{d}p_-\right)$. The plane wave mode functions (3.23) reflect the VTD behavior of the Bianchi I model. If a classical model has AVTD behavior, we can in general expect that such a plane wave mode expansion is always possible in the vicinity of the singularity.

Note that the mode functions are in WKB-form, that is, the WKB-approximation $\widetilde{\psi}^{\pm}_{p_+,p_-} = \widetilde{D}^{\frac{1}{2}}\,\mathrm{e}^{\mathrm{i}S_0}$ with S_0 satisfying the Hamilton-Jacobi equation and the Vleck factor being a constant

$\widetilde{D} = 1$ is exact in this case. The WKB-time vector field obtained from the modes reads

$$\frac{\partial}{\partial \widetilde{\tau}} = \mp\sqrt{p_+^2 + p_-^2}\frac{\partial}{\partial \alpha} + p_+\frac{\partial}{\partial \beta_+} + p_-\frac{\partial}{\partial \beta_-} \ . \tag{3.24}$$

Its integral curves as parametrized by WKB time are clearly the classical solutions

$$\alpha(\widetilde{\tau}) = -\sqrt{p_+^2 + p_-^2}\,\widetilde{\tau} + C_\alpha \ , \quad \beta_+(\widetilde{\tau}) = p_+\widetilde{\tau} + C_+ \ , \quad \beta_-(\widetilde{\tau}) = p_-\widetilde{\tau} + C_- \tag{3.25}$$

as expected. Note that in this case the WKB time $\widetilde{\tau}$ coincides with the coordinate time in the quasi-Gaussian gauge. This is the case exactly because we chose to do calculations in the representation in which the DeWitt metric is flat. This representation corresponds to the gauge $N = \mathrm{e}^{3\alpha}$.

We now choose the amplitudes

$$\mathcal{A}_+\left(p_+, p_-\right) = \frac{1}{2\pi\Delta p_+\Delta p_-}\exp\left(-\frac{\left[p_+ - p_{+,0}\right]^2}{2\Delta p_+^2} - \frac{\left[p_- - p_{-,0}\right]^2}{2\Delta p_-^2}\right) \ , \quad \mathcal{A}_-\left(p_+, p_-\right) = 0 \tag{3.26}$$

and assume that $\mathcal{A}_+$ is sharply peaked, i.e. Δp_+, $\Delta p_- \ll 1$. In addition we assume that $p_{+,0}$ and $p_{+,0}$ are sufficiently large such that we can approximate

$$\sqrt{p_+^2 + p_-^2} \approx \frac{p_{+,0}\ p_+ + p_{-,0}\ p_-}{\sqrt{p_{+,0}^2 + p_{-,0}^2}} \tag{3.27}$$

under the integral in (3.22). We can now evaluate the wave packet approximately as

$$\begin{aligned}\widetilde{\Psi}\left(\alpha, \beta_+, \beta_-\right) \approx\ & \exp\left(-\frac{1}{2\Delta\beta_+^2}\left[\frac{p_{+,0}\ \alpha}{\sqrt{p_{+,0}^2 + p_{-,0}^2}} - \beta_+\right]^2\right) \\ & \times\exp\left(-\frac{1}{2\Delta\beta_-^2}\left[\frac{p_{-,0}\ \alpha}{\sqrt{p_{+,0}^2 + p_{-,0}^2}} - \beta_-\right]^2\right) \ ,\end{aligned} \tag{3.28}$$

where $\Delta\beta_\pm = \frac{1}{\Delta p_\pm}$. The wave packet (3.28) represents now a Gaussian which is broadly peaked about one of the classical trajectories. As an artifact of the approximation (3.27), no spreading/decay of wave packets can be seen. This is because we replaced the non-linear dispersion relation by a linear one. As we shall argue in the following, spreading and decay will inevitably occur for reasonable wave packet and large enough $|\alpha|$; hence the approximation we employed here loses its validity. However, the larger $p_{+,0}$ and $p_{-,0}$ and the smaller Δp_+ and Δp_- the better the approximation will be (at least in some region of the minisuperspace).

We should therefore expect broadly peaked wave packets with large momentum to spread slower than sharply peaked wave packets with a lower momentum. Plots of a wave packet for which the approximation breaks down are shown in figure 3.2.

Singularity avoidance

Note that $\widetilde{\psi}_{p_+,p_-}$ does not approach zero as $\alpha \to -\infty$. Rather the limit is not well defined and all modes have an essential singularity at this point. The vanishing of the mode functions, however, is a sufficient but not a necessary criterion for the vanishing of the wave packets $\widetilde{\Psi}$ obtained by smearing out the mode functions.

We know that solutions to the $d = 1 + 1$ dimensional classical wave equation will not decay. If we give, for example, a Gaussian initial condition on a infinitely long and friction less violin string and let it evolve in time, we would see two Gaussian wave packets moving out in opposite directions. These wave packets would not decay in time and instead preserve their shape. In our case such a wave packet would run straight into the singularity. If we, however, go to higher dimensions $d > 2$, the situation changes. Now wave packets can propagate in infinitely many directions (Huygen's principle). This leads to a spreading of wave packets which is accompanied by a decay of the amplitude $|\Psi|$. In our case that means that a wave packet can never reach the singular boundary $\alpha \to -\infty$. Our statements can now be made more precise in the form of so called local decay rate estimates (see e.g. [107]). For the case of the Kasner quantum solution we can apply the theorem in appendix A.3.

To conclude the discussion on the Kasner quantum solution: No stable wave packets can be constructed in order to obtain wave packets that are fully peaked about a single classical trajectory. Note that this is true despite the fact that the WKB approximation is exact for the classical wave equation. Wave packets which satisfy the requirements of the theorem in appendix A.3 will be subject to spreading which goes along with the fact that both the amplitudes $|\widetilde{\Psi}|$ and the amplitudes of the derivatives $|\partial_A \widetilde{\Psi}|$ decay at least as fast as $1/\sqrt{|\alpha|}$. The Klein-Gordon current $\boldsymbol{J}$ therefore decays as fast as or faster than $1/|\alpha|$. Moreover, the density $\star|\Psi|^{\frac{2d}{d-2}} = \star|\Psi|^6$ decays as fast as or faster than $1/|\alpha|^3$. This leads to an avoidance of the singularity by criterion 1 and 2:

$$\boldsymbol{J} \to 0 \quad \text{and} \quad \star\,|\Psi|^6 \to 0 \quad \text{as} \;\; \alpha \to -\infty \; . \tag{3.29}$$

Our criteria, however, also predict an avoidance of the non-singular late stages ($\alpha \to \infty$) of the universe. This is an example where quantum effects are not restricted to small scales of Planck size. Because the superposition principle is universally valid in Quantum Cosmology, quantum effects can arise in principle at any scale. The question of how the situation changes if matter is added will be discussed in the following sections. For simplicity we will restrict our attention to the case of an effective potential.

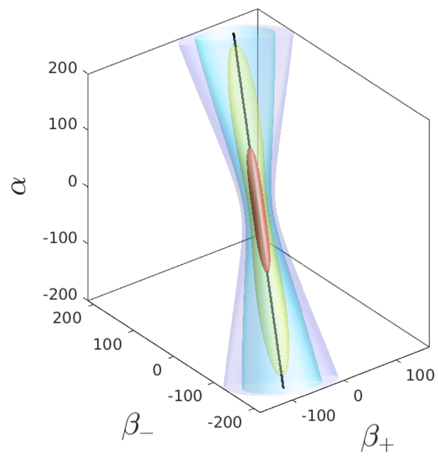


Figure 3.2: The plot shows the equipotential lines of the absolute value of a typical wave packet $\widetilde{\Psi}$ that was numerically evaluated from (3.22) by using Matlab's fast Fourier transform algorithm. For the amplitude $\mathcal{A}(p_+, p_-)$ we chose a Gaussian distribution peaked over some non–zero momenta. Our choice leads to wave packet which is only sharply peaked over the classical trajectory (marked by the black line) close to $\alpha = 0$. The spreading and the decay of the wave packet are both manifest in the plots.

3.1.3 Effective matter potential

In this section we treat matter in a phenomenological way. A hypersurface orthogonal (non-tilted) barotropic fluid with an equation of state $p = w\rho$ and energy density $\rho \propto a^{-3(1+w)}$ can be modeled by adding an effective matter potential of the form $\mathcal{V}(\alpha) = \mathcal{V}_0 \mathrm{e}^{-3(1+w)\alpha} \propto \rho$, with $\mathcal{V}_0 > 0$ being constant, to the Einstein-Hilbert action (3.3). The full action then reads

$$S = \int \mathrm{d}t\ \mathrm{e}^{3\alpha} \left(\frac{-\dot{\alpha}^2 + \dot{\beta}_+^2 + \dot{\beta}_-^2}{2N} - N\mathcal{V}_0 \mathrm{e}^{-3(1+w)\alpha} \right). \tag{3.30}$$

We recognize that the introduction of matter introduces an asymmetry with respect to α. The usual energy conditions require the following:

- Null energy condition: ($w \geq -1$ and $\mathcal{V}_0 \geq 0$) or ($w \leq -1$ and $\mathcal{V}_0 \leq 0$),
- Weak energy condition: $\mathcal{V}_0 \geq 0$ and $w \geq -1$,
- Dominant energy condition: $\mathcal{V}_0 \geq 0$ and $-1 \leq w \leq 1$,

- Strong energy condition: ($w \geq -1/3$ and $\mathcal{V}_0 \geq 0$) or ($w \leq -1$ and $\mathcal{V}_0 \leq 0$).

If we perform a rescaling of the lapse $N \mapsto \widetilde{N} = \mathrm{e}^{-3\alpha} N$ the Hamiltonian constraint can be written as

$$\widetilde{\mathcal{H}} = \frac{-p_\alpha^2 + p_+^2 + p_-^2}{2} + \widetilde{\mathcal{V}}(\alpha) = 0 \ , \tag{3.31}$$

where the rescaled minisuperspace potential is given by $\widetilde{\mathcal{V}}(\alpha) = \mathcal{V}_0 \mathrm{e}^{k\alpha}$ with $k := 3(1-w)$. In particular one obtains $\widetilde{\mathcal{V}}(\alpha) = \frac{\Lambda}{3}\mathrm{e}^{6\alpha}$ for a cosmological constant term, $\widetilde{\mathcal{V}}(\alpha) = a_m^3 \mathrm{e}^{3\alpha}/2$ for an effective dust potential, and $\mathcal{V}(\alpha) \equiv$ *constant* for a stiff fluid. If we assume that $\mathcal{V}_0 > 0$ and $0 < k \leq 6$, all energy conditions except the strong energy condition (which requires $0 < k \leq 4$) are satisfied. It is clear from (3.31) that the case $k < 0$ and $\mathcal{V}_0 > 0$ will replace the Big Bang singularity by a bounce. In the following we are therefore interested in the qualitative behavior of classical and quantum solution for the case that $k > 0$. We put to note that the general solution to the resulting field equations is known as the Heckmann-Schücking solution [108]. We will find that the case of phantom matter $k > 6$ ($w < -1$) generically leads to the appearance of a Big Rip singularity.

Variation with respect to N and employing the fact that β_+ and β_- are cyclic yields

$$\dot{a}^2 = N^2 \left(p_+^2 + p_-^2 + 2\mathcal{V}_0 a^k\right) a^{-4} \ . \tag{3.32}$$

In the following we assume that $p_+^2 + p_-^2 \neq 0$ and choose the the comoving gauge $N = 1$. Equation (3.32) is then solved by

$$t(a) = \frac{a^3}{3\sqrt{p_+^2 + p_-^2}} \, {}_2F_1\left(\frac{1}{2}, \frac{3}{k}; 1 + \frac{3}{k}; -\frac{2\mathcal{V}_0 a^k}{p_+^2 + p_-^2}\right) \ , \tag{3.33}$$

where ${}_2F_1(a, b; c; z)$ is the hypergeometric function. For small a, the hypergeometric function asymptotically equals 1, and we get for $a \to 0$:

$$t \sim \frac{a^3}{3\sqrt{p_+^2 + p_-^2}}. \tag{3.34}$$

Thus the universe starts with a Big Bang at $t = 0$, independent of the value for the barotropic index w. For large a and $w \neq -1$, the hypergeometric function can be simplified, too, and one gets from (3.33) in the limit $a \to \infty$:

$$t \sim \sqrt{\frac{2}{\mathcal{V}_0}} \frac{1}{6-k} a^{(6-k)/2} + t_*. \tag{3.35}$$

For $k < 6$ ($w > -1$), the universe expands infinitely, whereas in the phantom case, that is for

$k > 6$ ($w < -1$), the universe becomes infinitely large already at $t = t_*$ and ends with a Big Rip. We note that (3.35) is the full solution for the flat FLRW case: for $k < 6$ (non-phantom case) there is a Big Bang, but for $k > 6$ (phantom case) there is no past singularity. Therefore one can say that the anisotropy introduces the past singularity, leading to a model with Big Bang *and* Big Rip.

For the anisotropy factors one has

$$\beta_\pm = \frac{1}{k} \frac{p_\pm}{\sqrt{p_+^2 + p_-^2}} \log \left| \frac{1 - \sqrt{1 + \frac{2\mathcal{V}_0}{p_+^2 + p_-^2} a^k}}{1 + \sqrt{1 + \frac{2\mathcal{V}_0}{p_+^2 + p_-^2} a^k}} \right| ; \tag{3.36}$$

they become constant for large a. Thus in contrast to the vacuum solution, this universe isotropizes at late times. For small a, the asymptotic behavior corresponds to (3.8), which is again independent of the matter content. This property is sometimes called "matter doesn't matter". We conclude that in the limit $a \to 0$ and if the evolution is anisotropic the matter potential becomes irrelevant and the Kasner behavior is recovered. In other words: The approach to the singularity is AVTD. One might say that the universe evolves from a shape dominated phase to a matter dominated phase.

In contrast to the vacuum case the addition of matter allows now also for isotropic expansion. This is exactly the case when $p_+ = p_- = 0$ for which we obtain the flat Friedmann model. The approach to the singularity is not AVTD in this case. In the case $0 < k < 6$ the there is a Type I initial singularity. The case $k = 6$ (cosmological constant) yields the flat De Sitter universe, which is singularity free. For the case $k > 6$ there is no initial singularity. Instead the universe ends in a Big Rip type singularity.

Wheeler-DeWitt equation

The Wheeler-DeWitt equation in conformal factor ordering is given by

$$\left[\frac{\hbar^2}{2} \left(\frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial {\beta_+}^2} - \frac{\partial^2}{\partial {\beta_-}^2} \right) + \frac{\mathcal{V}_0 \mathrm{e}^{k\alpha}}{2} \right] \widetilde{\Psi} = 0 \; . \tag{3.37}$$

This is an essentially semi-classical model since we use an effective description for the matter content of the universe. Note that we already chose the representation $\widetilde{\Psi}$ of the wave function that corresponds to the gauge $N = \mathrm{e}^{3\alpha}$. We set again $\hbar = 1$ in the following. The solutions can be written in the form

$$\widetilde{\Psi}\left(\alpha, \beta_+, \beta_-\right) = \sum_{\sigma = \pm} \int_{\mathbb{R}^2} \mathrm{d}p_+ \mathrm{d}p_- \; \mathcal{A}_\sigma\left(p_+, p_-\right) \widetilde{\psi}^\sigma_{p_+, p_-}\left(\alpha, \beta_+, \beta_-\right) , \tag{3.38}$$

with the mode functions given by

$$\begin{aligned}\widetilde{\psi}^{\pm}_{p_+,p_-}(\alpha,\beta_+,\beta_-) =&\ \mathrm{e}^{-\mathrm{i}p_+\beta_+-\mathrm{i}p_-\beta_-}c^{\pm}_{p_+,p_-}J_{\pm\frac{2\mathrm{i}}{k}\sqrt{p_+^2+p_-^2}}\left(\frac{2}{k}\sqrt{\mathcal{V}_0}\mathrm{e}^{k\alpha/2}\right),\\ c^{\pm}_{p_+,p_-} :=&\ \Gamma\left(1\pm\frac{2\mathrm{i}}{k}\sqrt{p_+^2+p_-^2}\right)\left(\frac{\sqrt{\mathcal{V}_0}}{k}\right)^{\mp 2\mathrm{i}\sqrt{p_+^2+p_-^2}/k},\end{aligned} \tag{3.39}$$

where $J_\nu(z)$ and $\Gamma(z)$ denote the Bessel function of the first kind and the gamma function, respectively. Let us now investigate the asymptotic forms of the wave packet. In the limit $\alpha \to -\infty$ we can approximate the mode functions by

$$\widetilde{\psi}^{\pm}_{p_+,p_-}(\alpha,\beta_+,\beta_-) = \mathrm{e}^{\pm\mathrm{i}\sqrt{p_+^2+p_-^2}\ \alpha-\mathrm{i}p_+\beta_+-\mathrm{i}p_-\beta_-} + \mathcal{O}\left(\mathrm{e}^{k\alpha}\right), \tag{3.40}$$

which is independent of k. We conclude that the quantum Kasner behavior is recovered in this limit.

The discussion of the limit $\alpha \to \infty$ is slightly more complicated, but it turns out that a discussion of the mode functions in the WKB approximation

$$\widetilde{\psi} \approx \sqrt{D}\exp\left(\mathrm{i}S\right) \tag{3.41}$$

will be sufficient. A solution to the Hamilton-Jacobi equation is given by

$$\begin{aligned}S_{p_+,p_-}(\alpha,\beta_+,\beta_-) = \pm&\left(\frac{2}{k}\sqrt{p_+^2+p_-^2+\mathcal{V}_0\mathrm{e}^{k\alpha}}+\frac{1}{k}\sqrt{p_+^2+p_-^2}\log\left|\frac{1-\sqrt{1+\frac{\mathcal{V}_0}{p_+^2+p_-^2}\mathrm{e}^{k\alpha}}}{1+\sqrt{1+\frac{\mathcal{V}_0}{p_+^2+p_-^2}\mathrm{e}^{k\alpha}}}\right|\right)\\ &-p_+\beta_+-p_-\beta_-\ .\end{aligned} \tag{3.42}$$

The corresponding van Vleck factor reads

$$\widetilde{D}_{p_+,p_-}(\alpha) = \frac{1}{\sqrt{p_+^2+p_-^2+\mathcal{V}_0\mathrm{e}^{k\alpha}}}. \tag{3.43}$$

If we introduce the functions

$$\begin{aligned}\mathcal{B}_+(p_+,p_-) =&\sqrt{\frac{k}{8\pi}}(1-\mathrm{i})\left[c^{+}_{p_+,p_-}\mathrm{e}^{\frac{\pi}{k}\sqrt{p_+^2+p_-^2}}\mathcal{A}_+(p_+,p_-)+c^{-}_{p_+,p_-}\mathrm{e}^{-\frac{\pi}{k}\sqrt{p_+^2+p_-^2}}\mathcal{A}_-(p_+,p_-)\right],\\ \mathcal{B}_-(p_+,p_-) =&\sqrt{\frac{k}{8\pi}}(1+\mathrm{i})\left[c^{+}_{p_+,p_-}\mathrm{e}^{-\frac{\pi}{k}\sqrt{p_+^2+p_-^2}}\mathcal{A}_+(p_+,p_-)+c^{-}_{p_+,p_-}\mathrm{e}^{\frac{\pi}{k}\sqrt{p_+^2+p_-^2}}\mathcal{A}_-(p_+,p_-)\right],\end{aligned} \tag{3.44}$$

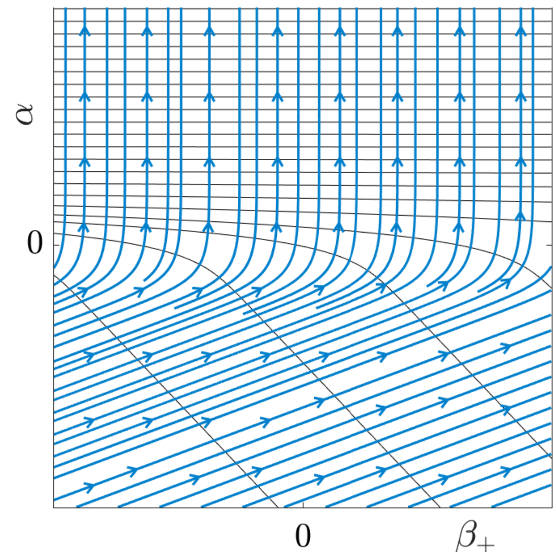


Figure 3.3: Contour plot of the Hamilton-Jacobi function $S_{p_+,0}(\alpha, \beta_+, 0)$ (black contour lines) and the corresponding flow of classical solutions (blue streamlines). We chose the dust case ($k = 3$) for the plot. Kasner solutions are flowing in from $\alpha \to -\infty$. The solutions then isotropize as $\alpha \to \infty$.

then the approximate wave packet with these coefficients,

$$\sum_{\sigma=\pm} \int_{\mathbb{R}^2} \mathrm{d}p_+ \mathrm{d}p_- \; \mathcal{B}_\sigma \sqrt{D} \exp(\sigma \mathrm{i} S), \tag{3.45}$$

matches the exact wave packet for large α at the leading order. This follows from the asymptotic expansion of the exact mode functions and an approximation of the WKB modes of the form

$$\widetilde{\psi} \approx \frac{1}{\sqrt[4]{\mathcal{V}_0}} \mathrm{e}^{-k\alpha/4} \exp\left[\pm \mathrm{i} \left(\frac{2}{k}\sqrt{\mathcal{V}_0}\mathrm{e}^{k\alpha/2}\right)\right]. \tag{3.46}$$

Then one has

$$\widetilde{\Psi}(\alpha, \beta_+, \beta_-) \approx \frac{\mathrm{e}^{-\frac{k}{4}\alpha}}{\sqrt[4]{\mathcal{V}_0}} \sum_{\sigma=\pm} \exp\left(\sigma \frac{2\mathrm{i}}{k} \sqrt{\mathcal{V}_0} \mathrm{e}^{\frac{k}{2}\alpha}\right) \int_{\mathbb{R}^2} \mathrm{d}p_+ \mathrm{d}p_- \; \mathcal{B}_\sigma(p_+, p_-) \, \mathrm{e}^{-\mathrm{i}p_+\beta_+ - \mathrm{i}p_-\beta_-}. \tag{3.47}$$

We can now draw a clear picture of the behavior of wave packets. In the limit $\alpha \to -\infty$, we recover the quantum Kasner behavior. Consequently, we expect a spreading with a resulting decay of amplitudes. The behavior in the limit $\alpha \to \infty$ can be inferred from (3.47): the term in the second line of this equation is just the Fourier transform of B_σ and is independent of α. If, for example, we choose B_σ to be Gaussian, its Fourier transform will be a Gaussian which is peaked about some particular values of β_+ and β_-. This strongly reflects the classical behavior of isotropization. Most importantly, wave packets do not spread in the region where

α is large. The wave packet is modulated by a strongly oscillating factor and an exponentially decaying factor. The exponentially decaying factor comes from the van Vleck factor (3.43) and can be interpreted as arising from the particular representation of the wave function.

The decay of the mode functions in this representation can be intuitively understood by inspecting the Hawking-Page formula (2.175): The representation of the wave function $\widetilde{\Psi}$ we are working corresponds to the gauge $N = \mathrm{e}^{3\alpha}$. In this gauge, classical solutions reach $\alpha = \infty$ in a finite time t. Hence they spend less and less time t in the region of minisuperspace where α is large. In this sense the decay of the density $\sqrt{-\widetilde{\mathcal{G}}}\widetilde{D}$ is implied by (2.175).

We can switch to the comoving time representation via a conformal rescaling with $\Omega = \mathrm{e}^{3\alpha/2}$. For our WKB modes this yields a comoving time density

$$\star|\psi| = \star D_{p_+,p_-} \propto a^{\frac{(1+3w)}{2}} \mathrm{d}a \wedge \mathrm{d}\beta_+ \wedge \mathrm{d}\beta_- \tag{3.48}$$

in the large a region. Note also that we switched from the variable α to the scale factor a. Consider the prefactor $a^{\frac{(1+3w)}{2}}$. It decays with a when $w < -\frac{1}{3}$ and grows with a for $w > -\frac{1}{3}$. This behavior precisely reflects the accelerated and decelerated late time expansion phases of the universe. Figure 3.4 displays the behavior of the wave packet in the model with dust. The asymmetry compared to Fig. 3.2 is clearly visible.

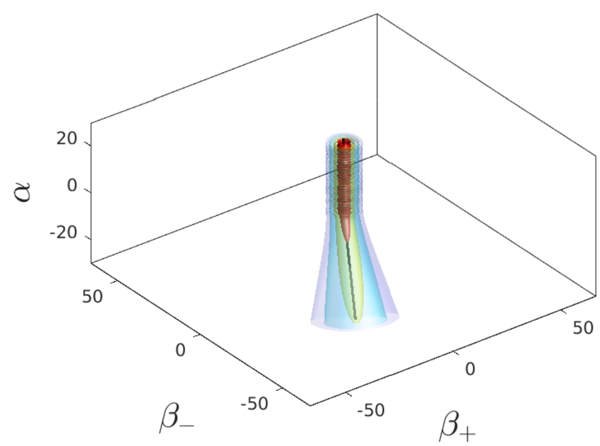


Figure 3.4: The plot shows equipotential surfaces of the absolute value of a (rescaled) wave packet Ψ constructed from (3.38). We chose dust ($k = 3$) and the amplitude $\mathcal{A}(p_+, p_-)$ to be Gaussian and peaked about some momenta $(p_+, p_-) = (\bar{p}_+, \bar{p}_-)$. It turned out to be appropriate to plot the equipotential surfaces of the rescaled wave packed $D^{-1/2}_{\bar{p}_+,\bar{p}_-}|\Psi|$ instead of $|\Psi|$ to counter the decrease in the amplitude. The black line marks the corresponding classical configuration space trajectory (3.36).

For simplicity we set $\mathcal{B}_- = 0$. Then the large-α limit of the Klein-Gordon current is given by

$$\boldsymbol{J}[\Psi,\Psi] = \left| \int_{\mathbb{R}^2} \mathrm{d}p_+ \mathrm{d}p_- \ \mathcal{B}_+ \mathrm{e}^{-\mathrm{i}p_+\beta_+ - \mathrm{i}p_-\beta_-} \right|^2 \mathrm{d}\beta_+ \wedge \mathrm{d}\beta_- + \mathcal{O}\left(\mathrm{e}^{-\frac{k}{4}\alpha}\right) . \tag{3.49}$$

Up to leading order, the current only has an α component given by the Fourier transform of $B_+ (p_+, p_-)$. If we assume that B_+ is peaked at some particular values p_+ and p_-, we will expect the Fourier transform of B_+ to be peaked at some particular value of β_+ and β_-. The current thus reflects the classical behavior in the region where α is large (in contrast to the vacuum Kasner case). We have, however, $\quad \star|\Psi|^6 \to 0 \quad$ as $\alpha \to \infty$. Note that the behavior is qualitatively independent of w, that is, there is no difference between the cases $w \geq -1$ and $w < -1$, although the latter case leads to a Big Rip. The Big Rip is thus only avoided by criterion 2.

3.1.4 Scalar fields

The symmetry reduced matter action for a minimally coupled scalar field ϕ can be brought into the form

$$S_m = \frac{1}{2} \int \mathrm{d}t \ a^3 \left[\frac{\dot{\phi}^2}{N} - NV(\phi) \right] \tag{3.50}$$

The full action then reads

$$S = \frac{1}{2} \int \mathrm{d}t \ \frac{\mathrm{e}^{3\alpha}}{N} \left[\left(-\dot{\alpha}^2 + \dot{\beta}_+^2 + \dot{\beta}_-^2 + \dot{\phi}^2 \right) - N^2 V(\phi) \right] \ . \tag{3.51}$$

Note that if we transform $N \to \bar{N} = N\mathrm{e}^{-3\alpha}$, it becomes manifest that the model is analogous to a massless relativistic particle in a potential $\mathrm{e}^{6\alpha}V(\phi)$.

Massless scalar field

In the region where $a \to 0$ the massless scalar field might be a good approximation for the general case if the universe enters a region in minisuperspace where the potential is negligible. In the gauge $N = \mathrm{e}^{3\alpha}$ it becomes clear that this can in particular be the case when approaching the initial singularity ($\alpha \to -\infty$) since then $\mathrm{e}^{6\alpha}V(\phi)$ might be negligible. The scalar field is then called kinetic-dominated.

In the comoving and in the quasi-Gaussian gauge the equations of motion are solved by

gauge $N =$	1	$\mathrm{e}^{3\alpha}$
$\alpha(t) =$	$\frac{1}{3}\log\left(\sqrt{p_+^2+p_-^2+p_\phi^2}[t-t_0]\right)$	$\sqrt{p_+^2+p_-^2+p_\phi^2}\,(t-t_0)$
$\beta_\pm(t) =$	$\frac{p_\pm}{3\sqrt{p_+^2+p_-^2+p_\phi^2}}\log(t-t_0)+C_\pm$	$p_\pm(t-t_0)+C_\pm$
$\phi(t) =$	$\frac{p_\phi}{3\sqrt{p_+^2+p_-^2+p_\phi^2}}\log(t-t_0)+C_\phi$	$p_\phi(t-t_0)+C_\phi$

In the quasi-Gaussian gauge it is manifest that the solution represents again straight lines in configuration space.

Are these solutions an exception to the phrase "matter doesn't matter"? Not really! The qualitative nature of the initial singularity is not affected, that is, it remains VTD. In addition, however, we obtain the possibility of an isotropic singularity, i.e. the universe can collapse into a point. This is exactly the case when $p_+ = p_- = 0$ and $p_\phi \neq 0$.

Wheeler-DeWitt equation

The DeWitt metric is given by

$$\mathrm{d}\mathcal{S}^2 = \mathrm{e}^{3\alpha}\left(-\mathrm{d}\alpha^2 + \mathrm{d}\beta_+^2 + \mathrm{d}\beta_-^2 + \mathrm{d}\phi^2\right) \ . \tag{3.52}$$

The Wheeler-DeWitt equation reads

$$\hat{\mathcal{H}}\Psi = \frac{\hbar^2\mathrm{e}^{-3\alpha}}{2}\left[\frac{\partial^2}{\partial\alpha^2} + 2f\frac{\partial}{\partial\alpha} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2} - \xi\mathcal{R}\mathrm{e}^{3\alpha} - \frac{\partial^2}{\partial\phi^2} + \frac{\mathrm{e}^{6\alpha}}{\hbar^2}V(\phi)\right]\Psi = 0 \ , \tag{3.53}$$

where the Ricci scalar on $\mathcal{M}$ is

$$\mathcal{R} = \frac{27}{2}\mathrm{e}^{-3\alpha} \ . \tag{3.54}$$

The Laplace-Beltrami factor ordering is now obtained for $f = 3/2$ and $\xi = 0$. Setting instead $\xi = \xi_4 = \frac{1}{6}$ we obtain the conformal factor. As in the vacuum case we define $\widetilde{\Psi} := \mathrm{e}^{f\alpha}\Psi$. The Wheeler-DeWitt equation then simplifies to

$$\left[\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2} - \frac{\partial^2}{\partial\phi^2} + \frac{\mathrm{e}^{6\alpha}}{\hbar^2}V(\phi) + f^2 - \frac{27}{2}\xi\right]\widetilde{\Psi} = 0 \ . \tag{3.55}$$

In the case of conformal factor ordering we then get

$$\left[\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2} - \frac{\partial^2}{\partial\phi^2} + \frac{\mathrm{e}^{6\alpha}}{\hbar^2}V(\phi)\right]\widetilde{\Psi} = 0 \ . \tag{3.56}$$

If the minisuperspace potential $\frac{\mathrm{e}^{6\alpha}}{\hbar^2}V(\phi)$ becomes negligible in the singular region $\alpha \to \infty$, we can conclude the avoidance of the singularity by applying the decay rate estimates for the classical wave equation in 3+1 dimensions. Both $|\widetilde{\Psi}|$ and $|\partial_A \widetilde{\Psi}|$ decay as fast or faster than $\frac{1}{|\alpha|}$ due to the spreading of wave packets. This implies an avoidance of the singularity by all three criteria imposed in section 2.2.5.

In [T3] the discussion was extended to the case of a phantom field (opposite sign in the kinetic term). The coupling of the phantom field can lead to the appearance of a Big Rip type future singularity. The singularity was found to be only avoided by criterion 2.

3.1.5 Electromagnetic fields

In the following we will couple an electromagnetic field to the general Bianchi I metric. The resulting model was to my knowledge first studied in [109].

We write the Bianchi I metric in the ADM form (2.18) where the basis one forms are $\sigma^1 = \mathrm{d}x$, $\sigma^2 = \mathrm{d}y$ and $\sigma^3 = \mathrm{d}z$. The structure coefficients of Bianchi I are all zero. Therefore the momentum constraints are trivially satisfied in the vacuum case, that is, $\mathcal{H}_i = 0$. The full Hamiltonian for the non-diagonal Bianchi I model is therefore given by

$$H = N\mathcal{H} = \frac{N\mathrm{e}^{-3\alpha}}{2}\left(-p_\alpha^2 + p_+^2 + p_-^2 + \frac{l_1^2}{I_1} + \frac{l_2^2}{I_2} + \frac{l_3^2}{I_3}\right) . \tag{3.57}$$

This result is independent of the choice of the diagonalizing group. Since there are no inner automorphisms there are no distinguished choices for the diagonalizing group. We will choose the diagonalizing group to be $SO(3, \mathbb{R})$ in the following. In the discussion of the Bianchi IX in section 3.4.2 we will diagonalize the spatial metric by using the so called Euler matrix which is parametrized by the three Euler angles θ, ϕ and ψ. We can do the same thing here by just using the result from section 3.4.2. Note that in the vacuum case the total angular momentum $l_1^2 + l_2^2 + l_3^2$ commutes with the total Hamiltonian and therefore constitutes a constant of motion.

The matter action is given by

$$S_{\text{Maxwell}} = \frac{1}{8\mu_0}\int \star\mathbf{F}\wedge\mathbf{F} . \tag{3.58}$$

We first need to perform the symmetry reduction in the matter sector. Matter fields should respect the symmetries of the gravitational system. This leads to the fact that vector fields can only be coupled to certain Bianchi models [110]. In the Bianchi I case the vector potential can be expanded as

$$\boldsymbol{A} = A_t\mathrm{d}t + A_x\mathrm{d}x + A_y\mathrm{d}y + A_z\mathrm{d}z . \tag{3.59}$$

The field strength tensor is then obtained by $\mathbf{F} = \mathrm{d}\boldsymbol{A}$. The gauge potential $\mathbf{A}$ might contain nonphysical degrees of freedom. The field strength $\mathbf{F}$, however, is physical and should respect the symmetries of Bianchi I. Hence we demand that $\mathcal{L}_{\mathbf{v}}\mathbf{F} = 0$ for all Killing vector fields $\mathbf{v}$. In the Bianchi I case $\mathbf{v} = \partial_x, \partial_y, \partial_z$ and the field strength tensor is restricted to be of the form

$$\mathbf{F} = E_i \mathrm{d}x^i \wedge \mathrm{d}t + \frac{1}{2} B_{ij} \mathrm{d}x^i \wedge \mathrm{d}x^j \tag{3.60}$$

with the components E_i and B_{ij} being functions of t only. Demanding, furthermore, $\mathbf{F}$ to be exact, already implies that $B_{ij} = const$. We conclude that the most general ansatz for a vector potential respecting the symmetries of Bianchi I reads

$$\begin{aligned} A_t &= xc_x + yc_y + zc_z \ , \\ A_x &= -\mathcal{A}_x + \frac{1}{2}\left(yB^z - zB^y\right) \ , \\ A_y &= -\mathcal{A}_y + \frac{1}{2}\left(zB^x - xB^z\right) \ , \\ A_z &= -\mathcal{A}_x + \frac{1}{2}\left(xB^y - yB^x\right) \ , \end{aligned} \tag{3.61}$$

where $c_i = c_i(t)$. The electric and magnetic field as measured by comoving observers are given by $E_i = \dot{\mathcal{A}}_i + c_i$ and $B_{ij} = \varepsilon_{ijk} B^k = constant$, respectively. It seems that we do no harm when setting $c_i = 0$. We can now rewrite the action (3.58) in the ADM form

$$S_{\text{Maxwell}} = \frac{1}{2} \int \mathrm{d}t \sqrt{h} \left[\frac{1}{N} h^{ij} \left(E_i + N^k B_{ki}\right)\left(E_j + N^l B_{lj}\right) - \frac{1}{2} N h^{ij} h^{lk} B_{il} B_{jk} \right] \ , \tag{3.62}$$

Where we absorbed the factor $\frac{1}{2\mu_0}\int_{\mathbb{R}^3} \mathrm{d}^3 x$ into the fields. Let us denote the momenta conjugate to $\mathcal{A}_i$ by

$$\Pi^i = \frac{\partial L}{\partial \dot{\mathcal{A}}_i} = \frac{\sqrt{h} h^{ij}}{N} \left(E_j + N^k B_{kj}\right) \ . \tag{3.63}$$

The Legendre transform yields the matter part of the Hamiltonian

$$H^{(m)} = N \mathcal{H}^{(m)} + N^i \mathcal{H}_i^{(m)} \ . \tag{3.64}$$

The matter part of the Hamiltonian constraint and momentum constraints are given by

$$\mathcal{H}^{(m)} = \frac{1}{2\sqrt{h}} h_{ij} \left(\Pi^i \Pi^j + B^i B^j\right) \ , \quad \mathcal{H}_i^{(m)} = -B_{ik} \Pi^k = \varepsilon_{ijk} B^j \Pi^k \ . \tag{3.65}$$

The full Hamiltonian is then given by

$$
\begin{aligned}
H &= \frac{N\mathrm{e}^{-3\alpha}}{2}\left[-p_\alpha^2 + p_+^2 + p_-^2 + \frac{l_1^2}{I_1} + \frac{l_2^2}{I_2} + \frac{l_3^2}{I_3} + h_{ij}\left(\Pi^i\Pi^j + B^iB^j\right)\right] - N^iB_{ij}\Pi^j \\
&=: N\mathcal{H} + N^i\mathcal{H}_i \ .
\end{aligned}
\tag{3.66}
$$

Note that the matter part of the Hamiltonian constraint now explicitly depends on the Euler angles. The total angular momentum $l_1^2 + l_2^2 + l_3^2$ is therefore not conserved in general. The momenta Π^i are constants of motion. The momentum constraints $\mathcal{H}_i = \mathcal{H}_i^{(m)} \simeq 0$ are enforcing the vanishing of the Poynting vector. The constraint algebra closes with the Poisson brackets given by

$$
\{\mathcal{H}, \mathcal{H}_i\} = 0 \quad \text{and} \quad \{\mathcal{H}_i, \mathcal{H}_j\} = 0 \ . \tag{3.67}
$$

Our result for the Hamiltonian agrees with the one obtained in [109]. It was also checked in [109] that the symmetry reduction works in the sense that it produces the correct Einstein-Maxwell equations.

The equations of motion are a rather complicated set of coupled second order differential equations. From the fact that the potential is positive, however, it is already clear that the scale factor α is strictly increasing (or decreasing depending on the choice of the direction of time). The authors of [109] have used diagrammatic methods to analyze the general case. In order to get some insight into the situation we restrict ourselves to the consideration of a more simple and symmetric situation for which the equations of motion are analytically solvable.

Diagonal case

We consider the subset of solutions for which the metric coefficients h_{ij} are diagonal at all times, i.e. the Euler angles are kept fixed ($\theta = \pi/2$, $\phi = 0 = \psi$). Without the loss of generality we can set $\Pi^x = \Pi^y = 0$ and $B^x = B^y = 0$ and keep only the z-components to be non-zero. Note that this is only possible because the equations of motion for the Euler angles now consistently imply $l_i = 0$. The momentum constraints are also satisfied by this ansatz. The dynamics of this universe is controlled by the Lagrangian

$$
L = \frac{\mathrm{e}^{3\alpha}}{2N}\left(-\dot{\alpha}^2 + \dot{\beta}_+^2 + \dot{\beta}_-^2\right) - \frac{N}{2}\left[(\Pi^z)^2 + (B^z)^2\right]\mathrm{e}^{-\alpha-4\beta_+} \tag{3.68}
$$

The dynamics are completely analogous to a relativistic particle that is reflected from one potential wall that moves in the β_+ direction as α (corresponding to time here) grows. There is a now an additional Noether symmetry in the system. We expose it by defining new configuration space variables. We first rescale the lapse function by $N \to \widetilde{N} = \mathrm{e}^{-3\alpha} N$. Now we can get rid of the "time" dependence in the potential by performing the Lorentz boost

$$T := \frac{2\alpha - \beta_+}{\sqrt{3}} \ , \quad X := \frac{2\beta_+ - \alpha}{\sqrt{3}} \ . \tag{3.69}$$

The Lagrangian now becomes

$$L = \frac{1}{2\widetilde{N}} \left(-\dot{T}^2 + \dot{X}^2 + \dot{\beta}_-^2 \right) + \frac{\widetilde{N}}{2} \left[(\Pi^z)^2 + (B^z)^2 \right] \mathrm{e}^{-2\sqrt{3}X} \ . \tag{3.70}$$

The symmetries are now exposed: since T and β_- are cyclic, their momenta p_T and p_- are constants of motion

$$p_T = -\frac{\dot{T}}{\widetilde{N}} = \frac{\dot{\beta}_+ - 2\dot{\alpha}}{\widetilde{N}\mathrm{e}^{2\alpha}} = \mathit{constant} \ . \tag{3.71}$$

Variation with respect to X yields

$$\ddot{X} = \sqrt{3} \left[(\Pi^z)^2 + (B^z)^2 \right] \mathrm{e}^{-2\sqrt{3}X} \ , \tag{3.72}$$

where we have fixed the gauge $\widetilde{N} = 1$ ($N = \mathrm{e}^{3\alpha}$). We can solve the equation and get

$$\begin{aligned} X(t) &= \frac{1}{\sqrt{3}} \log \left(\frac{1 + K^2 \left[(\Pi^z)^2 + (B^z)^2 \right] \mathrm{e}^{2\sqrt{3}K(t-t_0)}}{2K^2 \mathrm{e}^{\sqrt{3}K(t-t_0)}} \right) \ , \\ T(t) &= -p_T(t - t_0) + C_T \ , \\ \beta_-(t) &= p_-(t - t_0) + C_- \ , \end{aligned} \tag{3.73}$$

where $K, C_T, C_- \in \mathbb{R}$ are integration constants. We choose $C_T = C_- = 0$ since they can be absorbed into the coordinate functions anyways. Up to now we haven't taken the Hamiltonian constraint into account. The Hamiltonian constraint, obtained by varying with respect to $\widetilde{N}$, reads

$$-\dot{T}^2 + \dot{X}^2 + \dot{\beta}_-^2 + \left[(\Pi^z)^2 + (B^z)^2 \right] \mathrm{e}^{-2\sqrt{3}X} = 0 \ . \tag{3.74}$$

Plugging the solution (3.73) into the constraint implies that

$$p_T = \pm\sqrt{K^2 + p_-^2} \ . \tag{3.75}$$

Performing the Lorentz boost back to the Misner variables yields

$$\begin{aligned}\alpha(t) &= \pm 2\sqrt{\frac{p_-^2+K^2}{3}}\,(t-t_0)+\frac{1}{3}\log\left(\frac{1}{2K^2}\mathrm{e}^{-\sqrt{3}K(t-t_0)}+\frac{[(\Pi^z)^2+(B^z)^2]}{2}\mathrm{e}^{\sqrt{3}K(t-t_0)}\right)\\ \beta_+(t) &= \pm\sqrt{\frac{p_-^2+K^2}{3}}\,(t-t_0)+\frac{2}{3}\log\left(\frac{1}{2K^2}\mathrm{e}^{-\sqrt{3}K(t-t_0)}+\frac{[(\Pi^z)^2+(B^z)^2]}{2}\mathrm{e}^{\sqrt{3}K(t-t_0)}\right)\\ \beta_-(t) &= p_-(t-t_0)\ .\end{aligned} \tag{3.76}$$

We now discuss the limiting behavior. For brevity we set $t_0 = 0$ and restrict ourselves to the solutions with the +-sign and the case when $K > 0$ and $(\Pi^z)^2 + (B^z)^2 \neq 0$. For $t \to -\infty$ the asymptotics are

$$\begin{aligned}\alpha(t) &\approx \sqrt{p_{+,1}^2+p_-^2}\ t + const.\\ \beta_+(t) &\approx p_{+,1}\ t + const.\\ \beta_-(t) &\approx p_-\ t + const.\ ,\end{aligned} \tag{3.77}$$

where $p_{+,1} = \frac{-2K+\sqrt{p_-^2+K^2}}{\sqrt{3}} = \frac{|p_T|-2\sqrt{p_T^2-p_-^2}}{\sqrt{3}}$. For $t \to +\infty$ the asymptotics are

$$\begin{aligned}\alpha(t) &\approx \sqrt{p_{+,2}^2+p_-^2}\ t + const.\\ \beta_+(t) &\approx p_{+,2}\ t + const.\\ \beta_-(t) &\approx p_-\ t + const.\ ,\end{aligned} \tag{3.78}$$

where $p_{+,2} = \frac{2K+\sqrt{p_-^2+K^2}}{\sqrt{3}} = \frac{|p_T|+2\sqrt{p_T^2-p_-^2}}{\sqrt{3}}$. Both asymptotic solutions correspond to ingoing and outgoing Kasner solutions (3.14). From the asymptotic solutions we conclude that during the process of reflection at the potential wall a momentum of $\Delta p_+ = \frac{4K}{\sqrt{3}}$ is transferred.

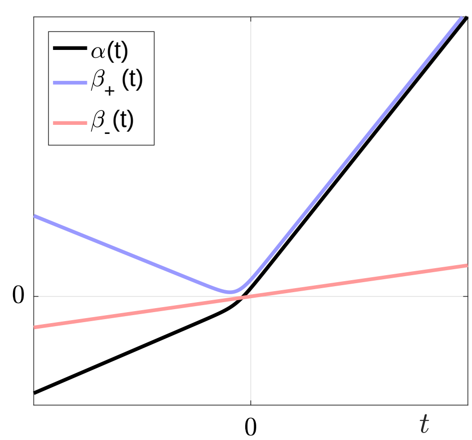


Figure 3.5: Plot of a particular solution in the gauge $N = \mathrm{e}^{3\alpha}$. One can clearly see the transition from one Kasner solution to the other

Let's now provide a physical interpretation of the situation. The components of the energy-momentum tensor are given by

$$\{T^{\mu}{}_{\nu}\} = \frac{\mathrm{e}^{-4\beta+}}{8\pi a^4}\left[(\Pi^z)^2 + (B^z)^2\right]\mathrm{diag}\,(-1,1,1,-1)\ . \tag{3.79}$$

If $p_- = 0$ (cylindrical symmetry), the universe starts to expand in the z-direction and it contracts in the other two directions. The pressure now starts to grow as the electric and magnetic field lines become denser, which finally leads to a bounce. After the bounce the universe contracts in the z-direction and expands in the other two directions.

Wheeler-DeWitt equation

Starting from the Hamiltonian (3.66) we can read off the DeWitt metric, compute the volume element, and the Ricci curvature scalar of the 4–dimensional minisuperspace

$$\begin{gathered}\mathrm{d}\mathcal{S}^2 = \mathrm{e}^{2\alpha}\left(-\mathrm{d}\alpha^2 + \mathrm{d}\beta_+^2 + \mathrm{d}\beta_-^2\right) + \mathrm{e}^{4\beta_+}\mathrm{d}A_z^2\ , \quad \mathcal{R} = -6\mathrm{e}^{-2\alpha}\ , \\ \star 1 = \mathrm{e}^{3\alpha+2\beta_+}\mathrm{d}\alpha\wedge\mathrm{d}\beta_+\wedge\mathrm{d}\beta_-\wedge\mathrm{d}A_z\ .\end{gathered} \tag{3.80}$$

We started here from the conformal gauge which corresponds to $N = \mathrm{e}^{\alpha}$. Note that, in contrast to the previous models, the configuration space is not conformally flat. This follows from the fact that the Weyl squared scalar is given by $\mathcal{W}^2 = 12\mathrm{e}^{-4\alpha}$. The DeWitt metric, however, admits a representation for which the curvature scalar is constant. For simplicity we set the magnetic field B_i to zero in the following. The Laplace-Beltrami operator reads

$$\Box = \mathrm{e}^{-2\alpha}\left(-\frac{\partial^2}{\partial\alpha^2} + \frac{\partial^2}{\partial{\beta_+}^2} + \frac{\partial^2}{\partial{\beta_-}^2} - \frac{\partial}{\partial\alpha} + 2\frac{\partial}{\partial\beta_+}\right) + \mathrm{e}^{-4\beta_+}\frac{\partial^2}{\partial{A_z}^2}\ . \tag{3.81}$$

We pick the conformal factor ordering defined by

$$\hat{\mathcal{H}} := -\frac{1}{2}\left(\Box - \xi\mathcal{R}\right)\ , \tag{3.82}$$

with $\xi = \xi_4 = 1/6$. The conformal weight of the wave function is $w(\Psi) = -1$. The Hamiltonian constraint operator is then given by

$$2\hat{\mathcal{H}} = \mathrm{e}^{-2\alpha}\left(\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2} + \frac{\partial}{\partial\alpha} - 2\frac{\partial}{\partial\beta_+} + 6\xi\right) - \mathrm{e}^{-4\beta_+}\frac{\partial^2}{\partial{A_z}^2}\ . \tag{3.83}$$

We transform now $\Psi \to \widetilde{\Psi} = \mathrm{e}^{\frac{\alpha}{2}+\beta_+}\Psi$. The transformation corresponds to a conformal transformation $\Omega = \mathrm{e}^{-\frac{\alpha}{2}-\beta_+}$. The volume element is now given by

$$\widetilde{\star}1 = \sqrt{-\widetilde{\mathcal{G}}}\, \mathrm{d}\alpha \wedge \mathrm{d}\beta_+ \wedge \mathrm{d}\beta_- \wedge \mathrm{d}A_z = \mathrm{e}^{\alpha-2\beta_+}\mathrm{d}\alpha \wedge \mathrm{d}\beta_+ \wedge \mathrm{d}\beta_- \wedge \mathrm{d}A_z \ . \tag{3.84}$$

Most importantly note that $\sqrt{-\widetilde{\mathcal{G}}}\left\{\widetilde{\mathcal{G}}^{AB}\right\} = \mathrm{diag}\left(-1, 1, 1, \mathrm{e}^{2\alpha-4\beta_+}\right)$. After the conformal transformation, the Wheeler-DeWitt equation reads

$$\left[\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2} - \mathrm{e}^{2\alpha-4\beta_+}\frac{\partial^2}{\partial{A_z}^2} + \frac{3(1-8\xi)}{4}\right]\widetilde{\Psi}\left(\alpha, \beta_+, \beta_-, A_z\right) = 0 \ . \tag{3.85}$$

Due to the transformation we got rid of the first derivatives but we have picked up a mass^2 term of the form $\frac{3(1-8\xi)}{4}$. Note that it does not vanish for the usual conformal factor ordering with $\xi = 1/6$. Furthermore, note that $\hat{P}_z = \frac{\mathrm{i}}{\hbar}\frac{\partial}{\partial A_z}$ is a good quantum number. Therefore it suggests itself to perform the mode expansion

$$\widetilde{\Psi}\left(\alpha, \beta_+, \beta_-, A_z\right) = \widetilde{\psi}_{P_z}(\alpha, \beta_+, \beta_-)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}P_z A_z} \ . \tag{3.86}$$

We then obtain

$$\left[\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2} + P_z^2\mathrm{e}^{2\alpha-4\beta_+} + \frac{3(1-8\xi)}{4}\right]\widetilde{\psi}_{P_z}(\alpha, \beta_+, \beta_-) = 0 \ . \tag{3.87}$$

The modes with quantum number $P_z = 0$ (vanishing electric field) then obey the equation

$$\left[\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2} - \frac{1}{4}\right]\widetilde{\psi}_0(\alpha, \beta_+, \beta_-) = 0 \ . \tag{3.88}$$

As we would wish to recover the behavior of the vacuum Bianchi I model, we remove the mass squared term from the Wheeler-DeWitt equation, that is, we consider instead of (3.90) the equation

$$\left[\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2} + P_z^2\mathrm{e}^{2\alpha-4\beta_+}\right]\widetilde{\psi}_{P_z}(\alpha, \beta_+, \beta_-) = 0 \ . \tag{3.89}$$

The Wheeler-DeWitt equation is solved analogously to the classical case. We first perform the Lorentz boost (3.69) to get

$$\left[\frac{\partial^2}{\partial T^2} - \frac{\partial^2}{\partial X^2} - \frac{\partial^2}{\partial{\beta_-}^2} + P_z^2\mathrm{e}^{-2\sqrt{3}X}\right]\widetilde{\psi}_{P_z}(T, X, \beta_-) = 0 \ . \tag{3.90}$$

This is solved by a superposition of the mode functions

$$\widetilde{\psi}^{\pm}_{P_z,p_T,p_-}\left(T,X,\beta_-,A_z\right)=c^{\pm}_{p_T,p_-}I_{\pm\mathrm{i}\sqrt{\frac{p_T^2-p_-^2}{3}}}\left(\frac{P_z\mathrm{e}^{-\sqrt{3}X}}{\sqrt{3}}\right)\mathrm{e}^{-\mathrm{i}p_TT}\mathrm{e}^{\mathrm{i}p_-\beta_-}\mathrm{e}^{\mathrm{i}P_zA_z}\ . \tag{3.91}$$

Now remind yourself that in the classical model the trajectory comes in from the region where $X\to\infty$. In this region the universes asymptotic behavior corresponds to that of the Kasner solution. The trajectory then hits the potential barrier and is reflected back to $X=\infty$. The region $X\to-\infty$ is therefore classically forbidden if $P_z\neq 0$. After boosting back to the Misner variables, we obtain the general solution

$$\begin{aligned}
&\widetilde{\Psi}\left(\alpha,\beta_+,\beta_-,A_z\right)=\int\limits_{-\infty}^{\infty}\mathrm{d}P_z\int\limits_{-\infty}^{\infty}\mathrm{d}p_T\int\limits_{-\infty}^{\infty}\mathrm{d}p_-\ \mathcal{A}_l\left(P_z,p_T,p_-\right)\widetilde{\psi}^{l}_{P_z,p_T,p_-}\left(\alpha,\beta_+,\beta_-,A_z\right)\\
&\text{where}\quad \widetilde{\psi}^{\pm}_{P_z,p_T,p_-}\left(\alpha,\beta_+,\beta_-,A_z\right)=c^{\pm}_{p_T,p_-,P_z}I_{\pm\mathrm{i}\sqrt{\frac{p_T^2-p_-^2}{3}}}\left(\frac{P_z\mathrm{e}^{\alpha-2\beta_+}}{\sqrt{3}}\right)\mathrm{e}^{-\mathrm{i}p_T\frac{2\alpha-\beta_+}{\sqrt{3}}}\mathrm{e}^{\mathrm{i}p_-\beta_-}\mathrm{e}^{\mathrm{i}P_zA_z}\\
&\text{with}\quad c^{\pm}_{p_T,p_-,P_z}=\Gamma\left(1\pm\mathrm{i}\sqrt{\frac{p_T^2-p_-^2}{3}}\right)\mathrm{e}^{\pm\mathrm{i}\sqrt{\frac{p_T^2-p_-^2}{3}}\left[\log\left(2\sqrt{3}\right)-P_z\right]}\ .
\end{aligned}\tag{3.92}$$

We should choose $\mathcal{A}_{\pm}\left(P_z,p_T,p_-\right)$ such that $\mathrm{supp}(\mathcal{A}_{\pm})\subseteq\left\{(P_z,p_T,p_-)\in\mathbb{R}\mid p_T^2-p_-^2\geq 0\right\}$. The coefficients $c^{\pm}_{p_T,p_-,P_z}$ were chosen such that for small $\mathrm{e}^{-\sqrt{3}X}=\mathrm{e}^{\alpha-2\beta_+}$ the mode functions behave as

$$\begin{aligned}
\widetilde{\psi}^{\pm}_{P_z,p_T,p_-}\left(\alpha,\beta_+,\beta_-,A_z\right)&=\mathrm{e}^{\pm\mathrm{i}\sqrt{\frac{p_T^2-p_-^2}{3}}(\alpha-2\beta_+)}\left[1+\mathcal{O}\left(P_z^2\mathrm{e}^{2(\alpha-2\beta_+)}\right)\right]\mathrm{e}^{-\mathrm{i}p_T\frac{2\alpha-\beta_+}{\sqrt{3}}}\mathrm{e}^{\mathrm{i}p_-\beta_-}\mathrm{e}^{\mathrm{i}P_zA_z}\\
&=\left[1+\mathcal{O}\left(P_z^2\mathrm{e}^{2(\alpha-2\beta_+)}\right)\right]\mathrm{e}^{-\mathrm{i}\frac{2p_T\mp\sqrt{p_T^2-p_-^2}}{\sqrt{3}}\alpha}\mathrm{e}^{\mathrm{i}\frac{p_T\mp2\sqrt{p_T^2-p_-^2}}{\sqrt{3}}\beta_+}\mathrm{e}^{\mathrm{i}p_-\beta_-}\mathrm{e}^{\mathrm{i}P_zA_z}\ .
\end{aligned}\tag{3.93}$$

Identifying now

$$p_{+,1}:=\frac{p_T-2\sqrt{p_T^2-p_-^2}}{\sqrt{3}}\quad\text{and}\quad p_{+,2}:=\frac{p_T+2\sqrt{p_T^2-p_-^2}}{\sqrt{3}}\tag{3.94}$$

and restricting attention to the oscillating modes with $p_T\geq|p_-|$ we can write

$$\begin{aligned}
\widetilde{\psi}^{+}_{P_z,p_T,p_-}\left(\alpha,\beta_+,\beta_-,A_z\right)&=\left[1+\mathcal{O}\left(P_z^2\mathrm{e}^{2(\alpha-2\beta_+)}\right)\right]\mathrm{e}^{-\mathrm{i}\sqrt{p_{+,1}^2+p_-^2}\alpha}\mathrm{e}^{\mathrm{i}p_{+,1}\beta_+}\mathrm{e}^{\mathrm{i}p_-\beta_-}\mathrm{e}^{\mathrm{i}P_zA_z}\ ,\\
\widetilde{\psi}^{-}_{P_z,p_T,p_-}\left(\alpha,\beta_+,\beta_-,A_z\right)&=\left[1+\mathcal{O}\left(P_z^2\mathrm{e}^{2(\alpha-2\beta_+)}\right)\right]\mathrm{e}^{-\mathrm{i}\sqrt{p_{+,2}^2+p_-^2}\alpha}\mathrm{e}^{\mathrm{i}p_{+,2}\beta_+}\mathrm{e}^{\mathrm{i}p_-\beta_-}\mathrm{e}^{\mathrm{i}P_zA_z}\ .
\end{aligned}\tag{3.95}$$

Therefore the plus modes $\widetilde{\psi}^{+}_{P_z,p_T,p_-}$ correspond to the asymptotics solutions of the classical model given by equations (3.77) and the minus modes $\widetilde{\psi}^{-}_{P_z,p_T,p_-}$ to the ones given by equations

(3.78).

Usually the problem of matching is solved after imposing the Hawking-Page boundary (see e.g. the example in [104]). The boundary condition demands that wave packets vanish deep inside of the classically forbidden region. As discussed in section 2.2.6, this criterion is questionable in view of the conformal covariance of the wave function. By studying the asymptotics of the modified Bessel functions [111] we find that the real part of the modes functions (3.91) blows up like $\exp\left(\exp\left(-\sqrt{3}X\right)/\sqrt{3}\right)$ as $X \to -\infty$. This problem is cured by choosing the Macdonald function $K_\nu(z)$ instead of the modified Bessel functions $I_\nu(z)$ in (3.91). Hence we get

$$\widetilde{\psi}_{P_z,p_T,p_-}\left(\alpha,\beta_+,\beta_-,A_z\right) = K_{\mathrm{i}\sqrt{\frac{p_T^2-p_-^2}{3}}}\left(\frac{P_z \mathrm{e}^{\alpha-2\beta_+}}{\sqrt{3}}\right)\mathrm{e}^{-\mathrm{i}p_T\frac{2\alpha-\beta_+}{\sqrt{3}}}\mathrm{e}^{\mathrm{i}p_-\beta_-}\mathrm{e}^{\mathrm{i}P_zA_z}\ . \tag{3.96}$$

The Macdonald function decays exponentially in the classically forbidden region. The mode function (3.96) is a certain linear combination of the plus and minus modes in (3.91). The choice of (3.96) thus leads to a matching of the ingoing and outgoing modes.

Singularity avoidance: Classically the electric field does not influence the spacetime dynamics close to the singularity, that is, “matter doesn’t matter” and we recover the Kasner behavior in the vicinity of the singularity. Interestingly the same holds for the quantum model in the following sense: The (1+3)–dimensional Wheeler-DeWitt equation becomes effectively $(1+2)$–dimensional as $\alpha \to -\infty$:

$$\left[\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2} - \mathrm{e}^{2\alpha-4\beta_+}\frac{\partial^2}{\partial{A_z}^2}\right]\widetilde{\Psi} \approx \left[\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2}\right]\widetilde{\Psi} = 0\ . \tag{3.97}$$

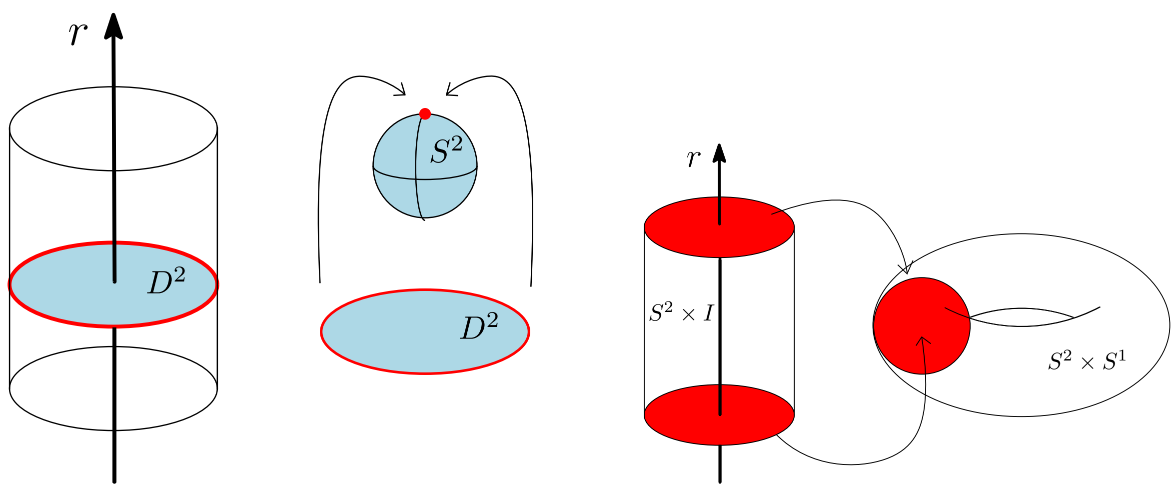
Note that this is different from the case of minimally coupled scalar fields. By using the decay rate estimate in appendix A.3 we find that $|\widetilde{\Psi}|$ and $|\partial_A\widetilde{\Psi}|$ decay as fast as or faster than $\frac{1}{\sqrt{|\alpha|}}$ as $\alpha \to -\infty$. We conclude that all components of the Klein-Gordon current $\boldsymbol{J}$ in the presently used coordinates decay like $1/|\alpha|$, that is, they decay in the same way as in the vacuum Bianchi I case. This is true for all components except for the A_z component in front of $\mathrm{d}\alpha\wedge\mathrm{d}\beta_+\wedge\mathrm{d}\beta_-$ which decays like $\exp(-2\sqrt{3}X)$. The conformally invariant density $\star|\Psi|^4 = \mathrm{e}^{-\sqrt{3}X}|\widetilde{\Psi}|^4\mathrm{d}\alpha\wedge\mathrm{d}\beta_+\wedge\mathrm{d}\beta_-\wedge\mathrm{d}A_z$ goes to zero at the singular boundary. We conclude that the singularity can be avoided by all three criteria imposed in section 2.2.5.

3.2 Kantowski-Sachs

As already mentioned in section 2.1.2, the Kantowski-Sachs spacetime is the only spatially homogeneous cosmological model which is not covered by the Bianchi classification. The isometry group of the models is $\mathbb{R} \times SO(3)$. The Kantowski-Sachs model is particularly interesting. It was already noticed by Kantowski and Sachs [112] that the vacuum solutions are in fact the interior part of the Schwarzschild spacetime.

3.2.1 The Kantowski-Sachs metric

We have visualized the topology of constant time hypersurfaces $\Sigma = \mathbb{R} \times S^2$ in figure 3.6a. Note that it is in principle possible to compactify the spatial hypersurfaces by imposing periodic boundary conditions as shown in figure 3.6b. The topology of the spatial hypersurfaces then becomes $S^1 \times S^2$. We will refer to this three–dimensional manifold as the Kantowski-Sachs torus.



(a) Kantowski-Sachs cylinder.

(b) Compactification to Kantowski-Sachs torus.

Figure 3.6: Visualization of the topology of the Kantowski-Sachs universe.

The spacetime manifold is given by $M = \mathbb{R} \times \Sigma$ and we equip it with the spherical class of Kantowski-Sachs metrics.[1] The line element is given by

$$\mathrm{d}s^2 = -N^2 \mathrm{d}t^2 + z^2 \mathrm{d}r^2 + b^2 \mathrm{d}\Omega^2 \ , \tag{3.98}$$

where $b = b(t)$, $z = z(t)$ and $\mathrm{d}\Omega^2 = \mathrm{d}\vartheta^2 + \sin^2 \vartheta \mathrm{d}\varphi^2$ is the standard metric on S^2. The model

[1] There also exists a flat and open version of the metric. These are however just special cases of the Bianchi type I and Bianchi type III model which are obtained by imposing additional symmetries [31].

possesses four spacelike Killing vector fields

$$\begin{aligned}\eta &= \partial_r \ , \quad \sigma_1 = \partial_\varphi \ , \\ \sigma_2 &= \sin\varphi\ \partial_\vartheta + \cot\vartheta\cos\varphi\ \partial_\varphi \ , \\ \sigma_3 &= \cos\varphi\ \partial_\vartheta - \cot\vartheta\sin\varphi\partial_\varphi\end{aligned} \tag{3.99}$$

that obey the Killing algebra

$$[\sigma_i, \sigma_j] = \sum_{i,j} \varepsilon_{ijk}\sigma_k \quad \text{and} \quad [\eta, \sigma_i] = 0 \quad \text{for } i, j, k = 1, 2, 3 \ . \tag{3.100}$$

It will turn out to be useful to switch to another set of configuration space variables defined by

$$a^3 := zb^2 \quad \text{and} \quad s := \mathrm{e}^{-3\sigma} := \frac{z}{b} \ . \tag{3.101}$$

The metric then becomes

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + a^2(\mathrm{e}^{-4\sigma}\mathrm{d}r^2 + \mathrm{e}^{2\sigma}\mathrm{d}\Omega^2) \ . \tag{3.102}$$

The shear factor s controls the shape of the universe and the scale factor a controls the volume of the spatially homogeneous hypersurfaces. If we define $\alpha := \ln a$ then α and σ play the role of Misner type variables. The inverse transformation reads

$$b = a\mathrm{e}^{\sigma} \ , \quad z = a\mathrm{e}^{-2\sigma}. \tag{3.103}$$

We will encounter the following types of singularities in this thesis:

- Disklike singularities with $z \to 0$ and therefore $a \to 0$ and $\sigma \to \infty$. As we will see, such singularities can be part of a horizon and hence coordinate singularities. If this is the case the model is incomplete.

- Cigarlike singularities for which $b \to 0$.

- We will see that also a third kind of singularity is possible for which both z and b approach zero at the same time.

The Weyl squared scalar of the Kantowski-Sachs universe reads

$$C_{\mu\nu\lambda\sigma}C^{\mu\nu\lambda\sigma} = \frac{3}{4}\left[\frac{1}{b^2} + \frac{N\ddot{z} - \dot{N}\dot{z}}{N^3 z}\right]^2 \ . \tag{3.104}$$

Therefore $b \to 0$ seems to be a good indicator for the presence of a curvature singularity.

Particles moving in the r-direction with a four velocity $\boldsymbol{u} = \frac{1}{N}\sqrt{\frac{P^2}{z^2} - K}\partial_t + \frac{P}{z^2}\partial_r$ move on geodesics. $K = -1$ for timelike geodesics and $K = 0$ for lightlike geodesics. The parameter P is the constant of motion associated with the spacelike killing vector field $\eta = \frac{\partial}{\partial r}$. In the case $K = -1$ it is the momentum per rest mass of the particle. If $K = 0$ the parameter P is the wave number of the lightlike particle. Setting $K = -1$ and $P = 0$ shows that observers comoving with the coordinates r, ϑ and φ move on geodesics. Furthermore, if we gauge $N = 1$ then t is the comoving time of these observers.

3.2.2 Hamiltonian formulation

The Ricci scalar of the Kantowski-Sachs spacetime reads

$$R = \frac{6}{N^2 a^2}\left(\dot{a}^2 + a^2\dot{\sigma}^2 + a\ddot{a} - a\dot{a}\frac{\dot{N}}{N}\right) + {}^{(3)}R\ , \tag{3.105}$$

where the three–curvature is given by ${}^{(3)}R = \frac{2e^{-2\sigma}}{a^2} = \frac{2}{b}$. The trace of the extrinsic curvature is given by

$$K = \frac{3\dot{a}}{Na}\ . \tag{3.106}$$

Furthermore, the determinants of the four and three metrics are given by

$$\begin{aligned} \sqrt{-g} &= Na^3 \sin\theta \\ \sqrt{h} &= a^3 \sin\theta \end{aligned} \tag{3.107}$$

By plugging the symmetry-reduced ansatz into the Einstein-Hilbert action (2.39) we obtain

$$S = \frac{\mathcal{I}}{2\mathrm{G}}\int \mathrm{d}t \left[-\frac{3a\dot{a}^2}{N} + \frac{3a^3\dot{\sigma}^2}{N} + N\left(a\mathrm{e}^{-2\sigma} - \Lambda a^3\right)\right]\ , \tag{3.108}$$

where $\mathcal{I} := \int_I \mathrm{d}r$ is a compactification parameter. We set $\mathrm{G} = 1$ in the following. The gravitational Lagrangian is then given by

$$L = \frac{\mathcal{I}}{2}\left[-\frac{3a\dot{a}^2}{N} + \frac{3a^3\dot{\sigma}^2}{N} + N\left(a\mathrm{e}^{-2\sigma} - \Lambda a^3\right)\right]\ . \tag{3.109}$$

If we switch to the variable $\alpha := \ln a$ it becomes

$$L = \frac{\mathcal{I}}{2}\left[\frac{3\mathrm{e}^{3\alpha}}{N}\left(-\dot{\alpha}^2 + \dot{\sigma}^2\right) - Ne^{3\alpha}\left(\Lambda - \mathrm{e}^{-2(\alpha+\sigma)}\right)\right]\ . \tag{3.110}$$

Expressed in terms of z and b the Lagrangian reads

$$L = \frac{\mathcal{I}}{2}\left(-\frac{2b\dot{b}\dot{z}}{N} - \frac{z\dot{b}^2}{N} - N\Lambda z b^2 + Nz\right) . \tag{3.111}$$

We can read off the minisuperspace potential $\mathcal{V}(z,b) = \frac{\mathcal{I}z(\Lambda b^2-1)}{2}$. In particular, if $\Lambda = 0$, the potential is negative everywhere. Consequently the trajectory of the universe point will be "spacelike" in $\mathcal{M}$ and the universe can recollapse. The conditions under which the matter filled model recollapses were studied in [60].

Note that under the transformation

$$z \mapsto c \cdot z \ , \quad \text{with } c \in \mathbb{R} \tag{3.112}$$

the gravitational Lagrangian transforms as $L \mapsto c \cdot L$. The resulting equations of motions will therefore be invariant under the transformation, i.e. the transformation (3.112) maps solutions into solutions. Furthermore, the rescaling symmetry enables us to absorb the compactification parameter $\mathcal{I}$ into z. This symmetry can be explicitly broken by adding matter to the system.

For the study of both the classical as well as the quantum dynamics it is helpful to introduce yet another parametrization of the minisuperspace. A useful set of minisuperspace coordinates is defined by the following transformation

$$\bar{\alpha} := \alpha - \frac{1}{2}\sigma \ , \qquad \bar{\phi} := \sigma - \frac{1}{2}\alpha \quad \text{and} \quad N =: 2\bar{N}\mathrm{e}^{\bar{\alpha}+2\bar{\phi}} \ . \tag{3.113}$$

The inverse transformation of the configuration space variables is

$$\alpha = \frac{4}{3}\bar{\alpha} + \frac{2}{3}\bar{\phi} \quad \text{and} \quad \sigma = \frac{4}{3}\bar{\phi} + \frac{2}{3}\bar{\alpha} \ . \tag{3.114}$$

Note that the transformation can be regarded as a combination of a Lorentz-boost and a rescaling of the minisuperspace coordinates. The Lagrangian now becomes

$$L = \mathcal{I}\left[\frac{\mathrm{e}^{3\bar{\alpha}}}{\bar{N}}\left(\dot{\bar{\phi}}^2 - \dot{\bar{\alpha}}^2\right) + \bar{N}\mathrm{e}^{\bar{\alpha}}\right] \ , \tag{3.115}$$

while the Hamiltonian constraint reads

$$\dot{\bar{\alpha}}^2 - \dot{\bar{\phi}}^2 + \bar{N}^2\mathrm{e}^{-2\bar{\alpha}} = 0 \ . \tag{3.116}$$

This corresponds to the Friedmann equation of a closed universe with a minimally coupled scalar field. Since $\bar{\phi}$ is cyclic we now have

$$\bar{\kappa} := \frac{2\mathcal{I}\mathrm{e}^{3\bar{\alpha}}}{\bar{N}}\dot{\bar{\phi}} = constant \; . \tag{3.117}$$

The transformation exposed an internal symmetry of the system. If we think about the Kantowski-Sachs as the Schwarzschild interior the corresponding constant of motion $\bar{\kappa}$ will be proportional to the Schwarzschild mass M. If we plug the constant of motion into the Friedmann equation we get

$$\frac{\mathrm{d}\bar{\phi}}{\mathrm{d}\bar{\alpha}} = \pm \frac{\frac{\bar{\kappa}}{2\mathcal{I}}}{\sqrt{\frac{\bar{\kappa}^2}{4\mathcal{I}^2} - \mathrm{e}^{4\bar{\alpha}}}} \; , \tag{3.118}$$

from which we obtain the configuration space trajectories

$$\bar{\phi}(\bar{\alpha}) = \pm\frac{1}{2}\mathrm{arcosh}\left(\frac{\bar{\kappa}}{2\mathcal{I}e^{2\bar{\alpha}}}\right) + C \; . \tag{3.119}$$

The Quantum Cosmology of the closed Friedmann universe with one minimally coupled massless scalar field was extensively discussed in [10] and in more detail in [104]. We will return to the discussion of the classical vacuum solution in section 3.2.3. We remark that the dust solution was first given by Kantowski and Sachs in their original paper [112]. The Quantum Cosmology of the model filled with dust was discussed in great detail by Conradi [113].

The canonical momenta conjugate to the configuration space variables a and p_σ are given by

$$p_a = -\frac{3\mathcal{I}a\dot{a}}{N} \; , \quad p_\sigma = \frac{3\mathcal{I}a^3\dot{\sigma}}{N} \; . \tag{3.120}$$

The Hamiltonian is then obtained by the usual Legendre transform

$$H = \frac{N}{2\mathcal{I}}\left[-\frac{p_a^2}{3a} + \frac{p_\sigma^2}{3a^3} + \mathcal{I}\left(\Lambda a^3 - a\mathrm{e}^{-2\sigma}\right)\right] = N\mathcal{H} \; . \tag{3.121}$$

If we switch to the variable $\alpha := \ln a$ and its conjugate momentum $p_\alpha = ap_a$ the Hamiltonian becomes

$$H = \frac{N}{2\mathcal{I}}\left[\frac{\mathrm{e}^{-3\alpha}}{3}\left(-p_\alpha^2 + p_\sigma^2\right) + \mathcal{I}^2\mathrm{e}^{3\alpha}\left(\Lambda - \mathrm{e}^{-2[\alpha+\sigma]}\right)\right] \; . \tag{3.122}$$

The diffeomorphism constraints are all trivially satisfied, that is H is the full Hamiltonian of the system. The canonical momenta of z and b are given by

$$p_z = -\frac{\mathcal{I}b\dot{b}}{N} \; , \qquad p_b = -\frac{\mathcal{I}(zb)^{\cdot}}{N} \; . \tag{3.123}$$

In these variables the Hamiltonian is given by

$$H = \frac{N}{2\mathcal{I}} \left[-\frac{2p_z p_b}{b} + \frac{z p_z^2}{b^2} + \mathcal{I}^2 \left(\Lambda z b^2 - z \right) \right] . \tag{3.124}$$

3.2.3 Cosmological constant and electromagnetic field

In this section we consider a Kantowski-Sachs universe filled with a cosmological constant and an electromagnetic field. The general solution to the classical field equations turns out to be the interior Reissner-Nordström-DeSitter solution as was already noted by the authors of [114]. The Wheeler-DeWitt equation also turns out to be analytically solvable by using the symmetries of the model.

Coupling of electromagnetic field

The Lagrangian density of Maxwell's theory minimally coupled to gravity is given by

$$\mathcal{L}_{\text{Maxwell}} = -\frac{1}{16\pi} F_{\mu\nu} F^{\mu\nu} . \tag{3.125}$$

We expand the one-form vector potential as

$$\boldsymbol{A} = A_t \mathrm{d}t + A_r \mathrm{d}r + A_\vartheta \mathrm{d}\vartheta + A_\varphi \mathrm{d}\varphi . \tag{3.126}$$

The field strength tensor is then obtained by $\mathbf{F} = \mathrm{d}\mathbf{A}$. The Faraday two-form should respect the symmetries of the Kantowski-Sachs spacetime. Therefore we demand that $\mathcal{L}_{\mathbf{v}}\mathbf{F} = 0$ for $\mathbf{v} = \eta, \sigma_i$ $(i = 1, 2, 3)$ being the Killing vector fields of the Kantowski-Sachs spacetime. This restricts the form of $\mathbf{F}$ to

$$\begin{aligned} &\mathbf{F} = -E_r \mathrm{d}t \wedge \mathrm{d}r + B_r \sin\vartheta \; \mathrm{d}\vartheta \wedge \mathrm{d}\varphi , \quad \text{where} \\ &E_r = E_r(t) \quad \text{and} \quad B_r = B_r(t) . \end{aligned} \tag{3.127}$$

Further demanding $\mathrm{d}\mathbf{F} = 0$ requires $B_r = \textit{constant}$. This fixes the four potential up to admissible gauge transformations to be of the form

$$\begin{aligned} A_t &= c_r(t) r , & A_r &= A_r(t) \\ A_\vartheta &= \int^\varphi c_\varphi(\vartheta, \phi) \mathrm{d}\phi , & A_\varphi &= c_\varphi(\vartheta, \varphi) - B_r \cos\vartheta \end{aligned} \tag{3.128}$$

Since c_r can in principle be absorbed into A_r we will set it to zero. The electric field is then given by $E_r = -\dot{A}_r$. The form of the function c_φ is irrelevant as well since it will not appear in the action anyways. The action for the four potential then becomes

$$
\begin{aligned}
S_{\text{Maxwell}} &= \int \mathrm{d}^4x \, \sqrt{-g} \, \mathcal{L}_{\text{Maxwell}} \\
&= \frac{\mathcal{I}}{2} \int \mathrm{d}t \left[\frac{a\mathrm{e}^{4\sigma}}{N} \dot{A}_r^2 - \frac{N\mathrm{e}^{-4\sigma}}{a} B_r^2 \right]
\end{aligned}
\tag{3.129}
$$

Note that, in contrast to a scalar field, A_r couples to both the scale and shape factors. Note also that the conformal invariance of Maxwell's theory enables us to cancel the coupling to the scale factor by rescaling the lapse according to $N \mapsto \bar{N} = N/a$ ($\bar{N} = 1$ is the conformal time gauge).

Electric field and cosmological constant

Expressed in terms of z and b the Lagrangian of the electromagnetic four potential reads

$$
L_{\text{Maxwell}} = \frac{\mathcal{I}}{2} \left[\frac{b^2 \dot{A}_r^2}{zN} - \frac{NzC_M^2}{b^2} \right] , \tag{3.130}
$$

where $C_M = B_r$ In the following we use the variable $A := -A_r$. Note that $\dot{A} = E_r$ is the electric field in the r-direction. The full Lagrangian is now given by

$$
L = \frac{\mathcal{I}}{2} \left(-\frac{2b\dot{b}\dot{z}}{N} - \frac{z\dot{b}^2}{N} + \frac{b^2 \dot{A}_r^2}{zN} - \frac{NzC_M^2}{b^2} - N\Lambda z b^2 + Nz \right) . \tag{3.131}
$$

As usual it should be checked if the symmetry reduced Lagrangian yields the correct equations of motion. We will not do so here. The correctness of the Lagrangian will only be justified later by the fact that it yields the correct solution to the field equations which is the Reissner-Nordström-DeSitter solution.

Since $\frac{\partial L}{\partial A} = 0$ the canonical momentum p_A is a constant of motion, that is

$$
C_E := \frac{b^2 \dot{A}}{zN} = \mathit{constant} . \tag{3.132}
$$

The constant C_E will later be identified as an electric charge while C_M can in principle be identified with a magnetic charge. Variation of the action with respect to N yields the Hamiltonian constraint

$$
z\dot{b}^2 + 2b\dot{z}\dot{b} + N^2 \left(1 - \Lambda b^2 - \frac{C_E^2 + C_M^2}{b^2} \right) z = 0 , \tag{3.133}
$$

where we already made use of equation (3.132). By varying the action in z we obtain the field equation

$$\dot{b}^2 + N^2\left(1 - \Lambda b^2 - \frac{C_E^2 + C_M^2}{b^2}\right) + 2\left(\ddot{b} - \frac{\dot{N}}{N}\dot{b}\right) b = 0 \ . \tag{3.134}$$

After multiplying this expression with $\dot{b}/N^2$ it can be written as a total time derivative:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[b\left(\frac{\dot{b}^2}{N^2} + 1 - \frac{\Lambda}{3}b^2 + \frac{C_E^2 + C_M^2}{b^2}\right)\right] = 0 \ . \tag{3.135}$$

Integration in t now yields

$$\frac{\dot{b}^2}{N^2} + 1 - \frac{\Lambda}{3}b^2 - \frac{b_*}{b} + \frac{C_E^2 + C_M^2}{b^2} = 0 \ , \tag{3.136}$$

where b_* is another constant of motion. If we now make the ansatz $z = z(b)$ and replace $\dot{b}^2$ in the Hamiltonian constraint (3.133), we obtain the equation

$$\frac{z'}{z} = \frac{1}{2}\left(\frac{1 - \Lambda b^2 - \frac{C_E^2}{b^2}}{b - \frac{\Lambda}{3}b^3 - b_* + \frac{C_E^2 + C_M^2}{b}} - \frac{1}{b}\right) \ . \tag{3.137}$$

Integration then yields the configuration space trajectory

$$z(b) = z_*\sqrt{\frac{b_*}{b} + \frac{\Lambda}{3}b^2 - \frac{C_E^2 + C_M^2}{b^2} - 1} \ . \tag{3.138}$$

Note that the integration constant z_* can be absorbed into the r-coordinate. After fixing the gauge $N = b$ the "energy" equation (3.136) can be written as

$$\dot{b}^2 + V_{\text{eff}}(b) = 0 \ , \quad \text{where} \quad V_{\text{eff}}(b) = b^2 - \frac{\Lambda}{3}b^4 - b_* b + C_E^2 + C_M^2 \ . \tag{3.139}$$

In this gauge the constant of motion $C_E^2 + C_M^2$ acts like an energy offset. One can now analyze the behavior of the solutions by plotting the effective potential for different cases (for an example see subsection 3.2.3).

Performing now the coordinate transformation defined by

$$t \to \bar{t} := b(t) \ , \qquad r \to \bar{r} := z_* r \ , \tag{3.140}$$

brings the metric into the form

$$\mathrm{d}s^2 = -\frac{1}{\frac{2M}{\bar{t}} + \frac{\Lambda}{3}\bar{t}^3 - \frac{Q_E^2+Q_M^2}{\bar{t}^2} - 1}\mathrm{d}\bar{t}^2 + \left(\frac{2M}{\bar{t}} + \frac{\Lambda}{3}\bar{t}^3 - \frac{Q_E^2 + Q_M^2}{\bar{t}^2} - 1\right)\mathrm{d}\bar{r}^2 + \bar{t}^2\mathrm{d}\Omega^2 \ , \quad (3.141)$$

where we made the identifications $b_* =: 2M$, $C_E =: Q_E$ and $C_M =: Q_M$. This metric is indeed the interior of the Reissner-Nordström-DeSitter solution. We conclude that it has a coordinate singularity and that it can be analytically extended beyond the horizons. This works of course only if no compactifications have been imposed. If, however, a compactification is imposed the magnetic and electric field lines are closed and there is no electric charge and also no magnetic monopole. This is why we decided to keep the parameter Q_M to be non-zero. In the following we take a look at special cases of this solution.

Vacuum solution

In the vacuum case the "energy" equation (3.136) reads

$$\frac{\dot{b}^2}{N^2} + 1 - \frac{\Lambda}{3}b^2 - \frac{b_*}{b} = 0 \ , \quad (3.142)$$

where b_* is a constant motion that arises after integration. The equation fixes the classical range of the constant of motion $b_* \geq b\,(1 - \Lambda b^2/3)$. If $\Lambda = 0$ the constant b_* is the maximum of $b(t)$. This will become important in the later study of the corresponding quantum model. In phase space the constant of motion reads

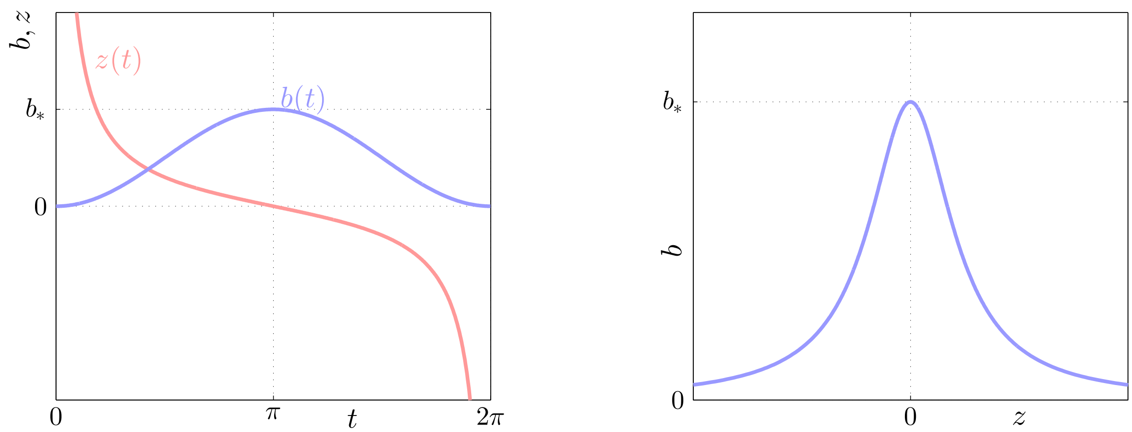
$$b_* = \frac{1}{\mathcal{I}^2 b}p_z^2 + b\left(1 - \frac{\Lambda}{3}b^2\right) \ . \quad (3.143)$$

In the case $\mathcal{I} = \infty$ the constant of motion can be identified as $b_* = 2M$, where M is the mass of the black hole, as we will see in the following . We now turn to the case $\Lambda = 0$ and choose the gauge $N = b$. Then

$$b(t) = b_* \sin^2\left(\frac{t - t_0}{2}\right) \quad \text{and} \quad z(t) = z_* \cot\left(\frac{t-t_0}{2}\right) \ , \quad (3.144)$$

where the constant $z_* \in \mathbb{R}$ is independent of b_* and can be absorbed into the coordinate r. The configurations space trajectory (3.138) reduces to

$$z(b) = z_*\sqrt{\frac{b_*}{b} - 1} \ . \quad (3.145)$$



(a) Plots of z and b versus t.

(b) Configuration space trajectory.

Figure 3.7: Plots of z and b. The universe emerges out of a cigarlike singularity collapses to a disklike singularity and goes back to the cigarlike singularity.

In terms of the scale and shear factor the solution reads

$$a(t) = a_* \sin\left(\frac{t-t_0}{2}\right)\cos^{\frac{1}{3}}\left(\frac{t-t_0}{2}\right) \quad \text{and} \quad s(t) := \frac{z(t)}{b(t)} = s_* \frac{\cos\left(\frac{t-t_0}{2}\right)}{\sin^3\left(\frac{t-t_0}{2}\right)} \, , \tag{3.146}$$

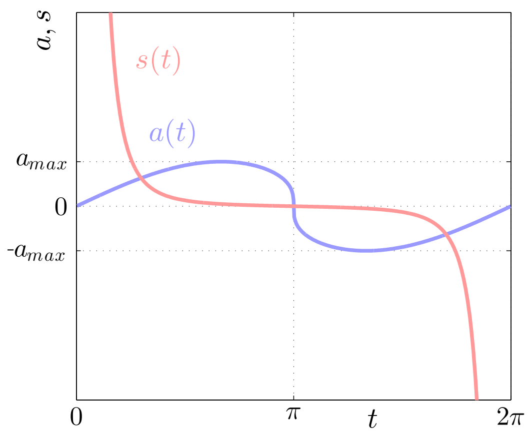
where $a_* = \sqrt[3]{z_* b_*^2}$ and $s_* = z_*/b_*$. The maximal and minimal scale factors $a_{max/min} = \pm 2^{-\frac{4}{3}}\sqrt{3} a_*$ are reached at $t - t_0 = \frac{2\pi}{3}$ and $t - t_0 = \frac{4\pi}{3}$. In the vacuum case the metric (3.141) reduces to the interior Schwarzschild metric:

$$\mathrm{d}s^2 = -\frac{1}{\frac{2M}{\bar{t}} - 1}\mathrm{d}\bar{t}^2 + \left(\frac{2M}{\bar{t}} - 1\right)\mathrm{d}\bar{r}^2 + \bar{t}^2 \mathrm{d}\Omega^2 \, . \tag{3.147}$$

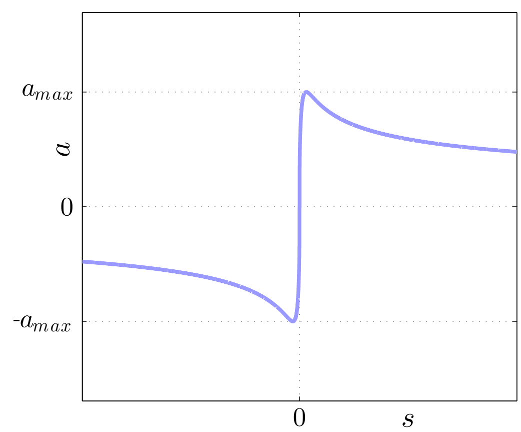
If we now choose $t \in (0, \pi)$ the coordinate $\bar{t}$ runs from 0 to $2M$ and the metric covers the white hole region IV in the Kruskal diagram 3.9. If we had chosen $t \in (\pi, 2\pi)$, then $\bar{t}$ would range from $2M$ to 0. We see now explicitly that the disklike singularity corresponds to the intersection of the Schwarzschild horizons.

It is instructive to visualize the compactified vacuum solution. Equivalence relations can be imposed at some constant values r_1 and $r_2 > r_1$. The resulting Kantowski-Sachs torus can then be plotted in a Kruskal diagram (see figure 3.9b).

Having the Oppenheimer-Snyder solution in mind, it should also be clear that it is possible to glue a Friedmann universe to the Kantowski-Sachs spacetime at some fixed radius. The matching and the Quantum Cosmology of the resulting model have been discussed by Conradi [113].

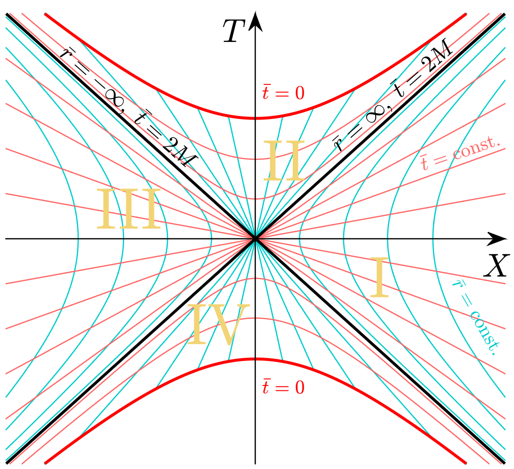


(a) a, s versus t

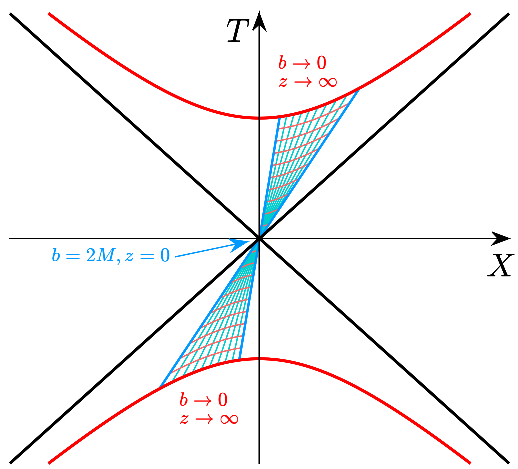


(b) configurations space trajectory

Figure 3.8: plots of a and s.



(a) The Kruskal diagram shows the maximally analytic extension of the Schwarzschild spacetime. The red lines in the interior regions (II and IV) correspond to the Kantowski-Sachs cylinder at different stages of its temporal evolution.



(b) This Kruskal diagram shows the Kantowski-Sachs torus for a specific choice of compactification. After compactification the disklike singularity (bifurcation point in the Kruskal diagram) turns into a conic singularity.

Figure 3.9: Kruskal diagrams.

Vanishing cosmological constant

In the following we concentrate on the solutions with $\Lambda = 0$ and a non-vanishing electromagnetic field. This case corresponds to the interior Reissner-Nördstrom solution if no compactifications are imposed. We choose the gauge $N = b$ and write the equation of motion for b as

$$\dot{b}^2 + \left(b - \frac{b_*}{2}\right)^2 = \frac{b_*^2}{4} - C_E^2 \, . \tag{3.148}$$

This is just the energy equation of a harmonic oscillator with an energy $\frac{b_*^2}{4} - C_E^2$ that oscillates around the minimum of the potential at $b_*/2$. The solution is given by

$$b(t) = \frac{1}{2}\left(b_* + \sqrt{b_*^2 - 4C_E^2}\,\sin(t - t_0)\ .\right) \tag{3.149}$$

For the solutions to be physically viable we have to demand that $|C_E| < b_*/2$. In the case $C_E = 0$ the solution reduces to that of the vacuum case with $\Lambda = 0$ and we obtain a cigarlike and disklike singularity. For $0 < |C_E| < b_*/2$ the cigarlike singularity vanishes and the solution oscillates through disklike coordinate singularities. This is plotted in figure 3.10. The plot in figure 3.10 can be identified with the black and white hole regions in the Penrose diagram of the Reissner-Nordström solution (see e.g. [1] for the Penrose diagramm). The points where $z = 0$ correspond to the bifurcation points.

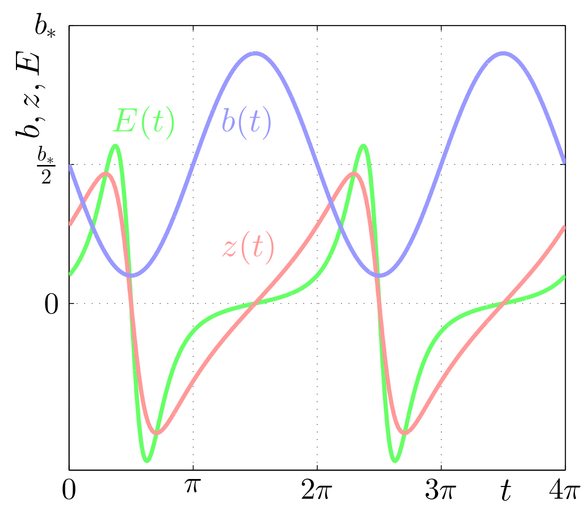


Figure 3.10: Plot of z, b and E versus t in the gauge $N = b$.

The energy momentum tensor of the electromagnetic field is given by

$$\{T^\mu{}_\nu\} = \frac{C_E^2}{8\pi b^4}\,\mathrm{diag}\,(-1,\ -1,\ 1,\ 1)\ . \tag{3.150}$$

We can now interpret the energy-momentum tensor as that of a fluid and read off energy density and pressure

$$\rho = -p_r = p_\theta = p_\varphi = \frac{C_E^2}{8\pi b^4}\ . \tag{3.151}$$

The pressure in the θ and φ direction rises when b approaches 0. Instead of a cigarlike singularity, as in the vacuum case, the universe encounters a bounce due to the increasing pressure in the θ and φ directions.

General solution for $M \neq 0$, $Q \neq 0$ and $\Lambda \neq 0$.

The configuration space trajectory is given by

$$z(b) = z_* \sqrt{\frac{b_*}{b} + \frac{\Lambda}{3} b^2 - \frac{C_E^2}{b^2} - 1}\,, \tag{3.152}$$

and the effective potential can be written as

$$V_{\text{eff}}(b) = \left(b - \frac{b_*}{2}\right)^2 - \frac{\Lambda}{3} b^4 + C_E^2 - \frac{b_*^2}{4}\,. \tag{3.153}$$

The potential and configuration space trajectory are plotted now for an exemplary case in figure 3.11. For the plot we choose the gauge $N = b$. Note that when $b \gg b_*$ and $\Lambda > 0$ we have $z \sim b$ and the shape becomes constant. The scale factor behaves as $a(t) \propto b(t) \sim \mathrm{e}^{\sqrt{\frac{\Lambda}{3}} t}$ in this limit. Consequently these solutions undergo inflation and isotropize at late times.

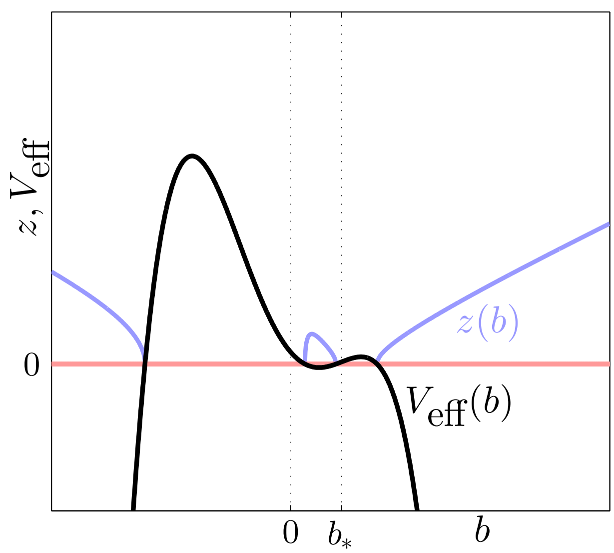


Figure 3.11: $\Lambda = 0.5$, $b_* = 1$ and $C_E = 0.45$. We see three particular solutions. The left one has no physical meaning. The middle one oscillates between two disklike singularities such as the solution in figure 3.10. The right solution is reflected at a disklike singularity. Its large b limit is the interior DeSitter solution. If no compactification is imposed the solutions correspond to a particular case of the Reissner-Nordström-DeSitter solution and the disklike singularities are in fact part of a horizon.

Wheeler-DeWitt equation

In this subsection we will derive and solve the Wheeler-DeWitt equation for a Kantowski-Sachs torus filled with a cosmological constant and an electromagnetic field. Conradi [113] already derived and solved the Wheeler-DeWitt equation for an effective dust potential and a cosmological constant. The Wheeler-DeWitt equation Conradi obtained in Laplace-Beltrami factor ordering for the vacuum case reads

$$\hat{\mathcal{H}}\Psi = \left[-\frac{1}{2b^2\mathcal{I}}\left(z\frac{\partial^2}{\partial z^2}+\frac{\partial}{\partial z}-2b\frac{\partial^2}{\partial z\partial b}\right)+\frac{\mathcal{I}}{2}\left(\Lambda z b^2 - z\right)\right]\Psi = 0\ . \tag{3.154}$$

An important step in Conradis deriviation of the solution to the Wheeler-DeWitt equation was the recovery of a quantum operator $\hat{b}_*$ that corresponds to the classical constant of motion (3.143). Most importantly $\hat{b}_*$ commutes with $\mathcal{H}$ and therefore its eigenvalues represent good quantum numbers. Hence the quantum model possesses the same symmetry as the classical model. The full Hamiltonian of the system under consideration is given by

$$H = \frac{N}{2\mathcal{I}}\left[-\frac{2p_z p_b}{b}+\frac{z}{b^2}(p_z^2+p_A^2+\mathcal{I}^2 Q_M^2)+\mathcal{I}^2\left(\Lambda z b^2 - z\right)\right] \tag{3.155}$$

By writing the Hamiltonian constraint as

$$\mathcal{H} = \frac{1}{2}\mathcal{G}^{AB}p_A p_B + \mathcal{V}(z,b)\ , \tag{3.156}$$

we can read off the components of the inverse DeWitt-metric and the minisuperspace potential

$$\{\mathcal{G}^{AB}\} = \frac{1}{\mathcal{I}b}\begin{pmatrix} z/b & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & z/b \end{pmatrix}\ , \qquad \mathcal{V}(z,b) = \frac{\mathcal{I}}{2}\left(\Lambda z b^2 - z\right)+\frac{z}{2\mathcal{I}b^2}\mathcal{I}^2 Q_M^2 \tag{3.157}$$

where $\{q^A\} = \{z, b, A\}$. The Ricci scalar is given by $\mathcal{R} = -\frac{5}{2\mathcal{I}zb^2}$. Note that the DeWitt metric is not conformally flat.[2] The Hamiltonian constraint operator in conformal factor ordering is given by

$$\hat{\mathcal{H}} = \frac{1}{4zb^2\mathcal{I}}\left[-2z^2\left(\frac{\partial^2}{\partial z^2}+\frac{\partial^2}{\partial A^2}\right)-\frac{b}{z}\frac{\partial}{\partial b}+z\frac{\partial}{\partial z}+4bz\frac{\partial^2}{\partial z\partial b}+5\xi\right]+\mathcal{V}(z,b)\ , \tag{3.158}$$

where $\xi = 1/8$. We now perform a conformal transformation of the DeWitt metric with a conformal factor $\Omega = \sqrt{z}/b$. The wave function then transforms as

$$\Psi \to \widetilde{\Psi} := \sqrt{\frac{b}{\sqrt{z}}}\Psi\ . \tag{3.159}$$

[2]Since the minisuperspace is 3-dimensional this can be checked by computing the Cotton tensor and seeing that its components are non-vanishing (e.g. by using the xAct package xCoba to get a quick answer).

From the relation $\hat{\mathcal{H}}\Psi = \Omega^{\frac{5}{2}}\hat{\tilde{\mathcal{H}}}\tilde{\Psi}$ we obtain

$$\hat{\tilde{\mathcal{H}}} = \frac{b^2}{2\mathcal{I}}\left[-\frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial A^2} - \frac{2}{z}\frac{\partial}{\partial z} + \frac{2b}{z}\frac{\partial^2}{\partial z \partial b} + \frac{40\xi - 5}{64 z^2}\right] + \frac{b^4}{z}\mathcal{V}(z,b) \ . \tag{3.160}$$

After inserting the value $\xi = 1/8$, the expression simplifies to

$$\hat{\tilde{\mathcal{H}}} = \frac{1}{\mathcal{I}z}\left[-\frac{z}{2}\left(\frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial A^2}\right) - \frac{1}{2}\frac{\partial}{\partial z} + b\frac{\partial^2}{\partial z \partial b}\right] + \frac{b^2}{z}\mathcal{V}(z,b) \ . \tag{3.161}$$

The kinetic term now coincides with that of (3.154) up to the additional term $-\partial^2/\partial A^2$ and a non-constant prefactor. Note that in contrast to the case of Bianchi I model with an electric field no (undesired) mass squared term appears in the Hamiltonian constraint operator. The Wheeler-DeWitt equation now reads

$$\left[z^2\left(\frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial A^2} - \mathcal{I}^2 Q_M^2\right) + \frac{z}{2}\frac{\partial}{\partial z} - 2zb\frac{\partial^2}{\partial z \partial b} + \mathcal{I}^2 z^2 b^2\left(1 - \Lambda b^2\right)\right]\Psi(z,b,A) = 0 \ , \tag{3.162}$$

where from now on we skip the tilde over Ψ and $\mathcal{H}$ (but keep in mind that we have performed a conformal transformation). We define the operators

$$\mathcal{I}^2\ \hat{b}_* := -\frac{1}{b}\frac{\partial^2}{\partial z^2} + \mathcal{I}^2\left(b - \frac{\Lambda}{3}b^3 + \frac{\hat{Q}_E^2 + Q_M^2}{b}\right) \quad \text{and} \quad \mathcal{I}\ \hat{Q}_E := -\mathrm{i}\frac{\partial}{\partial A} \ . \tag{3.163}$$

These operators correspond to the classical constants of motion b_* and Q_E. It holds now for the commutators of these operators that

$$\left[\hat{b}_*, zb^{-2}\hat{\mathcal{H}}\right] = 0 \ , \qquad \left[\hat{Q}_E, \hat{\mathcal{H}}\right] = 0 \quad \text{and} \quad \left[\hat{Q}_E, \hat{b}_*\right] = 0 \ . \tag{3.164}$$

Therefore they represent good quantum numbers and we can conclude that the physical symmetries were preserved during the process of quantization. The eigenvalue equations

$$\hat{Q}_E\psi = Q_E\psi \quad \text{and} \quad \hat{b}_*\Psi = 2M\psi \tag{3.165}$$

are solved by the mode functions

$$\psi^{\pm}_{M,Q_E}(z,b,A) = \Phi_{M,Q_E}(b)\exp\left[\pm\mathrm{i}\ g_{M,Q}(b)\ z + \mathrm{i}\frac{Q_E}{\mathcal{I}}A\right] \tag{3.166}$$

where

$$g_{M,Q}(b) := \mathcal{I}|b|\sqrt{\frac{\Lambda}{3}b^2 + \frac{2M}{b} - \frac{Q^2}{b^2} - 1} \tag{3.167}$$

and $Q := \sqrt{Q_M^2 + Q_E^2}$. The functional form of $\Phi_{M,Q}(b)$ is determined by plugging (3.166) into the Wheeler-DeWitt equation. This way we obtain the equation

$$\frac{\partial_b \Phi_{M,Q_E}}{\Phi_{M,Q_E}} = \frac{1}{4b} - \frac{\partial_b g_{M,Q_E}}{g_{M,Q_E}} \ , \tag{3.168}$$

which is readily solved by

$$\Phi_{M,Q}(b) \propto \frac{b^{1/4}}{g_{M,Q_E}(b)} = \frac{b^{-3/4}}{\sqrt{\frac{\Lambda}{3}b^2 + \frac{2M}{b} - \frac{Q^2}{b^2} - 1}} \ . \tag{3.169}$$

The mode functions are then obtained as

$$\psi^{\pm}_{M,Q_E,Q_M}(z,b,A) = \frac{b^{-3/4}}{\sqrt{\frac{\Lambda}{3}b^2 + \frac{2M}{b} - \frac{Q^2}{b^2} - 1}} \exp\left(\pm \mathrm{i}\mathcal{I}z|b|\sqrt{\frac{\Lambda}{3}b^2 + \frac{2M}{b} - \frac{Q^2}{b^2} - 1} + \mathrm{i}\frac{Q_E}{\mathcal{I}}A \right) \ . \tag{3.170}$$

We note the interesting fact that the mode functions are in the WKB form, that is

$$\psi^{\pm}_{M,Q_E,Q_M}(z,b,A) = \sqrt{D_{M,Q_E,Q_M}(z,b)} \exp\left(\mathrm{i}S_{M,Q_E,Q_M}(z,b,A)\right) \ , \tag{3.171}$$

where $S_{M,Q_E,Q_M}(z,b,A)$ is a solution of the Hamilton-Jacobi equation and

$$D_{M,Q_E,Q_M}(z,b) = \frac{b^{-3/2}}{\frac{\Lambda}{3}b^2 + \frac{2M}{b} - \frac{Q^2}{b^2} - 1} \tag{3.172}$$

is the corresponding Van Vleck factor. Conradi [113] also found mode functions which were in WKB form in the case of the dust model.

In the following we set $\Lambda = 0$ for simplicity. In order to obtain mode functions that are exponentially damped in the classically forbidden region and wave packets that fulfill

$$\Psi \to 0 \quad \text{as} \quad b \to \infty \tag{3.173}$$

we have to choose the mode with the plus sign. Otherwise the mode functions blow up in the classical classically forbidden region. Even if this is not a conformally invariant condition it seems reasonable to disregard the modes with the minus sign (at least in the $\Lambda = 0$ case). Wave packets are then constructed by smearing out the mode functions against a suitable momentum distribution $\mathcal{A}(M, Q_E)$:

$$\Psi(z, b, A) = \int_0^\infty \mathrm{d}M \int_{-\infty}^\infty \mathrm{d}Q_E \; \mathcal{A}(M, Q_E)\psi^+_{M,Q_E}(z, b, A) \; . \tag{3.174}$$

Singularity avoidance

A discussion of singularity avoidance, of course, only makes sense if there is a singularity. This is not the case for the model with an electromagnetic field (more precisely the singularity is located behind the horizon which is not part of the minisuperspace model under consideration). For the vacuum case (we can ignore the cosmological constant in the singular region) the Hamiltonian constraint reads

$$\mathcal{H} = \frac{1}{2\mathcal{I}} \left[\frac{\mathrm{e}^{-3\alpha}}{3} \left(-p_\alpha^2 + p_\sigma^2\right) - \mathcal{I}^2 \mathrm{e}^{3\alpha} \mathrm{e}^{-2[\alpha+\sigma]} \right] \; . \tag{3.175}$$

Close to the singular boundary of minisuperspace where $\alpha \to -\infty$ the Wheeler-DeWitt equation in conformal ordering becomes

$$\left[\frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \sigma^2} \right] \Psi = 0, \quad \text{where} \quad w(\Psi) = 0 \; . \tag{3.176}$$

This is just the $(1 + 1)$–dimensional wave equation. Hence no spreading occurs and wave packets run straight into the singular boundary without any decay of their amplitudes. To conclude: the vacuum model does not have a sufficiently large number of degrees of freedom to avoid the singularity.

3.2.4 Scalar field

In this section we couple a scalar field to the Kantowski-Sachs spacetime via the minimal coupling procedure.

The Lagrangian of a minimally coupled scalar field

The action of a homogeneous scalar field minimally coupled to the Kantowski-Sachs spacetime metric is given by

$$S_\phi = \frac{1}{2} \int \mathrm{d}^4x \, \sqrt{-g} \left[-\partial_\mu \phi \partial^\mu \phi - V(\phi) \right] = 2\pi \mathcal{I} \int \mathrm{d}t \; a^3 \left[\frac{\dot{\phi}^2}{N} - NV(\phi) \right] \; . \tag{3.177}$$

For brevity we rescale the scalar field and the potential to absorb a factor of 8π. We then get

$$L_\phi = \frac{\mathcal{I}a^3}{4}\left[\frac{\dot{\phi}^2}{N} - NV(\phi)\right] . \tag{3.178}$$

Note that the homogeneous scalar field ϕ couples only to the scale factor a and not to the sheer factor s of the Kantowski-Sachs spacetime. Furthermore, note that the coupling of the scalar field does not break the rescaling symmetry of z. The case of a non-vanishing potential is rather complicated and no exact solutions are known up to my knowledge.

Massless scalar field

We now restrict our attention to the case of a massless scalar field, that is, we set $V(\phi) = 0$. The corresponding solution was first derived in [115]. The same authors also studied a conformally coupled field in [116]. We choose here a different way for deriving the solution and make use of the fact that the dynamics of the Kantowski-Sachs universe with a minimally coupled massless scalar field are mathematically equivalent to the dynamics of a classical Friedmann universe with two minimally coupled massless scalar fields. Therefore both the classical as well as the Quantum Cosmology of these models appear to be most easily handled by using the bared variables $\bar{\alpha}$ and $\bar{\phi}$ introduced in section 3.2.1. The full Lagrangian of the system then takes the simple form

$$L = \mathcal{I}\left[\frac{\mathrm{e}^{3\bar{\alpha}}}{\bar{N}}\left(-\dot{\bar{\alpha}}^2 + \dot{\bar{\phi}}^2 + \dot{\phi}^2\right) + \bar{N}\mathrm{e}^{\bar{\alpha}}\right] . \tag{3.179}$$

Since both $\bar{\phi}$ and ϕ are cyclic variables we get

$$\frac{2\mathcal{I}\mathrm{e}^{3\bar{\alpha}}}{\bar{N}}\dot{\bar{\phi}} = \text{const.} =: \bar{\kappa} \qquad \text{and} \qquad \frac{2\mathcal{I}\mathrm{e}^{3\bar{\alpha}}}{\bar{N}}\dot{\phi} = \text{const.} =: \kappa . \tag{3.180}$$

We restrict our attention to the case $\kappa \neq 0$. This now yields that $\bar{\kappa}\dot{\phi} = \kappa\dot{\bar{\phi}}$ and integration gives

$$\kappa\bar{\phi} - \bar{\kappa}\phi = \text{const.} =: \kappa C_1 . \tag{3.181}$$

Since ϕ is either strictly increasing or decreasing we can use the scalar field as a time variable. The Hamiltonian constraint equation reads

$$\dot{\bar{\alpha}}^2 - \dot{\bar{\phi}}^2 - \dot{\phi}^2 + \bar{N}^2\mathrm{e}^{-2\bar{\alpha}} = 0 . \tag{3.182}$$

We can now eliminate $\bar{\phi}$ from the equation and obtain

$$\frac{\mathrm{d}\phi}{\mathrm{d}\bar{\alpha}} = \pm\frac{\kappa}{\sqrt{\kappa^2+\bar{\kappa}^2}}\frac{\frac{\sqrt{\kappa^2+\bar{\kappa}^2}}{2\mathcal{I}}}{\sqrt{\frac{\kappa^2+\bar{\kappa}^2}{4\mathcal{I}^2}-\mathrm{e}^{4\bar{\alpha}}}} \ . \tag{3.183}$$

An integration then gives

$$\phi(\bar{\alpha}) = \pm\frac{\kappa}{2\sqrt{\kappa^2+\bar{\kappa}^2}}\mathrm{arcosh}\left(\frac{\sqrt{\kappa^2+\bar{\kappa}^2}}{2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}}\right) + C_2 \ . \tag{3.184}$$

Finally we obtain a paramtrization of the configuration space trajectory in terms of the scalar field:

$$\begin{aligned} \exp\left(\bar{\alpha}(\phi)\right) &= \frac{\left(\kappa^2+\bar{\kappa}^2\right)^{1/4}}{\sqrt{2\mathcal{I}}}\cosh^{-1/2}\left(\frac{2\sqrt{\kappa^2+\bar{\kappa}^2}}{\kappa}\left[\phi - C_2\right]\right) \ , \\ \bar{\phi}(\phi) &= \frac{\bar{\kappa}}{\kappa}\phi - C_1 \ . \end{aligned} \tag{3.185}$$

By switching to the scale and shape variables we obtain

$$a(\phi) = \sqrt[3]{\frac{\kappa^2+\bar{\kappa}^2}{4\mathcal{I}^2}}\cosh^{-2/3}\left(\frac{2\sqrt{\kappa^2+\bar{\kappa}^2}}{\kappa}\left[\phi - C_2\right]\right)\exp\left(\frac{2}{3}\left[\frac{\bar{\kappa}}{\kappa}\phi - C_1\right]\right) \ , \tag{3.186}$$

$$s(\phi) = \frac{2\mathcal{I}}{\sqrt{\bar{\kappa}^2+\kappa^2}}\cosh\left(\frac{2\sqrt{\kappa^2+\bar{\kappa}^2}}{\kappa}\left[\phi - C_2\right]\right)\exp\left(-4\left[\frac{\bar{\kappa}}{\kappa}\phi - C_1\right]\right) \ . \tag{3.187}$$

The limits are given by

$$\begin{aligned} s(\phi) &\sim \exp\left(\frac{2}{\kappa}\left[\sqrt{\bar{\kappa}^2+\kappa^2} \mp 2\bar{\kappa}\right]|\phi|\right) \ , \\ a(\phi) &\sim \exp\left(-\frac{2}{3\kappa}\left[\sqrt{\bar{\kappa}^2+\kappa^2} \pm \bar{\kappa}\right]|\phi|\right) \qquad \text{as} \quad \phi \to \pm\infty \ . \end{aligned} \tag{3.188}$$

We now restrict attention to the case $\bar{\kappa} > 0$. Then s goes to zero if $|\kappa| < \sqrt{3}|\bar{\kappa}|$ and it blows up if $|\kappa| > \sqrt{3}|\bar{\kappa}|$ as $\phi \to \infty$. In the limiting case $|\kappa| = \sqrt{3}|\bar{\kappa}|$ it approaches a constant value. In all cases a goes to 0 when $\phi \to -\infty$.

We now derive the time dependence of the variables z and b in order to compare the solution with that of the vacuum case. By combing the equations (3.182) and (3.180) we get

$$\dot{\bar{\alpha}}^2 - \bar{N}^2\left(\frac{\kappa^2+\bar{\kappa}^2}{4\mathcal{I}^2\mathrm{e}^{6\bar{\alpha}}} - \mathrm{e}^{-2\bar{\alpha}}\right) = 0 \tag{3.189}$$

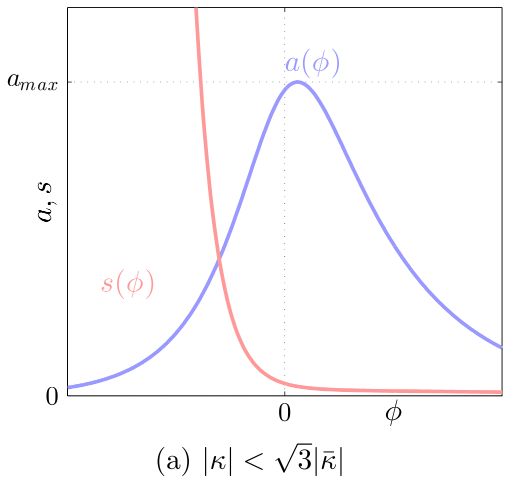


Figure 3.12: Plots of a and s versus ϕ. We choose $\bar{\kappa} > 0$ in both cases.

We now choose the gauge $\bar{N} = \mathrm{e}^{\bar{\alpha}}/2$ corresponding to $N = b$. Integration then yields

$$\mathrm{e}^{2\bar{\alpha}(t)} = \frac{\sqrt{\kappa^2 + \bar{\kappa}^2}}{2\mathcal{I}} \sin(\pm [t - t_0]) \ . \tag{3.190}$$

We choose the $+$ sign and set $t_0 = 0$ in the following. Furthermore, we take $t \in [0, \pi]$. The scalar field strength is then

$$\phi(t) - \phi(\pi/4) = \frac{\kappa}{2\sqrt{\kappa^2 + \bar{\kappa}^2}} \ln\left(\tan(t/2)\right) \ . \tag{3.191}$$

We now choose $\phi(\pi/4) = 0$. After some calculation we finally obtain

$$z(t) \propto [\tan(t/2)]^{-K} \ , \tag{3.192}$$

$$b(t) = \frac{\sqrt{\kappa^2 + \bar{\kappa}^2}}{2\mathcal{I}} \sin(t) \, [\tan(t/2)]^{K} \ . \tag{3.193}$$

where $K := \frac{\bar{\kappa}}{\sqrt{\kappa^2+\bar{\kappa}^2}}$ fulfills $-1 \leq K \leq 1$. Note that if we set the constant of motion $\kappa = 0$, identify $b_* = 2M = |\bar{\kappa}|/\mathcal{I}$ and replace $t \to t - t_0 + \pi/2$ the above expressions coincide with those obtained in the vacuum case. For the particular case $K = 0$ we have $b(t) = \frac{|\kappa|}{2\mathcal{I}} \sin(t)$ and $z(t) = const.$

What happens with the structure of the disklike singularity that was the bifurcation point of the horizon in the vacuum case? This singularity is at $t = \pi$ if $\kappa \geq 0$ and at $t = 0$ otherwise.

Let us consider the case $\kappa \geq 0$. The limits as $t \to \pi$ are then as follows:

$$z \to 0 \quad \text{for all } K \in (0, 1] \ , \tag{3.194}$$

$$b \to \begin{cases} b_* \ , & \text{when } K = 1 \\ 0 \ , & \text{when } 0 < K < 1 \ . \end{cases} \tag{3.195}$$

The energy-momentum tensor of the massless scalar field reads

$$\{T^\mu{}_\nu\} = \frac{\kappa^2}{16\mathcal{I}^2 a^6} \mathrm{diag}\,(-1,\ 1,\ 1,\ 1) \ . \tag{3.196}$$

Hence the energy density and pressure diverge as $a \to 0$. Consequently both singularities are physical. Note at this point that the massless scalar field mimics a stiff fluid, that is, it satisfies the equation of state $p = \rho$. We can obtain an expression for the Weyl squared scalar by plugging the solution $\{N(t), z(t), b(t)\}$ into (3.104). This way we obtain

$$C_{\mu\nu\lambda\sigma}C^{\mu\nu\lambda\sigma} = \frac{3\mathcal{I}\tan^{-2K}\left(\frac{t}{2}\right)\left(4\mathcal{I}\bar{\kappa}^2 + \sqrt{\kappa^2+\bar{\kappa}^2}\left[4\mathcal{I}\bar{\kappa}\cos(t) + (\kappa^2+\bar{\kappa}^2)\sin^3(t)\tan^K\left(\frac{t}{2}\right)\right]\right)}{2\left(\kappa^2+\bar{\kappa}^2\right)^2\sin^4(t)} \ . \tag{3.197}$$

For the vacuum case $\kappa = 0$ and $\bar{\kappa} > 0$ we have that $C_{\mu\nu\lambda\sigma}C^{\mu\nu\lambda\sigma} \to 3\mathcal{I}(\mathcal{I}+\bar{\kappa})/(2\bar{\kappa})^2$ as $t \to \pi$ (i.e. at the bifurcation point of the horizon). However for $\kappa > 0$ and $\bar{\kappa} > 0$ we have that $C_{\mu\nu\lambda\sigma}C^{\mu\nu\lambda\sigma} \to -\infty$ as $t \to \pi$. We conclude that the singularity at $t = \pi$ is a curvature singularity.

Let us at this point retain the following: the coupling of the massless scalar field changed the structure of the disklike singularity. It is replaced by a physical singularity for which both z and b approach zero.

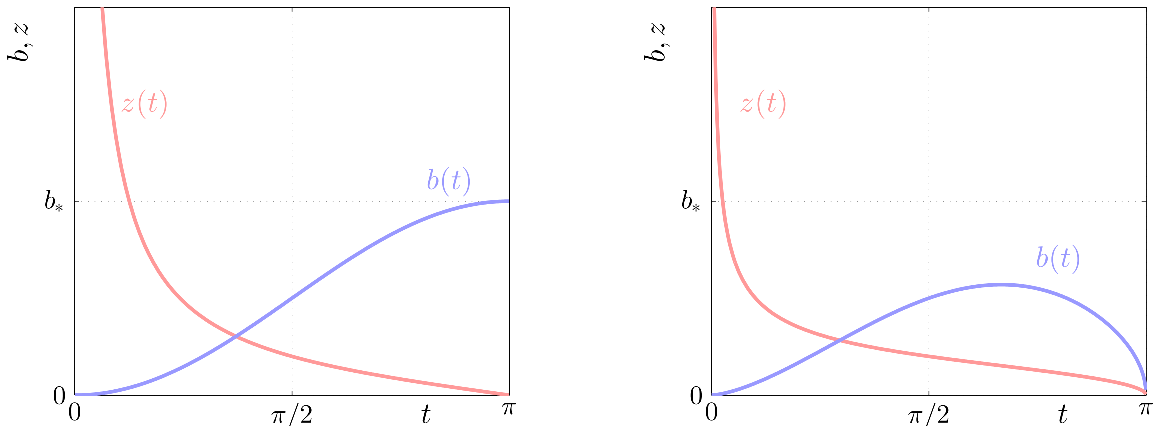
Next we perform the coordinate transformation

$$t \to \bar{t} := \frac{2M}{K}\sin^2(t/2) \ , \tag{3.198}$$

where $2M := \bar{\kappa}/\mathcal{I}$. In addition we absorb the prefactor of z into the r-coordinate. The metric then assumes the interior Schwarschild like form

$$\mathrm{d}s^2 = -\frac{1}{\left(\frac{2M}{K\bar{t}}-1\right)^K}\mathrm{d}\bar{t}^2 + \left(\frac{2M}{K\bar{t}}-1\right)^K\mathrm{d}\bar{r}^2 + \frac{\bar{t}^2}{\left(\frac{2M}{K\bar{t}}-1\right)^{K-1}}\mathrm{d}\Omega^2 \ , \tag{3.199}$$

which reduces to the interior Schwarzschild metric in the vacuum case, that is, $\kappa = 0$ and



(a) $K = 1$, corresponding to the vacuum case. The universe goes from a cigarlike singularity to a disklike singularity.

(b) $0 < K < 1$, i.e. $|\kappa| > 0$. If we switch on the scalar field the disklike singularity is turned into a physical singularity.

Figure 3.13: Plots of the t-dependence of z and b for different values of K.

$K = 1$. The $\bar{t}$ dependence of the scalar field is

$$\begin{aligned}\phi(\bar{t}) &= -\frac{\kappa}{4\sqrt{\kappa^2+\bar{\kappa}^2}}\ln\left(\frac{2M}{K\bar{t}}-1\right)\\ &= \pm\frac{1}{4}\sqrt{1-\frac{1}{K^2}}\ln\left(\frac{2M}{K\bar{t}}-1\right)\ .\end{aligned} \tag{3.200}$$

We remark on the formal similarities with the corresponding spherically symmetric solution with a massless scalar field. This is the so called Janis-Newman-Winicour-Wyman (JNWW) solution [117, 118]. This solution has a naked singularity at its center and hence violates the cosmic censorship hypothesis. It can formally be obtained from (3.199) and (3.200) by switching $\bar{r} \leftrightarrow \bar{t}$. $M = \frac{\bar{\kappa}}{2\mathcal{I}}$ will then become the ADM mass. In this sense one might formally regard the solution of the Kantowski-Sachs universe with a minimally coupled massless scalar field as the "interior" solution of a naked singularity.

Wheeler-DeWitt equation

The Hamiltonian of a scalar field coupled to the Kantowski-Sachs metric reads

$$H = \frac{N}{2\mathcal{I}}\left[\frac{\mathrm{e}^{-3\alpha}}{3}\left(-p_\alpha^2+p_\sigma^2+\frac{3}{4}p_\phi^2\right)+\mathcal{I}^2\mathrm{e}^{3\alpha}\left(\Lambda-\mathrm{e}^{-2(\alpha+\sigma)}+V(\phi)\right)\right] \tag{3.201}$$

Again, we restrict our attention to the simple case of a massless scalar field with $V = 0$ and $\Lambda = 0$. The DeWitt metric and the Ricci scalar are given by

$$\mathrm{d}\mathcal{S}^2 = 3\mathcal{I}\mathrm{e}^{3\alpha}\left(-\mathrm{d}\alpha^2 + \mathrm{d}\sigma^2 + \frac{4}{3}\mathrm{d}\phi^2\right) \quad \text{and} \quad \mathcal{R} = \frac{3}{2\mathcal{I}}\mathrm{e}^{-3\alpha}\ . \tag{3.202}$$

The Wheeler-DeWitt equation reads

$$\hat{\mathcal{H}}\Psi = \frac{1}{6\mathcal{I}\mathrm{e}^{3\alpha}}\left[\left(\frac{\partial}{\partial\alpha} + 2f\right)\frac{\partial}{\partial\alpha} - \frac{\partial^2}{\partial\sigma^2} - \frac{3}{4}\frac{\partial^2}{\partial\phi^2} - 3\mathcal{I}\xi\mathcal{R}\mathrm{e}^{3\alpha} - 3\mathcal{I}^2\mathrm{e}^{4\alpha-2\sigma}\right]\Psi = 0 \tag{3.203}$$

where the factor ordering is partially left open as indicated by the presence of the parameters f and ξ. The Laplace-Beltrami factor ordering is obtained by setting $f = 3/4$ and $\xi = 0$. Setting $\xi = 1/8$ instead gives the conformal factor ordering. Note that if $f < 0$ the wave equation is damped while for $f > 0$ it is driven. Now we define

$$\mathrm{e}^{-f\alpha}\widetilde{\Psi} := \Psi\ . \tag{3.204}$$

The Wheeler-DeWitt equation $\hat{\mathcal{H}}\Psi = 0$ then becomes

$$\left[\frac{\partial^2}{\partial\alpha^2} + f^2 - \frac{\partial^2}{\partial\sigma^2} - \frac{3}{4}\frac{\partial^2}{\partial\phi^2} - \frac{9\xi}{2} - 3\mathcal{I}^2\mathrm{e}^{4\alpha-2\sigma}\right]\widetilde{\Psi}\left(\alpha,\sigma,\phi\right) = 0 \tag{3.205}$$

In this representation $\frac{9\xi}{2} - f^2$ can be interpreted as a mass squared term. If $f^2 > \frac{9\xi}{2}$ the mass is imaginary and solutions to the Wheeler-DeWitt equation can develop tachyonic behavior. We now fix the factor ordering to the conformal one. This makes f^2 and $\frac{9\xi}{2}$ cancel exactly. If in addition we switch to the variables $\bar{\alpha}$ and $\bar{\phi}$ defined in section 3.2.1 we obtain

$$\left[\frac{\partial^2}{\partial\bar{\alpha}^2} - \frac{\partial^2}{\partial\bar{\phi}^2} - \frac{\partial^2}{\partial\phi^2} - 4\,\mathcal{I}^2\mathrm{e}^{4\bar{\alpha}}\right]\widetilde{\Psi}(\bar{\alpha},\bar{\phi},\phi) = 0. \tag{3.206}$$

The equation is now separable and we can perform the mode expansion

$$\widetilde{\Psi}_{\bar{\kappa},\kappa}(\bar{\alpha},\bar{\phi},\phi) = C_{\bar{\kappa},\kappa}(\bar{\alpha})\mathrm{e}^{\mathrm{i}\bar{\kappa}\bar{\phi}}\mathrm{e}^{\mathrm{i}\kappa\phi}\ , \tag{3.207}$$

which yields the equation

$$C''_{\bar{\kappa},\kappa}(\bar{\alpha}) + \left(\bar{\kappa}^2 + \kappa^2 - 4\,\mathcal{I}^2\mathrm{e}^{4\bar{\alpha}}\right)C_{\bar{\kappa},\kappa}(\bar{\alpha}) = 0\ . \tag{3.208}$$

This equation is solved by the modified Bessel functions

$$C^{\pm}_{\bar{\kappa},\kappa}(\bar{\alpha}) = I_{\pm\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}}\left(2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}\right) \ . \tag{3.209}$$

Now note that for large $\bar{\alpha}$ we can expand

$$I_{\pm\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}}\left(2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}\right) = \frac{\sqrt{\pi}\exp\left(-2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}\right)}{2\sqrt{2\mathcal{I}}}\left[\mathrm{i}\mathrm{e}^{-\bar{\alpha}}\exp\left(4\mathcal{I}\mathrm{e}^{2\bar{\alpha}} \mp \frac{\pi}{2}\sqrt{\bar{\kappa}^2+\kappa^2}\right) + \mathrm{e}^{-\alpha} + \mathcal{O}(\mathrm{e}^{-3\bar{\alpha}})\right] \ , \tag{3.210}$$

while for small $\bar{\alpha}$ we get

$$I_{\pm\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}}\left(2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}\right) = \frac{\mathcal{I}^{\pm\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}}}{\Gamma\left(1\pm\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}\right)}\mathrm{e}^{\pm\mathrm{i}\sqrt{\bar{\kappa}^2+\kappa^2}\bar{\alpha}} + \mathcal{O}\left(\mathrm{e}^{4\bar{\alpha}}\right). \tag{3.211}$$

We can now identify

$$\psi^{\pm}(\bar{\alpha},\bar{\phi},\phi) = \frac{\Gamma\left(1\pm\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}\right)}{\mathcal{I}^{\pm\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}}}C^{\pm}_{\bar{\kappa},\kappa}(\bar{\alpha})\mathrm{e}^{\mathrm{i}\bar{\kappa}\bar{\phi}}\mathrm{e}^{\mathrm{i}\kappa\phi} \ . \tag{3.212}$$

In order to obtain an exponentially decreasing wave function for $\bar{\alpha} \to \infty$ we choose the MacDonald function

$$C_{\bar{\kappa},\kappa}(\bar{\alpha}) = \frac{\pi\left[C^{-}_{\bar{\kappa},\kappa}(\bar{\alpha}) - C^{+}_{\bar{\kappa},\kappa}(\bar{\alpha})\right]}{2\mathrm{i}\sinh\left(\frac{\pi}{2}\sqrt{\bar{\kappa}^2+\kappa^2}\right)} = K_{\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}}\left(2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}\right) \ . \tag{3.213}$$

For large $\bar{\alpha}$ the expansion now reads

$$K_{\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}}\left(2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}\right) = \frac{\sqrt{\pi}\exp\left(-2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}\right)}{2\sqrt{\mathcal{I}}}\left[\mathrm{e}^{-\bar{\alpha}} + \mathcal{O}(\mathrm{e}^{-3\bar{\alpha}})\right] \ , \tag{3.214}$$

while for small $\bar{\alpha}$ we get

$$\begin{aligned} K_{\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}}\left(2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}\right) =& \frac{\mathcal{I}^{\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}}}{2}\Gamma\left(-\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}\right)\mathrm{e}^{\mathrm{i}\sqrt{\bar{\kappa}^2+\kappa^2}\bar{\alpha}} \\ &+\frac{\mathcal{I}^{-\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}}}{2}\Gamma\left(\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}\right)\mathrm{e}^{-\mathrm{i}\sqrt{\bar{\kappa}^2+\kappa^2}\bar{\alpha}} + \mathcal{O}\left(\mathrm{e}^{4\bar{\alpha}}\right) \ . \end{aligned} \tag{3.215}$$

Note that our criterion for picking the MacDonald function is in principle the Hawking-Page boundary condition which is not conformally invariant. Nevertheless we will later see that only this choice leads to wave packets which are peaked over the full classical trajectory. This is completely analogous to the case of a closed Friedmann model with one massless scalar field as discussed in [10, 104].

Wave packets are then formed via

$$
\begin{aligned}
\widetilde{\Psi}(\alpha,\sigma,\phi) &= \int\limits_{-\infty}^{\infty} \mathrm{d}\bar{\kappa} \int\limits_{-\infty}^{\infty} \mathrm{d}\kappa \; \mathcal{A}(\bar{\kappa},\kappa)\; \widetilde{\psi}_{\bar{\kappa}\kappa}(\alpha,\sigma,\phi) \quad \text{where} \\
\widetilde{\psi}_{\bar{\kappa}\kappa}(\alpha,\sigma,\phi) &:= K_{\frac{\mathrm{i}}{2}\sqrt{\bar{\kappa}^2+\kappa^2}}\left(2\mathcal{I}\mathrm{e}^{2\alpha-\sigma}\right)\; \exp\left(\mathrm{i}\bar{\kappa}\left[\sigma - \frac{1}{2}\alpha\right] + \mathrm{i}\kappa\phi\right)
\end{aligned}
\tag{3.216}
$$

and $\mathcal{A}(\bar{\kappa},\kappa)$ is some momentum distribution. We remark that the wave packet (3.216) might be regarded as an integral transform $\mathcal{A}(\bar{\kappa},\kappa) \mapsto \widetilde{\Psi}(\alpha,\sigma,\phi)$ which is closely related to the so-called Kontorovich-Lebedev transform. A similar solution to the Wheeler-DeWitt equations was discussed by Misner in [17].

Construction of wave packets

We now show that by choosing $\mathcal{A}(\bar{\kappa},\kappa)$ to be peaked about certain values of $\bar{\kappa}$ and κ we obtain wave packets that are peaked over a classical configuration space trajectory. This works analogously to the case of a closed Friedmann universe with a minimally coupled scalar field. We can therefore use [104] as a guideline.

The equation (3.208) for $C_{\bar{\kappa},\kappa}(\bar{\alpha})$ has the form of a zero-energy Schrödinger equation with a "potential"

$$
E_{\bar{\kappa},\kappa}(\bar{\alpha}) := \bar{\kappa}^2 + \kappa^2 - 4\,\mathcal{I}^2\mathrm{e}^{4\bar{\alpha}} \tag{3.217}
$$

If $\bar{\kappa}^2+\kappa^2$ is sufficiently large we can solve this equation in a WKB approximation. The turning point of the potential is given by $E_{\bar{\kappa},\kappa}(\bar{\alpha}_{\bar{\kappa},\kappa}) = 0$, i.e. $\bar{\alpha}_{\bar{\kappa},\kappa} = \frac{1}{4}\ln\frac{\bar{\kappa}^2+\kappa^2}{4\mathcal{I}^2}$. The WKB solution for $\bar{\alpha} < \bar{\alpha}_{\bar{\kappa},\kappa}$ reads

$$
\begin{aligned}
C_{\bar{\kappa},\kappa}(\bar{\alpha}) &\approx \left[E_{\bar{\kappa},\kappa}(\bar{\alpha})\right]^{-\frac{1}{4}} \cos\left(\left|\int_{\bar{\alpha}_{\bar{\kappa},\kappa}}^{\bar{\alpha}} \mathrm{d}\tilde{\alpha}\,\sqrt{E_{\bar{\kappa},\kappa}(\tilde{\alpha})}\right| - \frac{\pi}{4}\right) \\
&= \frac{\cos\left(\frac{\sqrt{\bar{\kappa}^2+\kappa^2}}{2}\operatorname{arcosh}\left(\frac{\sqrt{\bar{\kappa}^2+\kappa^2}}{2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}}\right) - \frac{1}{2}\sqrt{\bar{\kappa}^2+\kappa^2-4\mathcal{I}^2\mathrm{e}^{4\bar{\alpha}}} - \frac{\pi}{4}\right)}{\left(\bar{\kappa}^2+\kappa^2-4\mathcal{I}^2\mathrm{e}^{4\bar{\alpha}}\right)^{\frac{1}{4}}}\,.
\end{aligned}
\tag{3.218}
$$

The WKB solution of course corresponds, up to a constant prefactor, to the expansion of the exact solution $C_{\bar{\kappa},\kappa}(\bar{\alpha})$ if one neglects terms off the order less or equal to $\mathrm{e}^{-2\bar{\alpha}}$. For $\bar{\alpha} > \bar{\alpha}_{\bar{\kappa},\kappa}$ the corresponding WKB solution is exponentially decreasing. We can also read of the van Vleck factor:

$$
\widetilde{D}_{\bar{\kappa},\kappa}(\bar{\alpha}) \propto \frac{1}{\sqrt{\bar{\kappa}^2+\kappa^2-4\mathcal{I}^2\mathrm{e}^{4\bar{\alpha}}}}\,. \tag{3.219}
$$

In order to calculate the explicit form of a wave packet we choose $\mathcal{A}(\bar{\kappa},\kappa)$ as a symmetric

Gaussian function with center $(\bar{k}, k)$ and width Δk:

$$\mathcal{A}(\bar{\kappa}, \kappa) = \frac{1}{\pi \Delta k} \exp\left(-\frac{\left[\bar{\kappa} - \bar{k}\right]^2 + \left[\kappa - k\right]^2}{2\Delta k^2} \right) . \tag{3.220}$$

Furthermore, we choose it to be sharply peaked around the center, i.e. $\Delta k \ll 1$. The integration can then be performed in an approximate manner by replacing all terms that vary slowly with κ or $\bar{\kappa}$ with their values at $\kappa = k$ and $\bar{\kappa} = \bar{k}$, respectively. In this way the wave packet can be approximated as

$$\begin{aligned} \widetilde{\Psi}(\bar{\alpha}, \bar{\phi}, \phi) \approx d_{k,\bar{k}}(\bar{\alpha}) \int_{-\infty}^{\infty} \mathrm{d}\kappa \int_{-\infty}^{\infty} \mathrm{d}\bar{\kappa} \exp\left(-\frac{\left[\bar{\kappa} - \bar{k}\right]^2 + \left[\kappa - k\right]^2}{2\Delta k^2} \right) \\ \times \cos\left(\frac{\sqrt{\bar{\kappa}^2 + \kappa^2}}{2} \operatorname{arcosh}\left(\frac{\sqrt{\bar{k}^2 + k^2}}{2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}} \right) - \frac{1}{2}\sqrt{\bar{\kappa}^2 + \kappa^2 - 4\mathcal{I}^2\mathrm{e}^{4\bar{\alpha}}} - \frac{\pi}{4} \right) \mathrm{e}^{-\mathrm{i}\left(\bar{\kappa}\bar{\phi} + \kappa\phi\right)} , \end{aligned} \tag{3.221}$$

where

$$d_{\bar{k},k}(\bar{\alpha}) = \frac{1}{2\sqrt{\pi}\Delta k} \frac{\mathrm{e}^{-\frac{\pi}{4}\sqrt{\bar{k}^2 + k^2}}}{\left(\bar{k}^2 + k^2 - 4\mathcal{I}^2\mathrm{e}^{4\bar{\alpha}}\right)^{\frac{1}{4}}} . \tag{3.222}$$

Since

$$\sqrt{\bar{\kappa}^2 + \kappa^2} \operatorname{arcosh}\left(\frac{\sqrt{\bar{k}^2 + k^2}}{2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}} \right) \gg \frac{1}{2}\sqrt{\bar{\kappa}^2 + \kappa^2 - 4\mathcal{I}^2\mathrm{e}^{4\bar{\alpha}}} \tag{3.223}$$

the second term in the cosine corresponds to a much lower frequency. Therefore it is also reasonable to replace κ and $\bar{\kappa}$ by k and $\bar{k}$ here. In addition we expand the square root in front of the arcosh around the center of the Gaussian and approximate the term by

$$\sqrt{\bar{\kappa}^2 + \kappa^2} \approx \sqrt{\bar{k}^2 + k^2} + \frac{\bar{k}(\bar{\kappa} - \bar{k}) + k(\kappa - k)}{\sqrt{\bar{k}^2 + k^2}} . \tag{3.224}$$

The integral in (3.221) may now be evaluated by employing the calculus of Gaussian integrals.

The real part of the resulting wave packet is given by

$$\begin{aligned}\mathrm{Re}\ \widetilde{\Psi}(\bar{\alpha},\bar{\phi},\phi) \approx{}& \frac{\pi d_{k,\bar{k}}(\bar{\alpha})}{4\Delta k^2} \\ &\times\left[f^{+}_{k,\bar{k}}(\bar{\alpha},\bar{\phi},\phi)\ \exp\left(-\frac{\Delta k^2}{2}\left[\left(\frac{\bar{k}}{2\sqrt{\bar{k}^2+k^2}}\mathrm{arcosh}\left(\frac{\sqrt{\bar{k}^2+k^2}}{2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}}\right)-\bar{\phi}\right)^2\right.\right.\right. \\ &\left.\left.+\left(\frac{k}{2\sqrt{\bar{k}^2+k^2}}\mathrm{arcosh}\left(\frac{\sqrt{\bar{k}^2+k^2}}{2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}}\right)-\phi\right)^2\right]\right) \\ &+f^{-}_{k,\bar{k}}(\bar{\alpha},\bar{\phi},\phi)\ \exp\left(-\frac{\Delta k^2}{2}\left[\left(\frac{\bar{k}}{2\sqrt{\bar{k}^2+k^2}}\mathrm{arcosh}\left(\frac{\sqrt{\bar{k}^2+k^2}}{2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}}\right)+\bar{\phi}\right)^2\right.\right. \\ &\left.\left.\left.+\left(\frac{k}{2\sqrt{\bar{k}^2+k^2}}\mathrm{arcosh}\left(\frac{\sqrt{\bar{k}^2+k^2}}{2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}}\right)+\phi\right)^2\right]\right)\right]\ ,\end{aligned} \tag{3.225}$$

where

$$f^{\pm}_{k,\bar{k}}(\bar{\alpha},\bar{\phi},\phi) := \cos\left(\bar{k}\bar{\phi}+k\phi\pm\frac{1}{2}\left[\sqrt{\bar{k}^2+k^2}\mathrm{arcosh}\left(\frac{\sqrt{\bar{k}^2+k^2}}{2\mathcal{I}\mathrm{e}^{2\bar{\alpha}}}\right)-\sqrt{\bar{k}^2+k^2-4\mathcal{I}^2\mathrm{e}^{4\bar{\alpha}}}\right]\mp\frac{\pi}{4}\right)\ . \tag{3.226}$$

This represents a sum of two modulated Gaussians of width Δk^{-1} whose centers follow the classical configuration space trajectory (3.185).

The validity of the WKB solution breaks down near the turning point $\bar{\alpha}=\bar{\alpha}_{\bar{\kappa},\kappa}$. Therefore a separate discussion is appropriate for this region. Consider again equation [3.208] in the linear approximation in $\bar{\alpha}-\bar{\alpha}_{\bar{\kappa},\kappa}$ around the turning point:

$$E_{\bar{\kappa},\kappa}(\bar{\alpha}) \approx 4\left(\bar{\kappa}^2+\kappa^2\right)\left(\bar{\alpha}-\bar{\alpha}_{\bar{\kappa},\kappa}\right)\ . \tag{3.227}$$

The solution of equation (3.208) that matches the WKB solution is given by

$$C_{\bar{\kappa},\kappa}(\bar{\alpha}) \sim \left(\bar{\kappa}^2+\kappa^2\right)^{-1/6}\mathrm{Ai}\left(\sqrt[3]{4\left(\bar{\kappa}^2+\kappa^2\right)}\left[\bar{\alpha}-\bar{\alpha}_{\bar{\kappa},\kappa}\right]\right)\ , \tag{3.228}$$

where Ai is the Airy function which for small arguments can be written as

$$\begin{aligned}\left(4\left[\bar{\kappa}^2+\kappa^2\right]\right)^{-1/6}\mathrm{Ai}\left(\sqrt[3]{4\left(\bar{\kappa}^2+\kappa^2\right)}\left[\bar{\alpha}-\bar{\alpha}_{\bar{\kappa},\kappa}\right]\right) \approx& \\ -\frac{\left(4\left[\bar{\kappa}^2+\kappa^2\right]\right)^{-1/6}}{3^{\frac{1}{3}}\Gamma\left(-\frac{1}{3}\right)}-\frac{\left(4\left[\bar{\kappa}^2+\kappa^2\right]\right)^{1/6}}{3^{\frac{1}{3}}\Gamma\left(\frac{1}{3}\right)}\left(\bar{\alpha}_{\bar{\kappa},\kappa}-\bar{\alpha}\right)\ .&\end{aligned} \tag{3.229}$$

As in the limit $\bar{\alpha} \to \bar{\alpha}_{\bar{k},k}$ the difference $\bar{\alpha}_{\bar{\kappa},\kappa} - \bar{\alpha}$ goes to $\frac{1}{4}\ln\left(\frac{\bar{\kappa}^2+\kappa^2}{\bar{k}^2+k^2}\right)$ only the first term is relevant. We then obtain the form of the wave packet in the close vicinity of the turning point:

$$\mathrm{Re}\,\widetilde{\Psi}(\bar{\alpha},\bar{\phi},\phi) \sim \cos\left(\bar{k}\bar{\phi} + k\phi\right)\exp\left(-\frac{\Delta k^2}{2}\left[\bar{\phi}^2 + \phi^2\right]\right) \tag{3.230}$$

There is no noticeable spreading of the wave packet in the region of the classical turning point.

To conclude: We have recovered the classical behavior from the quantum model in the sense that wave packets are peaked about classical trajectories. There is, however, a caveat: The computations in this section are to be taken with a grain of salt. By employing the approximation (3.224) we neglected the spreading of the wave packet. Since close to the singular regions in minisuperspace the Wheeler-DeWitt equation becomes the classical wave equation in 2+1 dimensions, the wave packet will spread. We can conclude that the wave packet becomes “maximally sharp” during the bounce from the potential wall. This can be seen in the plot in fig. 3.14. When approaching the singularity the situation is the same as for the vacuum Bianchi I model. The singularity is therefore avoided by all three criteria. The plot 3.14 confirms the qualitative features we just discussed in this section.

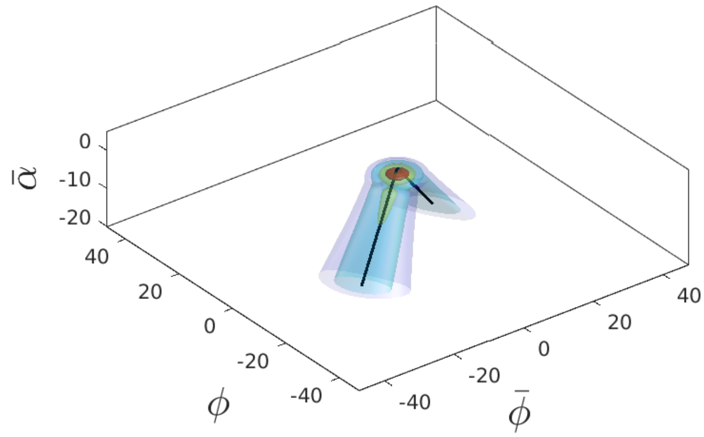


Figure 3.14: Plot of a the equipotential surfaces of a rescaled wave packet $\widetilde{\Psi}$ obtained from numerical evaluation of (3.216). The black line is the corresponding classical trajectory. The plot was obtained analogously to the one shown in fig. 3.4.

3.3 Bianchi II

We study the Bianchi II model in preparation for the study of the more complicated Bianchi IX. Misner [42] showed that during the bounces from the potential the Mixmaster universe can be well approximated by a Bianchi II model. Our attention shall be restricted to the vacuum case. The isometry group of the universe can be identified as the Heisenberg group. A basis on $T^*\Sigma$ is given by

$$\sigma^1 = \mathrm{d}x \ , \quad \sigma^2 = \mathrm{d}y \ , \quad \sigma^3 = \mathrm{d}z - x\mathrm{d}y \ . \tag{3.231}$$

Let us now perform the diagonal/off-diagonal decomposition. We construct the diagonalizing matrix $\boldsymbol{S} = \mathrm{e}^{\theta^1 \kappa_1}\mathrm{e}^{\theta^2 \kappa_2}\mathrm{e}^{\theta^3 \kappa_3}$ by choosing

$$\boldsymbol{\kappa}_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \ , \quad \boldsymbol{\kappa}_2 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \boldsymbol{\kappa}_3 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \ . \tag{3.232}$$

Note that $\boldsymbol{\kappa}_1$ and $\boldsymbol{\kappa}_2$ are generators of inner automorphisms, while $\boldsymbol{\kappa}_3$ generates a particular outer automorphism. This yields that $\{\rho_i{}^j\} = \mathrm{diag}(1,1,0)$. The algebra of the generators reads

$$[\boldsymbol{\kappa}_1, \boldsymbol{\kappa}_2] = 0 \ , \quad [\boldsymbol{\kappa}_1, \boldsymbol{\kappa}_3] = \boldsymbol{\kappa}_2 \ , \quad [\boldsymbol{\kappa}_2, \boldsymbol{\kappa}_3] = -\boldsymbol{\kappa}_1 \ . \tag{3.233}$$

Following the description in section 2.1.3 we obtain the "angular velocities" and the "moment of inertia tensor"

$$\begin{aligned} &\omega^1 = \cos\left(\theta^3\right)\dot\theta^1 - \sin\left(\theta^3\right)\dot\theta^2 \ , \quad \omega^2 = \sin\left(\theta^3\right)\dot\theta^1 + \cos\left(\theta^3\right)\dot\theta^2 \ , \quad \omega^3 = \dot\theta^3 \ , \\ &\{I_{ij}\} = \mathrm{diag}\left(I_1, I_2, I_3\right) = \frac{1}{12}\mathrm{diag}\left(\mathrm{e}^{-6\beta_+ + 2\sqrt{3}\beta_-}, \mathrm{e}^{-6\beta_+ - 2\sqrt{3}\beta_-}, 4\sinh^2\left(2\sqrt{3}\beta_-\right)\right) \ . \end{aligned} \tag{3.234}$$

The momenta p_i conjugate to the θ^i are given by

$$\begin{aligned} p_1 &= \frac{\mathrm{e}^{3\alpha}}{N}\left[I_1\cos\left(\theta^3\right)\omega^1 + I_2\sin\left(\theta^3\right)\omega^2\right] = \cos\left(\theta^3\right)\ell_1 + \sin\left(\theta^3\right)\ell_2 \ , \\ p_2 &= \frac{\mathrm{e}^{3\alpha}}{N}\left[-I_1\sin\left(\theta^3\right)\omega^1 + I_2\cos\left(\theta^3\right)\omega^2\right] = -\sin\left(\theta^3\right)\ell_1 + \cos\left(\theta^3\right)\ell_2 \ , \\ p_3 &= \frac{\mathrm{e}^{3\alpha}}{N}I_3\omega^3 = \ell_3 \ , \end{aligned} \tag{3.235}$$

where the angular momentum variables $\ell_i = \frac{\mathrm{e}^{3\alpha}}{N}I_{ij}\omega^j$ are found to obey the Poisson bracket algebra

$$\{\ell_1, \ell_2\} = 0 \ , \quad \{\ell_1, \ell_3\} = -\ell_2 \quad \text{and} \quad \{\ell_2, \ell_3\} = \ell_1 \ . \tag{3.236}$$

This is in accordance with the results from section 2.1.3. The three dimensional Ricci scalar obtained from (2.61) is given by

$${}^{(3)}R = -\frac{1}{2}\mathrm{e}^{-2\alpha}\mathrm{e}^{8\beta_+} \ . \tag{3.237}$$

The constraints now take the form

$$\begin{aligned} \mathcal{H}_0 &= \frac{\mathrm{e}^{3\alpha}}{2}\left(-p_\alpha^2 + p_+^2 + p_-^2 + \frac{\ell_1^2}{I_1} + \frac{\ell_2^2}{I_2} + \frac{\ell_2^2}{I_3} - \frac{\mathrm{e}^{-6\alpha}}{6}\,{}^{(3)}R\right) \ , \\ \mathcal{H}_1 &= \cos\left(\theta^3\right)\ell_1 - \sin\left(\theta^3\right)\ell_2 \ , \quad \mathcal{H}_2 = \sin\left(\theta^3\right)\ell_1 + \cos\left(\theta^3\right)\ell_2 \ . \end{aligned} \tag{3.238}$$

The third momentum constraint is trivially satisfied, that is, $\mathcal{H}_3 = 0$. The two momentum constraints effectively account to $\ell_1 \simeq 0$ and $\ell_2 \simeq 0$. This is expected since $\ell_{1/2}$ are the phase space generators of inner automorphisms. Furthermore, we find that the three Poisson brackets $\{l_3, \mathcal{H}_\mu\}$, where $\mu = 0, 1, 2$, all vanish. Accordingly ℓ_3 is a constant of motion. This is expected as well since ℓ_3 is the generator of an outer automorphism by construction.

Classical and Quantum Cosmology

We will focus on the diagonal vacuum case from now on.

Diagonal case

Our main aim in this section is to study the bounce from the curvature potential wall. For that purpose we reduce to the diagonal case, that is, we fix the generalized angles θ^i to be zero. The momentum constraints are then trivially satisfied and the gravitational Lagrangian becomes

$$L = \frac{-\dot{\alpha}^2 + \dot{\beta}_+^2 + \dot{\beta}_-^2}{2\widetilde{N}} - \widetilde{N}\frac{\mathrm{e}^{8\left(\frac{1}{2}\alpha+\beta_+\right)}}{24} \ , \tag{3.239}$$

where we have performed a rescaling of the lapse $N \mapsto \widetilde{N} = N\mathrm{e}^{3\alpha}$. The curvature potential thus presents an exponentially steep moving wall and we expect it to lead to a transition between two Kasner type solutions. The problem of solving the equations of motion is now equivalent to a relativistic scattering problem on a flat $1+2$ dimensional background. In order to expose an additional symmetry, we perform a Lorentz boost with velocity $-\frac{1}{2}$ in β_+-direction via the change of variables

$$T := \frac{2}{\sqrt{3}}\left(\alpha + \frac{1}{2}\beta_+\right) \quad X := \frac{2}{\sqrt{3}}\left(\beta_+ + \frac{1}{2}\alpha\right) \quad Y := \beta_- \ . \tag{3.240}$$

Thus we obtain

$$L = \frac{1}{\widetilde{N}}\left[\frac{-\dot{T}^2 + \dot{X}^2 + \dot{Y}^2}{2} - \frac{\widetilde{N}^2}{24}\mathrm{e}^{4\sqrt{3}X}\right] \ . \tag{3.241}$$

The symmetries of the system are now exposed. Variation with respect to $\widetilde{N}$ gives the Hamiltonian constraint

$$\frac{-\dot{T}^2 + \dot{X}^2 + \dot{Y}^2}{2} + \frac{1}{24}\mathrm{e}^{4\sqrt{3}X} = 0 \ , \tag{3.242}$$

where we have chosen the quasi-Gaussian gauge $\widetilde{N} = 1$ ($N = \mathrm{e}^{3\alpha}$). Since in the Lagrangian both T and Y are cyclic variables their conjugate momenta are constants of motion, i.e.

$$p_T = -\dot{T} = const. \quad \text{and} \quad p_Y = \dot{Y} = const. \tag{3.243}$$

The Hamiltonian constraint gives a differential equation for the variable X:

$$\dot{X} = \pm\sqrt{p_T^2 - p_Y^2 - \frac{1}{12}\mathrm{e}^{4\sqrt{3}X}} \ . \tag{3.244}$$

We choose the plus sign in the following. We see that we require $p_T^2 - p_Y^2 > 0$ in order to obtain real solutions. After solving the differential equation we obtain a family of trajectories of the universe point parametrized by t

$$\begin{aligned} X(t) =& \frac{1}{4\sqrt{3}} \log\left(12[p_T^2 - p_Y^2]\left[1 - \tanh^2\left(2\sqrt{3(p_T^2 - p_Y^2)}[t - t_0]\right)\right]\right) \\ T(t) =& - p_T(t - t_0) + C_T \ , \qquad Y(t) = p_Y(t - t_0) + C_Y \ , \end{aligned} \tag{3.245}$$

where $t_0, C_T, C_Y \in \mathbb{R}$ are integration constants. The inverse Lorentz transformation back to the Misner variables yields the solution

$$\alpha(t) = \frac{2}{\sqrt{3}}\left(T(t) - \frac{1}{2}X(t)\right) \ , \quad \beta_+(t) = \frac{2}{\sqrt{3}}\left(X(t) - \frac{1}{2}T(t)\right) \ , \quad \beta_-(t) = Y(t) \ . \tag{3.246}$$

We now study the asymptotic limits when $t \to \pm\infty$. Without the loss of generality we can set $C_T = C_Y = t_0 = 0$. First, we have to take a closer look at the functional form of $X(t)$. An asymptotic expansion of the expression yields that

$$X(t) \approx -\sqrt{p_T^2 - p_Y^2}|t| + \frac{1}{4\sqrt{3}} \log\left(48[p_T^2 - p_Y^2]\right) \ , \tag{3.247}$$

when $|t|$ is large. In the following we choose $p_T > 0$. This choice leads to a scale factor $a = \mathrm{e}^\alpha$ that decreases with t, i.e. the universe hits the singularity when $t \to \infty$. In the limit $t \to -\infty$ the Misner variables can then be approximated by

$$\begin{aligned} &\alpha(t) = -\sqrt{p_{+,\mathrm{in}}^2 + p_{-,\mathrm{in}}^2}\ t - C \\ &\beta_+(t) = p_{+,\mathrm{in}}\ t + C \ , \qquad \beta_-(t) = p_{-,\mathrm{in}}\ t \quad \text{with} \\ &p_{+,\mathrm{in}} = \sqrt{\frac{p_T^2 - p_Y^2}{3}} + \frac{p_T}{2\sqrt{3}} \ , \quad p_{-,\mathrm{in}} = p_Y \end{aligned} \tag{3.248}$$

and $C = \log\left(48[p_T^2 - p_Y^2]\right)/12$ is an irrelevant constant that can be absorbed into the coordinates. In the limit $t \to +\infty$ we obtain

$$\begin{aligned} &\alpha(t) = -\sqrt{p_{+,\mathrm{out}}^2 + p_{-,\mathrm{out}}^2}\ t - C \\ &\beta_+(t) = p_{+,\mathrm{out}} t + C \ , \qquad \beta_-(t) = p_{-,\mathrm{out}} t + \sqrt{3}C \quad \text{with} \\ &p_{+,\mathrm{out}} = -\sqrt{\frac{p_T^2 - p_Y^2}{3}} + \frac{p_T}{2\sqrt{3}} \ , \quad p_{-,\mathrm{out}} = p_Y \end{aligned} \tag{3.249}$$

Note that $\sqrt{p_{+,\mathrm{in}}^2 + p_{-,\mathrm{in}}^2} - \sqrt{p_{+,\mathrm{out}}^2 + p_{-,\mathrm{out}}^2} = 2\sqrt{\frac{p_T^2 - p_Y^2}{3}}$. Therefore the momentum of the universe point in the $(\alpha, \beta_+, \beta_-)$-coordinates decreases when it is scattered from the potential wall while moving towards the singularity.

With the help of some computer algebra, we can compute the Weyl squared scalar. The expression is lengthy and we refer to appendix C.2. We find that

$$C_{\mu\nu\lambda\sigma}C^{\mu\nu\lambda\sigma} \to \infty \quad \text{as } t \to \infty \ , \tag{3.250}$$

independent of the values of p_T, p_Y and C_T. Hence the universe indeed encounters a curvature singularity as $t \to \infty$.

Let us now turn to the corresponding quantum model. The Hamiltonian constraint is given by

$$\mathcal{H}_0 = \frac{\mathrm{e}^{3\alpha}}{2}\left(-p_\alpha^2 + p_+^2 + p_-^2 - \frac{\mathrm{e}^{-6\alpha}}{6}\,{}^{(3)}R\right) \ . \tag{3.251}$$

The Wheeler-DeWitt equation in conformal ordering is given by

$$\left[\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_-}^2} + \frac{1}{12}\mathrm{e}^{8\left(\frac{1}{2}\alpha+\beta_+\right)}\right]\widetilde{\Psi} = 0 \tag{3.252}$$

where we performed a conformal transformation to switch to the representation that corresponds to the gauge $N = \mathrm{e}^{3\alpha}$. The DeWitt metric is flat in this representation. The Lorentz boost (3.240) yields

$$\left[\frac{\partial^2}{\partial T^2} - \frac{\partial^2}{\partial X^2} - \frac{\partial^2}{\partial Y^2} + \frac{\mathrm{e}^{4\sqrt{3}X}}{12}\right]\Psi = 0 \tag{3.253}$$

This equation is readily solved by the mode functions

$$\begin{aligned} \psi^\pm_{p_T,p_Y}(T,X,Y) &= c^\pm_{p_T,p_Y} I_{\pm\frac{\mathrm{i}}{2}\sqrt{\frac{p_T^2-p_Y^2}{3}}}\left(\frac{\mathrm{e}^{2\sqrt{3}X}}{12}\right)\mathrm{e}^{\mathrm{i}p_T T}\mathrm{e}^{-\mathrm{i}p_Y Y} \quad \text{with} \\ c^\pm_{p_T,p_Y} &= \exp\left(\mp\frac{\pi}{4}\sqrt{\frac{p_T^2-p_Y^2}{3}}\right)\Gamma\left(1\pm\frac{\mathrm{i}}{2}\sqrt{\frac{p_T^2-p_Y^2}{3}}\right) \ . \end{aligned} \tag{3.254}$$

For the same reason as in the Kantowski-Sachs case, we choose to construct wave packets from the MacDonald function, that is, we consider wave packets of the form

$$\begin{aligned} \Psi(T,X,Y) &= \int_{\mathbb{R}^2} \mathrm{d}p_T\mathrm{d}p_Y\ \mathcal{A}(p_T,p_Y)\psi_{p_T,p_Y}(T,X,Y) \\ \text{where} \quad \psi_{p_T,p_Y}(T,X,Y) &= K_{\frac{\mathrm{i}}{2}\sqrt{\frac{p_T^2-p_Y^2}{3}}}\left(\frac{\mathrm{e}^{2\sqrt{3}X}}{12}\right)\mathrm{e}^{\mathrm{i}p_T T}\mathrm{e}^{-\mathrm{i}p_Y Y} \ . \end{aligned} \tag{3.255}$$

The amplitude $\mathcal{A}$ should be chosen such that its support lies in the region where $p_T^2 > p_Y^2$.

In the region of minisuperspace where $X \to -\infty$ the asymptotics of the mode functions are

$$\begin{aligned}\psi_{p_T,p_Y}(T,X,Y) &\approx \frac{1}{2}\left(d^+_{p_T,p_Y}\mathrm{e}^{-\mathrm{i}\sqrt{p_T^2-p_Y^2}X} + d^-_{p_T,p_Y}\mathrm{e}^{\mathrm{i}\sqrt{p_T^2-p_Y^2}X}\right)\mathrm{e}^{\mathrm{i}p_T T}\mathrm{e}^{-\mathrm{i}p_Y Y} ,\\ \text{where}\quad d^\pm_{p_T,p_Y} &= 24^{\pm\frac{\mathrm{i}}{2}\sqrt{\frac{p_T^2-p_Y^2}{3}}}\Gamma\left(\pm\frac{\mathrm{i}}{2}\sqrt{\frac{p_T^2-p_Y^2}{3}}\right) .\end{aligned} \tag{3.256}$$

The asymptotic expansion allows us to identify an ingoing and outgoing part of the wave packet $\Psi = \Psi_{\mathrm{in}} + \Psi_{\mathrm{out}}$, which we choose to write as

$$\begin{aligned}\Psi_{\mathrm{in}}(T,X,Y) &\approx \int_{\mathbb{R}^2} \mathrm{d}p_T\mathrm{d}p_Y\ \mathcal{B}(p_T,p_Y)\mathrm{e}^{\mathrm{i}p_T T}\mathrm{e}^{-\mathrm{i}\sqrt{p_T^2-p_Y^2}\left[X-\frac{1}{4\sqrt{3}}\log\left(48\left[p_T^2-p_Y^2\right]\right)\right]}\mathrm{e}^{-\mathrm{i}p_Y Y}\\ \Psi_{\mathrm{out}}(T,X,Y) &\approx \int_{\mathbb{R}^2} \mathrm{d}p_T\mathrm{d}p_Y\ \mathrm{e}^{2\mathrm{i}\delta(p_T,p_Y)}\mathcal{B}(p_T,p_Y)\mathrm{e}^{\mathrm{i}p_T T}\mathrm{e}^{+\mathrm{i}\sqrt{p_T^2-p_Y^2}X}\mathrm{e}^{-\mathrm{i}p_Y Y} ,\end{aligned} \tag{3.257}$$

where the rescaled amplitude $\mathcal{B}(p_T,p_Y)$ and the phase shift $\delta(p_T,p_Y)$ are defined by

$$\begin{aligned}\mathcal{B}(p_T,p_Y) &:= \frac{1}{2}d^+_{p_T,p_Y}\mathcal{A}(p_T,p_Y)\mathrm{e}^{-\mathrm{i}\sqrt{p_T^2-p_Y^2}\frac{1}{4\sqrt{3}}\log\left(48\left[p_T^2-p_Y^2\right]\right)}\\ \mathrm{e}^{2\mathrm{i}\delta(p_T,p_Y)} &:= d^-_{p_T,p_Y}/d^+_{p_T,p_Y}\mathrm{e}^{\mathrm{i}\sqrt{p_T^2-p_Y^2}\frac{1}{4\sqrt{3}}\log\left(48\left[p_T^2-p_Y^2\right]\right)} .\end{aligned} \tag{3.258}$$

Since both the incoming and outgoing waves are Kasner like we expect a spreading of the wave packets on both sides, that is, before and after the bounce from the curvature potential wall. However, the ingoing and outgoing wave might not be peaked about their corresponding classical trajectories due to the complicated behavior of the phase shift $\delta(p_T,p_Y)$. For large values of $\sqrt{p_T^2-p_Y^2}$ we can approximate

$$\mathrm{e}^{2\mathrm{i}\delta(p_T,p_Y)} \approx \mathrm{e}^{-\mathrm{i}\frac{\sqrt{p_T^2-p_Y^2}}{4\sqrt{3}}\left[\log\left(48\left[p_T^2-p_Y^2\right]\right)+\mathcal{O}\left(\left[p_T^2-p_Y^2\right]^{-1/2}\right)\right]} . \tag{3.259}$$

That is if $\mathcal{B}(p_T,p_Y)$ has support only over large values of $\sqrt{p_T^2-p_Y^2}$, the outgoing wave packet can be approximated as

$$\Psi_{\mathrm{out}}(T,X,Y) \approx \int_{\mathbb{R}^2} \mathrm{d}p_T\mathrm{d}p_Y\ e^{2\mathrm{i}\varepsilon}\mathcal{B}(p_T,p_Y)\mathrm{e}^{\mathrm{i}p_T T}\mathrm{e}^{+\mathrm{i}\sqrt{p_T^2-p_Y^2}\left[X-\frac{1}{4\sqrt{3}}\log\left(48\left[p_T^2-p_Y^2\right]\right)\right]}\mathrm{e}^{-\mathrm{i}p_Y Y} , \tag{3.260}$$

where $\varepsilon \in \mathbb{R}$ varies only slowly in $\sqrt{p_T^2-p_Y^2}$ when compared to the other functions. Consequently such wave packets are expected to be sharply peaked (apart from spreading) around the classical trajectories whose asymptotics were given by (3.247). We conclude that wave packets constructed with amplitudes $\mathcal{B}(p_T,p_Y)$ that have only support in the region where $\sqrt{p_T^2-p_Y^2}$

is large behave “more classically”.[3] It seems that the bounce from the potential will not have a big effect on the spreading of wave packets in the sense that it neither enhances nor weakens the spreading.

So far we have only considered the diagonal case. The quantization of the non-diagonal Bianchi II model is particularly interesting because the model possesses inner and outer automorphisms. Since it is not clear how to construct a factor ordering for this situation the investigation is left for future research.

3.4 Bianchi IX

In view of the BKL conjecture the Bianchi types VIII and IX are certainly the most interesting spatially homogeneous models. In this section we put focus on the latter. In particular by assuming that the minisuperspace approximation has some informative value a quantum avoidance of the singularity might be interpreted as a strong indication for the avoidance of the general singularity in a full theory of Quantum Gravity.

The Bianchi IX model and the BKL conjecture have been subject to many studies. Overviews can be found in the articles by Belinski [65] and the one by Heinzle and Uggla [119].

Studies of the dynamics of the general Bianchi IX spacetime were first carried out by BKL in the context of the BKL conjecture [66]. The dynamics of the diagonal Bianchi IX model were independently studied by Misner [42, 43]. Misner intention, however, was the search for a possible solution to the horizon problem via a process he called mixing. This is how the diagonal Bianchi IX model received the synonymous name mixmaster universe. It turned out later, however, that the mechanism suggested by Misner is not sufficient to resolve the issue (see e.g. [64]). Ryan, who was a student of Misner, generalized the analysis to the non-diagonal case [46, 47].

In contrast to the models we considered in the previous sections of this chapter the approach to the singularity is in general not AVTD. This is because the curvature potential plays a significant role in the vicinity of the singularity. Coupling a scalar field, however, can change the situation both quantitatively and qualitatively: The approach to the singularity becomes AVTD (see e.g. [64]). Similar results hold for spinor fields [120].

The general solution cannot be given in a closed form and apart from a few particular solutions no exact solutions are known. A series of approximations (see e.g. [66]), however,

[3] Supposing that $p_T > 0$, we infer from (3.248) and (3.249) that for $p_T^2 \gg p_Y^2$ we have that $p_{+,\mathrm{in}} \approx \frac{\sqrt{3}}{2} p_T$ and $p_{+,\mathrm{out}} \approx -\frac{1}{2\sqrt{3}} p_T$ while $p_{-,\mathrm{in}} = p_{-,\mathrm{out}} = p_Y$.

gives a clear picture of the Bianchi IX dynamics in the regime close to the singularity: The approach to the singularity is characterized by an infinite series of oscillations of the directional scale factors. The same picture is obtained by applying heuristic considerations as done by Misner [42] and Ryan [45–47]. Furthermore, these oscillations give rise to a chaotic character of the solutions [121]. Moreover, it is known that under the assumption of general energy condition a recollapse always occurs. In other words, the universe starts from an initial singularity, expands and then recollapses into a second singularity. This was proven by Lin and Wald in [59]. It is expected that in the approach towards the singularity the Kretschmann scalar becomes unbounded. This was proven by [122] in the case of the mixmaster model. A proof for the general model does not exist up to my knowledge.

Our analysis concerns the BKL scenario and our main interest lies in the asymptotic behavior of the general solutions close to the singularity. We begin by examining the diagonal case and discuss the more complicated non-diagonal case afterwards. We will restrict ourselves to qualitative and heuristic considerations which will be supported by numerical simulations.

3.4.1 Kinematics of the general Bianchi IX model

Spatial hypersurfaces in the spacetime are regarded as topological S^3, which can be parametrized by using the Euler angles $\left\{\bar\theta,\bar\phi,\bar\psi\right\}\in[0,\pi]\times[0,2\pi]\times[0,\pi]$. We write the Bianchi IX metric in a synchronous frame:

$$\mathrm{d}s^2=-N^2\mathrm{d}t^2+h_{ij}\sigma^i\otimes\sigma^j \tag{3.261}$$

where the basis 1-forms are given by

$$\begin{aligned}\sigma^1&=\cos(\bar\psi)\mathrm{d}\bar\phi+\sin(\bar\psi)\sin(\bar\phi)\mathrm{d}\bar\theta\\ \sigma^2&=\sin(\bar\psi)\mathrm{d}\bar\phi-\cos(\bar\psi)\sin(\bar\phi)\mathrm{d}\bar\theta\\ \sigma^3&=\cos(\bar\phi)\mathrm{d}\bar\theta+\mathrm{d}\bar\psi\ .\end{aligned} \tag{3.262}$$

The isometry group of the metric is $SO(3,\mathbb{R})$. The structure coefficients $C^i_{jk}=\varepsilon_{ijk}$ are in the standard diagonal form with $n^{(1)}=n^{(2)}=n^{(3)}=1$. The group $S\mathrm{Aut}(\mathfrak{g})$ coincides with the isometry group $SO(3,\mathbb{R})$ and hence it is convenient to use the special orthogonal group for the diagonalization of the spatial metric, i.e. we set

$$h_{ij}=O_i{}^kO_j{}^l\bar h_{kl}\ , \tag{3.263}$$

where $\{O_i{}^j\} \in SO(3)$. We choose here a slightly common but slightly different route for the parametrization of $O_i{}^j$ than the one discussed in section 2.1.3. More precisely we choose $O = \{O_i{}^j\} = O_\theta O_\phi O_\psi$ ($i\hat{=}$rows, $j\hat{=}$columns) to be the so-called Euler matrix which is parametrized by a set of Euler angles , that is

$$O_\psi = \begin{pmatrix} \cos(\psi) & \sin(\psi) & 0 \\ -\sin(\psi) & \cos(\psi) & 0 \\ 0 & 0 & 1 \end{pmatrix} , \quad O_\phi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\phi) & \sin(\phi) \\ 0 & -\sin(\theta) & \cos(\phi) \end{pmatrix}$$
$$O_\theta = \begin{pmatrix} \cos(\theta) & \sin(\theta) & 0 \\ -\sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix} . \tag{3.264}$$

The Euler angles θ, ϕ and ψ describe nutation, precession and pure rotation of the principal axes, respectively.

3.4.2 Hamiltonian formulation

In the following we shall be concerned with deriving the Hamiltonian formulation of the general Bianchi IX model. In order to keep track of the momentum constraints we insert the shift functions and replace the metric (3.261) by the more general ansatz

$$\mathrm{d}s^2 = -N^2\mathrm{d}t^2 + h_{ij}\left(N^i\mathrm{d}t + \sigma^i\right) \otimes \left(N^j\mathrm{d}t + \sigma^j\right) , \quad \text{where} \quad h_{ij} = \mathrm{e}^{2\alpha} O_j{}^l O_i{}^k b_{kl} . \tag{3.265}$$

The Hamiltonian formulation of the non-diagonal was first derived in a series of papers by Ryan. The so called symmetric/non-tumbling case which is obtained by constraining ψ and ϕ to be constant but keeping θ dynamical was discussed in [46]. The general case is discussed in [47]. We now write the Einstein-Hilbert action in the ADM form,

$$S_{EH} = \frac{1}{16\pi G}\int \sigma^1 \wedge \sigma^2 \wedge \sigma^3 \int \mathrm{d}t\; N\sqrt{h}\left[\left(h^{ik}h^{jl} - h^{ij}h^{kl}\right)K_{ij}K_{kl} + {}^{(3)}R\right] , \tag{3.266}$$

where $K_{ij} := \frac{1}{2N}\left(\dot{h}_{ij} - 2D_{(i}N_{j)}\right)$ is the second fundamental form and D_i denotes the covariant derivative in the non-coordinate basis. We will again set $\frac{3}{4\pi G}\int \sigma^1 \wedge \sigma^2 \wedge \sigma^3 = 1$ for simplicity. The three dimensional Ricci curvature scalar ${}^{(3)}R$ can be read off from (2.61) and is given by

$$\begin{aligned}\widetilde{\mathcal{V}}(\alpha,\beta_+,\beta_-) &= \frac{\mathrm{e}^{4\alpha}}{24}\left(\mathrm{e}^{-8\beta_+} - 4\mathrm{e}^{-2\beta_+}\cosh\left(2\sqrt{3}\beta_-\right) + 2\mathrm{e}^{4\beta_+}\left[\cosh\left(4\sqrt{3}\beta_-\right) - 1\right]\right) \\ &= -\frac{{}^{(3)}R\ \mathrm{e}^{6\alpha}}{12} \ .\end{aligned} \tag{3.267}$$

We will also make use of the variables that BKL used in their original analysis [66]. They chose the set of variables Γ_i to parametrize the diagonal metric

$$\left\{\bar{h}_{ij}\right\} = \mathrm{diag}\left(\Gamma_1, \Gamma_2, \Gamma_3\right) \ . \tag{3.268}$$

The relation to the Misner variables is as follows:

$$\Gamma_1 = \mathrm{e}^{2\alpha}\mathrm{e}^{2\beta_+ + 2\sqrt{3}\beta_-}, \quad \Gamma_2 = \mathrm{e}^{2\alpha}\mathrm{e}^{2\beta_+ - 2\sqrt{3}\beta_-}, \quad \Gamma_3 = \mathrm{e}^{2\alpha}\mathrm{e}^{-4\beta_+} \ . \tag{3.269}$$

Let us now turn to the computation of the momentum constraints. We proceed as in section 2.1.3 and define the anti-symmetric angular velocity tensor $\omega^i{}_j$ via the matrix equation

$$\boldsymbol{\omega} = \left\{\omega^i{}_j\right\} = \begin{pmatrix} 0 & \omega^1{}_2 & -\omega^3{}_1 \\ -\omega^1{}_2 & 0 & \omega^2{}_3 \\ \omega^3{}_1 & -\omega^2{}_3 & 0 \end{pmatrix} := O^T\dot{O}. \tag{3.270}$$

An explicit calculation of the right hand side shows that

$$\omega^2{}_3 = \cos(\psi)\dot{\phi} + \sin(\psi)\sin(\phi)\dot{\theta} \ , \tag{3.271}$$

$$\omega^3{}_1 = \sin(\psi)\dot{\phi} - \cos(\psi)\sin(\phi)\dot{\theta} \ , \tag{3.272}$$

$$\omega^1{}_2 = \dot{\psi} + \cos(\phi)\dot{\theta} \ . \tag{3.273}$$

The Lagrangian in the gauge $N^i = 0$ then takes the form

$$L = N\mathrm{e}^{3\alpha}\left[\frac{-\dot{\alpha}^2 + \dot{\beta}_+^2 + \dot{\beta}_-^2 + I_1\left(\omega^2{}_3\right)^2 + I_2\left(\omega^3{}_1\right)^2 + I_3\left(\omega^1{}_2\right)^2}{2N^2} + {}^{(3)}R/12\right] \ , \tag{3.274}$$

where the moments of inertia are given by

$$3I_1 = \sinh^2\left(3\beta_+ - \sqrt{3}\beta_-\right) \ , \quad 3I_2 = \sinh^2\left(3\beta_+ + \sqrt{3}\beta_-\right) \ , \quad 3I_3 = \sinh^2\left(2\sqrt{3}\beta_-\right) \ . \tag{3.275}$$

Note in particular that the term $\frac{1}{2}\left[I_1\left(\omega^2{}_3\right)^2+I_2\left(\omega^3{}_1\right)^2+I_3\left(\omega^1{}_2\right)^2\right]$ would identically correspond to the rotational energy of a rigid body if the moments of inertia were constant. The canonical momenta conjugate to the Euler angles are given by

$$\begin{aligned}
p_\theta &= \frac{\mathrm{e}^{3\alpha}}{N}\left[I_1\sin(\psi)\sin(\phi)\omega^2{}_3 - I_2\cos(\psi)\sin(\phi)\omega^3{}_1 + I_3\cos(\phi)\omega^1{}_2\right] \\
p_\phi &= \frac{\mathrm{e}^{3\alpha}}{N}\left[I_1\cos(\psi)\omega^2{}_3 + I_2\sin(\psi)\omega^3{}_1\right] \\
p_\psi &= \frac{\mathrm{e}^{3\alpha}}{N}\ I_3\omega^1{}_2
\end{aligned} \quad . \tag{3.276}$$

As in section 2.1.3 it is now convenient to introduce the (non-canonical) angular momentum like variables

$$\ell_1 = \frac{\mathrm{e}^{3\alpha}}{N}I_1\omega^2{}_3\ , \quad \ell_2 = \frac{\mathrm{e}^{3\alpha}}{N}I_2\omega^3{}_1\ , \quad \ell_3 = \frac{\mathrm{e}^{3\alpha}}{N}I_3\omega^1{}_2\ . \tag{3.277}$$

The relation to the canonical momenta can be given explicitly via the equations

$$\begin{aligned}
p_\theta &= \sin(\psi)\sin(\phi)\ell_1 - \cos(\psi)\sin(\phi)\ell_2 + \cos(\phi)\ell_3\ , & \ell_1 &= \frac{\sin(\psi)}{\sin(\phi)}\left[p_\theta - \cos(\phi)p_\psi\right] + \cos(\psi)p_\phi \\
p_\phi &= \cos(\psi)\ell_1 + \sin(\psi)\ell_2\ , & \ell_2 &= -\frac{\cos(\psi)}{\sin(\phi)}\left[p_\theta - \cos(\phi)p_\psi\right] + \sin(\psi)p_\phi\ . \\
p_\psi &= \ell_3
\end{aligned} \tag{3.278}$$

It is readily shown that the variables ℓ_i obey the Poisson bracket algebra $\{\ell_i,\ell_j\} = -C^k_{ij}\ell_k$, with C^k_{ij} being the structure constants of Bianchi IX. By performing the usual Legendre transform we obtain the Hamiltonian constraint

$$\mathcal{H} = \frac{\mathrm{e}^{-3\alpha}}{2}\left(-p_\alpha^2 + p_+^2 + p_-^2 + \frac{\ell_1^2}{I_1} + \frac{\ell_2^2}{I_2} + \frac{\ell_3^2}{I_3} - \frac{\mathrm{e}^{6\alpha}}{6}{}^{(3)}R\right)\ . \tag{3.279}$$

From (3.266) we obtain that the momentum constraints ($\partial L/\partial N^i = 0$) can be written as

$$\mathcal{H}_i = 2C^j{}_{il}h_{jk}p^{kl}\ , \tag{3.280}$$

where $p^{ij} = \frac{\sqrt{h}}{24N}\left(h^{ik}h^{jl} - h^{ij}h^{kl}\right)K_{kl}$ is the ADM momentum. From this expression we can finally compute the momentum constraints in terms of the angular momentum like variables and obtain

$$\mathcal{H}_i = O_i{}^j\ell_j\ , \tag{3.281}$$

that is we can as usual identify the momentum constraints with a basis of the generators of $SO(3,\mathbb{R})$. The full gravitational Hamiltonian now reads

$$H = N\mathcal{H} + N^i\mathcal{H}_i \ . \tag{3.282}$$

From the form of the diffeomorphism constraints we conclude that in the vacuum case $\ell_i = 0$ and no rotation is possible, that is, we obtain the diagonal case. If we want to obtain a rotating Bianchi IX universe we are consequently forced to add matter to the system. A formalism for obtaining equations of motion for general Bianchi class A models filled with fluid matter was developed by Ryan [44]. The equations of motion for all Bianchi models coupled to ideal fluids can also be found in [31]. For simplicity we will only consider the case of dust here. If we were interested in the study of the Quantum Cosmology of this model it would be desirable to couple a fundamental matter field instead. Usual scalar fields alone, however, cannot make Bianchi IX rotate. The easiest way, to my knowledge, is to couple a Dirac field as it has been done by the authors of [123]. We remark that the symmetries of the model do not allow for the coupling of electromagnetic fields as implied by the hairy ball theorem. We will use the formalism developed by Kuchař and Brown in [125] to couple dust and then reduce the symmetry in the matter sector of the model. Before doing so let us, however, have a look at the vacuum model, that is, the mixmaster universe.

3.4.3 Mixmaster dynamics

In the Taub gauge $N = \mathrm{e}^{3\alpha}$ the universe point behaves like a particle moving in a time dependent trapping potential. As with the other Bianchi models it is therefore instructive to visualize the curvature potential $\widetilde{\mathcal{V}} = -\frac{\mathrm{e}^{6\alpha}}{12}{}^{(3)}R$ to get some qualitative insights concerning the dynamics. The plot can be found in figure 3.15.

By using the analogy of a relativistic particle it is possible to explain some of the main features of the dynamics by considering the form of the potential $\widetilde{\mathcal{V}}$. It consists of three exponentially steep potential walls which form three valleys. When approaching the singularity ($\alpha \to -\infty$) the walls move away from the origin $\beta_+ = 0 = \beta_-$, which allows the universe to become more and more anisotropic. The universe point can enter any of the three valleys of the potential. Thereby it oscillates between the potential walls that form the valley.[4] In the asymptotic regime close to the singularity the walls become effectively hard walls. Thus during the time between two successive bounces the potential is negligible

[4]This is true except for the special case when the universe point goes perfectly straight into one of the valleys. This solution is known to be the Taub-NUT solution [45], which is a particular solution that can be given in closed form.

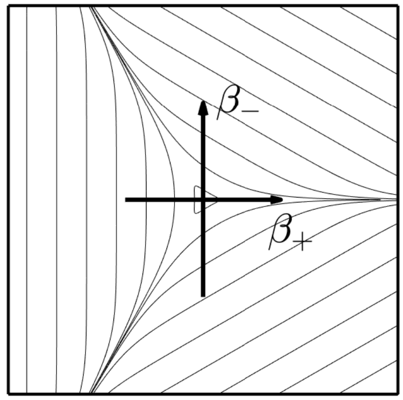


Figure 3.15: Logarithmic contour plot of the mixmaster potential $\widetilde{\mathcal{V}}(\alpha, \beta_+, \beta_-)$ for fixed α. When α becomes smaller the potential walls move away from the origin with speed 1/2 (when α is viewed as time and $\beta_\pm$ as positions). The potential is form invariant under rotations in the $\beta_\pm$ plane by angles that are integer multiples of $2\pi/3$. The potential assumes negative values in a region around the origin $\beta_+ = 0 = \beta_-$. This is essential for the existence of a rebounce.

and the dynamics can be well approximated by those of the Kasner model. The period between two successive bounces is thus called a Kasner epoch. The period between entering and exiting a valley is called a Kasner era. The approach towards the singularity consists of an infinite sequence of Kasner eras which themselves consist of a finite sequence of Kasner epochs. Note also that the potential $\widetilde{\mathcal{V}}$ is negative in a region around the origin $\beta_+ = 0 = \beta_-$. This essentially allows for the recollapse of the Bianchi IX model.

Furthermore, we remark that in the vacuum case the Lagrangian (3.274) transforms as $L \to \mathfrak{c}^2 L$ under the rescaling

$$\alpha \to \alpha + \log(\mathfrak{c}) \ , \quad \text{and} \quad N \to \mathfrak{c} N \tag{3.283}$$

for all constants $\mathfrak{c} > 0$. This means that the equations of motions are unaffected by the transformation. Consequently (3.283) maps solutions into solutions. The transformation (3.283) is equivalent to the transformation

$$\alpha \to \alpha + \log(\mathfrak{c}) \ , \quad \text{and} \quad t \to \mathfrak{c}^{-1} t \ . \tag{3.284}$$

Numerical analysis

Numerical simulations of the Bianchi IX dynamics were already carried out in the late 1980's and early 1990's (see e.g. [127, 128]). Recall that the evolution of Bianchi IX towards the singularity is characterized by an infinite number of bounces from the potential wall. The universe then hits the singularity in a finite comoving time. In order to resolve the bounces in the temporal evolution it is practical to work in the quasi-Gaussian gauge $N = \mathrm{e}^{3\alpha}$. In this time gauge the singularities lie at $t = \pm\inf$.

In terms of the variables Γ_i as defined by (3.269) the constraint reads

$$\begin{aligned} 0 = &-(\log\Gamma_1)^{\cdot}(\log\Gamma_2)^{\cdot} - (\log\Gamma_3)^{\cdot}(\log\Gamma_2)^{\cdot} - (\log\Gamma_1)^{\cdot}(\log\Gamma_3)^{\cdot} \\ &+ \Gamma_1^2 + \Gamma_2^2 + \Gamma_3^2 - 2(\Gamma_1\Gamma_2 + \Gamma_3\Gamma_1 + \Gamma_2\Gamma_3)\ , \end{aligned} \tag{3.285}$$

while the equations of motion are given by

$$(\log\Gamma_1)^{\cdot\cdot} = (\Gamma_2 - \Gamma_3)^2 - \Gamma_1^2\ , \quad (\log\Gamma_2)^{\cdot\cdot} = (\Gamma_3 - \Gamma_1)^2 - \Gamma_2^2\ , \quad (\log\Gamma_3)^{\cdot\cdot} = (\Gamma_1 - \Gamma_2)^2 - \Gamma_3^2\ . \tag{3.286}$$

With given initial conditions (obeying the constraint $\mathcal{H} = 0$) the system can now be integrated by using a suitable shooting method, e.g. Runge-Kutta. In this work we employ the MATLAB R2016b solver ode113 [126]. This code is an implementation of a linear multistep method, the so called Adams-Bashforth-Moulton method. It turned out to lead to better results when compared with the other MATLAB solvers. The relative error tolerance of the solver was chosen of the order 10^{-14}. A numerical vacuum solution obtained by the method is plotted in the figures 3.16.

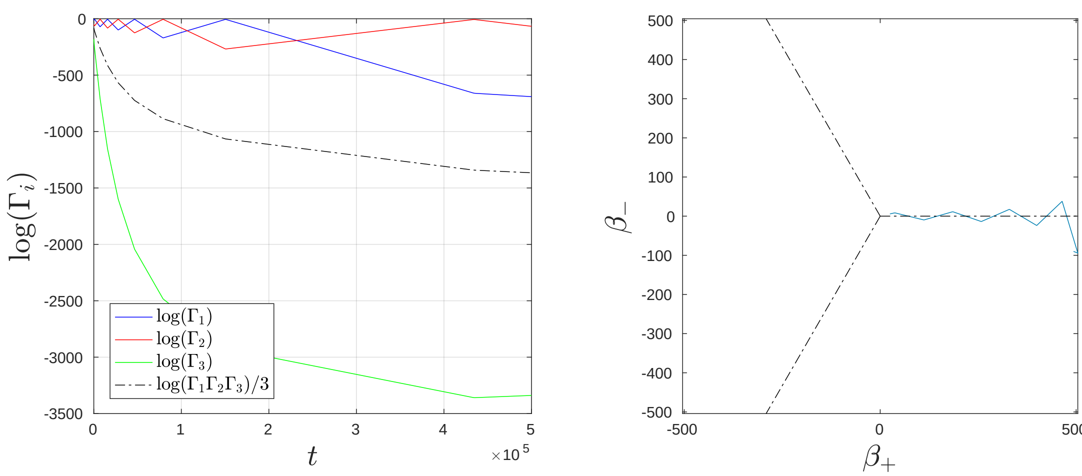


Figure 3.16: Numerical solution of the mixmaster model. The plots show a typical Kasner era where the solution bounces around in one of the potential valleys. The black dotted lines in the left figure represent the potential valleys.

A major problem in numerical relativity is that the Hamiltonian constraint is usually not preserved exactly by the numerical procedure. Similar to [127, 128] we find that the error in the Hamiltonian constraint varies most significantly right after starting the simulation.

Furthermore, it varies very strongly when the evolution of the universe is close to the point of maximal expansion. While approaching the singularity the error settles down and approaches an approximately constant value. Therefore we minimize the error when we choose the initial conditions such that we start the simulations further away from the point of maximal expansion. Moreover, it turned out that the error can be further reduced when we constrain the solvers maximally allowed time step size from above. This size should, however, not be too small since this can drive the propagation of round off errors. By manually fine tuning the initial conditions and the maximally allowed time step size it was possible to get the order of the error as low as 10^{-18}. In most of the simulations, however, the error was smaller than of the order of 10^{-10}, which turned out to be sufficient for short time simulations. Another check is obtained by plotting the value of the expression

$$|p_\alpha|^{-1}\sqrt{p_+^2 + p_-^2} = \sqrt{\left(\frac{\partial\beta_+}{\partial\alpha}\right)^2 + \left(\frac{\partial\beta_-}{\partial\alpha}\right)^2}\,. \tag{3.287}$$

This is nothing but the velocity of the universe point in the β-plane as measured in α-time. Since in the asymptotic regime close to the singularity the hard wall approximation becomes valid we expect the universe point to spend much time close to the Kasner circle $\mathcal{K}^\circ$, that is, the set in momentum space where $|p_\alpha|^{-1}\sqrt{p_+^2 + p_-^2} = 1$. If this ceases to be true it indicates a breakdown of the validity of the numerical method due to an increasing relevance of the error in the Hamiltonian constraint when approaching the singularity.

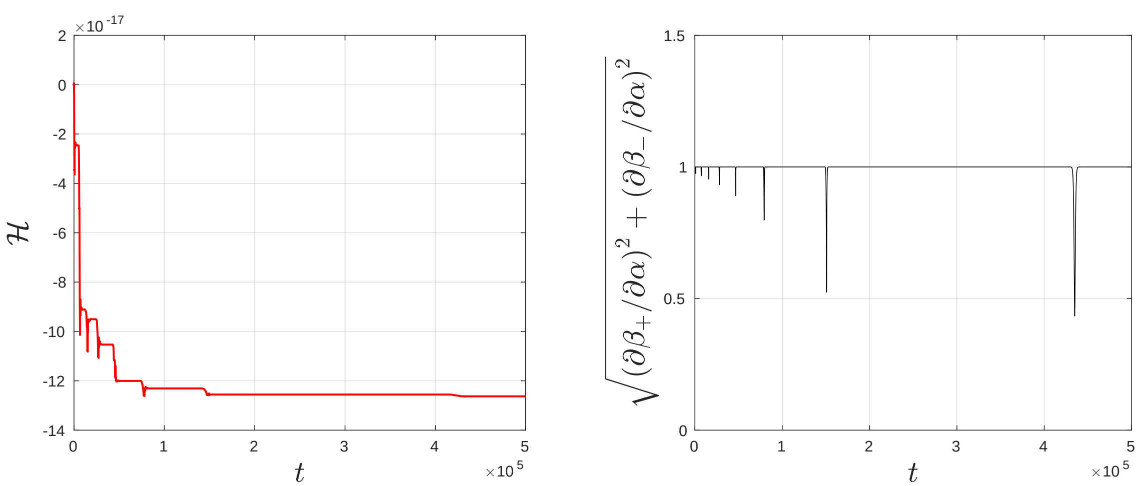


Figure 3.17: Plot of the error in the Hamiltonian constraint and the velocity in the β-plane corresponding to Figure 3.16.

3.4.4 Wheeler-DeWitt equation of the mixmaster universe

We include some heuristic considerations regarding the solutions to the conformally covariant Wheeler-DeWitt equation of the vacuum mixmaster model. The Bianchi IX model is also suitable for checking the factor ordering proposals. Some other aspect of the Wheeler-DeWitt Quantum Cosmology have been studied before [43, 124].

We start from the Hamiltonian constraint (3.279) and implement the momentum constraints (3.281). This yields the Hamiltonian constraint of the mixmaster universe

$$\mathcal{H} = \frac{\mathrm{e}^{-3\alpha}}{2}\left(-p_\alpha^2 + p_+^2 + p_-^2 - \frac{\mathrm{e}^{6\alpha}}{6}{}^{(3)}R\right) . \tag{3.288}$$

Implementing the momentum constraints (3.281) reduced the dimension of minisuperspace effectively to $d = 3$. We now quantize the system using the conformal ordering to obtain

$$\left[\frac{\partial^2}{\partial\alpha^2} - \frac{\partial^2}{\partial{\beta_+}^2} - \frac{\partial^2}{\partial{\beta_+}^2} + 2\widetilde{\mathcal{V}}\right]\widetilde{\Psi} = 0 . \tag{3.289}$$

Note that we already switched to the Wheeler-DeWitt equation in the representation that corresponds to the Taub gauge $N = \mathrm{e}^{3\alpha}$ by performing a conformal transformation with $\Omega = \mathrm{e}^{3\alpha/4}$.

I conjecture on the avoidance of the BKL singularity by spreading of the wave packet accompanied by a decay of its amplitude. This conjecture is can be rooted on the BKL scenario: Classical solutions are made up of an infinite sequence of Kasner eras which themselves consist of epochs. Our considerations on the Quantum Kasner solution in the previous section show that wave packets spread during Kasner epochs. During bounces from one epoch into another the solutions effectively behave like solutions to Bianchi II which we discussed in section 3.3. In a particular bounces from the Bianchi II potential wall did not seem to have a noticeable effect on the spreading. The author of [130] employed numerical techniques to solve the Wheeler-DeWitt equation by using a hard wall approximation. His findings support our conjecture on the spreading of wave packets. It might, however, be desirable to make this statement mathematically more precise. A possible way to do this is the application of decay rate estimates for the classical wave equation with a time dependent trapping potential. Up to my knowledge there are so far no results which are directly applicable to the situation in question.

Let us now turn to a discussion of the factor ordering. The Wheeler-DeWitt equation (3.289) of the vacuum mixmaster universe was obtained by first implementing the momementum constraints and a subsequent quantization of the 3-dimensional reduced system. In view of the full theory, however, it might be desirable to first quantize the full system and then implement the momentum constraints at the quantum level. One might expect that after a successful quantization it should somehow be possible to relate the resulting Wheeler-DeWitt equation back to the one of the mixmaster universe (3.289). We illustrate that this is not the case if we employ the naive conformal factor ordering.

We transform the momentum constraints $\mathcal{H}_i \mapsto \bar{\mathcal{H}}_i := (O^{-1})_i{}^j \mathcal{H}_j = \ell_i$. For brevity we skip the bar from here on and simply write $\mathcal{H}_i = \ell_i$. The Poisson bracket algebra of the constraints is then given by

$$\begin{aligned}\{\mathcal{H}_0, \mathcal{H}_i\} &= 2\mathrm{e}^{3\alpha} \sum_j C_{ij}^k \frac{\ell_j}{I_j} \ell_k = \mathcal{C}_{0i}^{\mu} \mathcal{H}_\mu \\ \{\mathcal{H}_i, \mathcal{H}_j\} &= -C_{ij}^k \ell_k = \mathcal{C}_{ij}^k \mathcal{H}_k \ .\end{aligned} \tag{3.290}$$

Consequently the non-vanishing components of the structure function of the constraint algebra read

$$\mathcal{C}_{0i}^k = 2\mathrm{e}^{3\alpha} \sum_j C_{ji}^k \frac{\ell_j}{I_j} \ , \quad \text{and} \quad \mathcal{C}_{ij}^k = -C_{ij}^k \ . \tag{3.291}$$

Note that $\lambda_i \equiv 0$. The minisuperspace is $\mathcal{M} = \mathbb{R}^3 \times SO(3, \mathbb{R})$ and it is equipped with the conformal DeWitt metric $[\mathrm{d}\mathcal{S}^2]$. As was already pointed out by Misner [42] a representation of the conformal DeWitt metric is given by

$$\mathrm{d}\widetilde{\mathcal{S}}^2 = -\mathrm{d}\alpha^2 + \mathrm{d}\beta_+^2 + \mathrm{d}\beta_-^2 + \sum_{i=1}^{3} I_i (\boldsymbol{B}^i)^2 \tag{3.292}$$

where

$$\begin{aligned}\boldsymbol{B}^1 &= \sin(\psi)\sin(\phi)\mathrm{d}\theta + \cos(\psi)\mathrm{d}\phi \\ \boldsymbol{B}^2 &= -\cos(\psi)\sin(\phi)\mathrm{d}\theta + \sin(\psi)\mathrm{d}\phi \\ \boldsymbol{B}^3 &= \cos(\phi)\mathrm{d}\theta + \mathrm{d}\psi \ .\end{aligned} \tag{3.293}$$

Note that in this representation the DeWitt metric is singular on the three lines in the (β_+, β_-)-plane where $\beta_- = 0$, $\beta_- = \pm\sqrt{3}\beta_+$. The Ricci scalar is given by $\widetilde{\mathcal{R}} = -90$ and the volume element reads

$$\widetilde{\star}1 = \sqrt{I_1 I_2 I_3}\,\sin(\phi)\mathrm{d}\alpha \wedge \mathrm{d}\beta_+ \wedge \mathrm{d}\beta_- \wedge \mathrm{d}\theta \wedge \mathrm{d}\phi \wedge \mathrm{d}\psi \ . \tag{3.294}$$

We shall define angular momentum operators via

$$\begin{aligned}\hat{\ell}_1 &= \frac{\sin(\psi)}{\sin(\phi)}\left[\hat{p}_\theta - \cos(\phi)\hat{p}_\psi\right] + \cos(\psi)\hat{p}_\phi \\ \hat{\ell}_2 &= -\frac{\cos(\psi)}{\sin(\phi)}\left[\hat{p}_\theta - \cos(\phi)\hat{p}_\psi\right] + \sin(\psi)\hat{p}_\phi \ , \\ \hat{\ell}_3 &= \hat{p}_\psi\end{aligned} \tag{3.295}$$

where $\hat{p}_\theta = -\mathrm{i}\partial_\theta$ etc.

We now quantize the system. We make first use of the naive conformal factor ordering $\hat{\mathcal{H}} = -\frac{1}{2}(\Box - \xi\mathcal{R}) + \mathcal{V}$. Since the dimension of the minisuperspace is $d = 6$ the wave function carries the conformal weight $w(\Psi) = -2$. This is different from the case where we first implemented the momentum constraints and then quantized the resulting 3 dimensional system. In that case the conformal weight of the wave function was $w(\Psi) = -\frac{1}{2}$.

We obtain the Wheeler-DeWitt equation

$$\begin{aligned}\hat{\widetilde{\mathcal{H}}}\widetilde{\Psi} = -\frac{1}{2}\Bigg[&-\frac{\partial^2}{\partial\alpha^2} + \frac{\partial^2}{\partial{\beta_+}^2} + \frac{\partial^2}{\partial{\beta_-}^2} - \frac{\hat{\ell}_1^2}{I_1} - \frac{\hat{\ell}_2^2}{I_2} - \frac{\hat{\ell}_3^2}{I_3} - 2\widetilde{\mathcal{V}} + 90\xi \\ &+\frac{1}{2}\frac{\partial\log\left(I_1I_2I_3\right)}{\partial\beta_+}\frac{\partial}{\partial\beta_+} + \frac{1}{2}\frac{\partial\log\left(I_1I_2I_3\right)}{\partial\beta_-}\frac{\partial}{\partial\beta_-}\Bigg]\widetilde{\Psi} = 0 \ .\end{aligned} \tag{3.296}$$

We already wrote the Wheeler-DeWitt equation in the representation that corresponds to the Taub gauge. Note that the factor ordering generated friction terms of the form

$$\partial_A\left(\sqrt{I_1I_2I_3}G^{AB}\right)\partial_B\widetilde{\Psi} = \frac{1}{2}\left(\frac{\partial\log\left(I_1I_2I_3\right)}{\partial\beta_+}\frac{\partial}{\partial\beta_+} + \frac{\partial\log\left(I_1I_2I_3\right)}{\partial\beta_-}\frac{\partial}{\partial\beta_-}\right)\widetilde{\Psi} \ . \tag{3.297}$$

In addition to the Wheeler-DeWitt equation we have quantum diffeomorphism constraints. According to the discussion in section 2.2.7, we implement them as

$$\hat{\mathcal{H}}_i\Psi = \hat{\ell}_j\Psi = 0 \ . \tag{3.298}$$

It is readily shown that they satisfy the commutation relations $[\hat{\mathcal{H}}_i, \hat{\mathcal{H}}_j]\widetilde{\Psi} = \mathrm{i}C_{ij}^k\hat{\mathcal{H}}_k\widetilde{\Psi}$. Furthermore,

$$[\hat{\mathcal{H}}, \hat{\mathcal{H}}_i] = 2\mathrm{e}^{3\alpha}\sum_{j,k} C_{ij}^k\frac{\hat{\ell}_j}{I_j}\hat{\ell}_k. \tag{3.299}$$

Hence the quantum system of equations is Dirac consistent. Since in this gauge the Wheeler-DeWitt equation still contains friction terms we perform a conformal transformation with $\Omega^{-4} = \sqrt{I_1I_2I_3}$, i.e. we transform $\widetilde{\Psi} \to \Psi := \Omega^{-2}\widetilde{\Psi}$. The Wheeler-DeWitt equation then becomes

$$\left[-\frac{\partial^2}{\partial\alpha^2}+\frac{\partial^2}{\partial{\beta_+}^2}+\frac{\partial^2}{\partial{\beta_-}^2}-\frac{\hat{\ell}_1^2}{I_1}-\frac{\hat{\ell}_2^2}{I_2}-\frac{\hat{\ell}_3^2}{I_3}-\widetilde{\mathcal{V}}+90\xi-\mathcal{U}\right]\Psi=0\ . \tag{3.300}$$

where $\mathcal{U}=12-\frac{1}{I_1}-\frac{1}{I_2}-\frac{1}{I_3}$. If we now implement the constraints $\hat{\ell}_i\Psi=0$ we do not obtain the Wheeler-DeWitt equation (3.289) that we got by implementing the momentum constraints before quantization. This is because of the presence of the additional potential term $\mathcal{U}$. The presence of this term spoils the Kasner like behavior in between two successive bounces. In this sense we interpret its presence as a failure of the naive conformal ordering. If we use the modified ordering defined by (2.216), the above mentioned problem is absent. The reduced Wheeler-DeWitt equation is then given by

$$\hat{\widetilde{\mathcal{H}}}_0^{(r)}\widetilde{\Psi}=\frac{1}{2}\left[\frac{\partial^2}{\partial\alpha^2}-\frac{\partial^2}{\partial{\beta_+}^2}-\frac{\partial^2}{\partial{\beta_+}^2}+2\widetilde{\mathcal{V}}\right]\widetilde{\Psi}=0\ , \tag{3.301}$$

which coincides with (3.288). The constraint algebra obeys the same relations as in the case of the naive ordering. The undesired potential terms, however, are absent.

3.4.5 The dust filled Bianchi IX spacetime

We now add pressure less matter to the system. This is rather straightforward when considering comoving dust. In order to make the Bianchi IX universe rotate, however, we require the dust velocities to have non-vanishing spatial components. In order to obtain equations of motion for this system we use the formalism developed by Ryan (to be found in [44, 46, 47] and for other Bianchi models in [31]). This formalism, however, has the disadvantage that it is not quite canonical. It is therefore not suitable for quantization without employing additional approximations.

The energy momentum tensor for dust reads $T_{\mu\nu}=\rho\ u_\mu u_\nu$, where ρ is the rest mass density of the dust field. As it is well known, the local energy conservation $\nabla_\mu T^{\mu\nu}=0$ leads to a geodesic equation for the positions of the dust particles. Let us start therefore by considering the geodesic equation for a single dust particle, whose four-velocity we express in the non-coordinate frame via the Pfaffian form

$$\boldsymbol{u}=u_0\mathrm{d}t+u_i\sigma^i\quad\text{with}\quad\langle\boldsymbol{u},\boldsymbol{u}\rangle=-1\ . \tag{3.302}$$

We partially fixed the gauge by setting $N^i = 0$. The normalization condition implies

$$u_0 = -N\sqrt{1 + h^{ij}u_i u_j}\ . \tag{3.303}$$

We chose the minus sign because it ensures that the dust time T runs in the same direction as the coordinate time t. The geodesic equation for the spatial components of the four velocity can then be written as

$$u^0(\partial_t u_i) - C^k_{ij} u_k u^j = 0\ . \tag{3.304}$$

The geodesic equation implies the existence of an additional constant of motion. To see this explicitly we compute the expression $\sum\limits_{i=1,2,3} \dot{u}_i u_i$ under the employment of the geodesic equation and convince ourselves that it vanishes identically. Thus the euclidean sum

$$C^2 := (u_1)^2 + (u_2)^2 + (u_3)^2 \tag{3.305}$$

is a constant of motion and we are left with 2 degrees of freedom. When we now define $\vec{u} := (u_1,\ u_2,\ u_3)^T$ the geodesic equation (3.304) can be re-written in the vector notation

$$\partial_t \vec{u} = \frac{N \mathrm{e}^{-2\alpha} \left[\vec{u} \times (Ob^{-1}O^T\vec{u})\right]}{\sqrt{1 + \mathrm{e}^{-2\alpha}\vec{u}^T Ob^{-1}O^T\vec{u}}}\ , \tag{3.306}$$

where "$\times$" denotes the usual cross product on three dimensional euclidean space. It is now convenient to define $\vec{v} := O^T\vec{u}/C$. This vector is normalized in the sense that $(v_1)^2 + (v_2)^2 + (v_3)^2 = 1$ and the geodesic equation simplifies to[5]

$$(\partial_t + \boldsymbol{\omega})\,\vec{v} \ = \frac{NC\mathrm{e}^{-2\alpha}\left[\vec{v} \times (b^{-1}\vec{v})\right]}{\sqrt{1 + C^2\mathrm{e}^{-2\alpha}\vec{v}^T b^{-1}\vec{v}}} \tag{3.307}$$

Note that we can also write $\boldsymbol{\omega}\vec{v} = \vec{v} \times \vec{\omega}$ where $\vec{\omega} = \{\omega^i\} = \frac{N}{\mathrm{e}^{3\alpha}}\left(\frac{\ell_1}{I_1},\ \frac{\ell_2}{I_2},\ \frac{\ell_3}{I_3}\right)^T$. It will therefore be possible to eliminate $\boldsymbol{\omega}$ from the geodesic equation by using the diffeomorphism constraints. We now couple the dust to the system by using the Kuchař and Brown formalism [125]. The full Hamiltonian of the Bianchi IX universe coupled to dust reads

$$\begin{gathered} H = N\left(\mathcal{H} + \mathcal{H}^{(m)}\right) + N^i\left(\mathcal{H}_i + \mathcal{H}_i^{(m)}\right)\ , \quad \text{where} \\ \mathcal{H}^{(m)} = \sqrt{p_T^2 + h^{ij}\mathcal{H}_i^{(m)}\mathcal{H}_j^{(m)}} \quad \text{and} \quad \mathcal{H}_i^{(m)} = -p_T u_i \end{gathered} \tag{3.308}$$

[5]Note that our result here differs from Ryan's by a factor 1/2.

The Hamiltonian constraint and diffeomorphism constraints read

$$\begin{aligned}
\mathcal{H}+\mathcal{H}^{(m)} &= \frac{\mathrm{e}^{-3\alpha}}{2}\left(-p_\alpha^2+p_+^2+p_-^2+\frac{\ell_1^2}{I_1}+\frac{\ell_2^2}{I_2}+\frac{\ell_3^2}{I_3}-\frac{\mathrm{e}^{6\alpha}}{6}{}^{(3)}R+2\mathrm{e}^{3\alpha}p_T\sqrt{1+h^{ij}u_iu_j}\right)\\
\mathcal{H}_i+\mathcal{H}_i^{(m)} &= O_i^{\ j}\left(\ell_j-Cp_Tv_j\right)\ .
\end{aligned} \tag{3.309}$$

The parameter $p_T > 0$ is the momentum conjugate to the dust proper time T. Since the Hamiltonian does not explicitly depend on T the momentum p_T is a constant of motion. Moreover, p_T controls the dust density which is given by

$$\rho = \frac{p_T\ \mathrm{e}^{-3\alpha}}{\sqrt{1+h^{ij}u_iu_j}}\ . \tag{3.310}$$

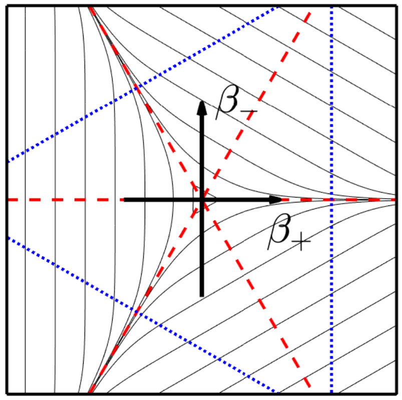
The formalism we derived is not quite canonical in the sense that it must be supplemented with the geodesic equation for the dust particles (3.304). The fact that $\ell_1^2+\ell_2^2+\ell_3^2$ commutes with $\mathcal{H}$ implies that $\ell_1^2+\ell_2^2+\ell_3^2=(Cp_T)^2$ is a conserved quantity. This is consistent with the fact that $(u_1)^2+(u_2)^2+(u_3)^2=C^2$ which itself now follows from the canonical description. In addition to the curvature potential $-\frac{\mathrm{e}^{6\alpha}}{12}{}^{(3)}R$ we have two additional "potentials". The term $\mathrm{e}^{3\alpha}p_T\sqrt{1+h^{ij}u_iu_j}$ can be interpreted as three rotational potential walls. These potentials are rather unimportant close to the singularity since they move away from the origin $\beta_\pm=0$ with speed 1. The term $\frac{\ell_1^2}{I_1}+\frac{\ell_2^2}{I_2}+\frac{\ell_3^2}{I_3}$ can be interpreted as three centrifugal potential walls. Asymptotically these walls are expected to become static. In general, however, all potential walls are dynamical and change in a complicated manner dictated by the motion of the dust particles. The centrifugal walls prevent the universe point from penetrating certain regions of the configuration space (see figure 3.18). Ryan [46, 47] employed these facts to obtain approximate solutions in a diagrammatic form.

For numerical purposes it is convenient to write the equations of motion using the variables Γ_i. Furthermore, we shall pick the gauges $N=\mathrm{e}^{3\alpha}=\sqrt{\Gamma_1\Gamma_2\Gamma_3}$ and $N^i=0$. The Hamiltonian constraint then becomes

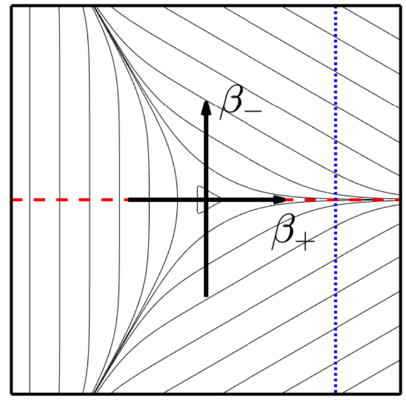
$$\begin{aligned}
&-(\log\Gamma_1)^{\cdot}(\log\Gamma_2)^{\cdot}-(\log\Gamma_2)^{\cdot}(\log\Gamma_3)^{\cdot}-(\log\Gamma_1)^{\cdot}(\log\Gamma_3)^{\cdot}\\
&+\Gamma_1^2+\Gamma_2^2+\Gamma_3^2-2(\Gamma_1\Gamma_2+\Gamma_3\Gamma_1+\Gamma_2\Gamma_3)\\
&+24\left[\frac{\ell_1^2}{I_1}+\frac{\ell_2^2}{I_2}+\frac{\ell_3^2}{I_3}+2|p_T|\sqrt{\Gamma_1\Gamma_2\Gamma_3+C^2\left(\Gamma_2\Gamma_3v_1^2+\Gamma_1\Gamma_3v_2^2+\Gamma_1\Gamma_2v_3^2\right)}\right]=0
\end{aligned} \tag{3.311}$$

where the moments of inertia are

$$I_1=\frac{(\Gamma_3-\Gamma_2)^2}{12\Gamma_3\Gamma_2}\ ,\quad I_2=\frac{(\Gamma_1-\Gamma_3)^2}{12\Gamma_1\Gamma_3}\ ,\quad I_3=\frac{(\Gamma_1-\Gamma_2)^2}{12\Gamma_1\Gamma_2}\ . \tag{3.312}$$



(a) General case.



(b) Non-tumbling case

.

Figure 3.18: When rotating dust is coupled the potential becomes modified. The dashed red lines represent the singular centrifugal walls which might appear and disappear during the temporal evolution. The dotted blue lines represent the exponentially steep rotation walls which move outwards with speed 1 when approaching the singularity. These walls might open and close again during the temporal evolution of the universe. The rotation walls are rather unimportant in the study of the dynamics towards the singularity since they cannot be reached by the universe point. They are only relevant for the dynamics in the vicinity of the rebounce.

The diffeomorphism constraints read $\ell_i = p_T C v_i$ and can be used to eliminate the angular momentum variables from the equations of motion. The equations of motion can then be written as

$$\begin{aligned}
(\log\Gamma_1)^{\cdot\cdot} =&(\Gamma_2-\Gamma_3)^2-\Gamma_1^2+2p_T'^2C^2\left[\frac{\Gamma_1\Gamma_3(\Gamma_1+\Gamma_3)v_2^2}{(\Gamma_1-\Gamma_3)^3}+\frac{\Gamma_1\Gamma_2(\Gamma_1+\Gamma_2)v_3^2}{(\Gamma_1-\Gamma_2)^3}\right]\\
&+\frac{p_T'(\Gamma_1\Gamma_2\Gamma_3+2C^2v_1^2\Gamma_2\Gamma_3)}{\sqrt{\Gamma_1\Gamma_2\Gamma_3+C^2\left(\Gamma_2\Gamma_3v_1^2+\Gamma_1\Gamma_3v_2^2+\Gamma_1\Gamma_2v_3^2\right)}}\\
(\log\Gamma_2)^{\cdot\cdot} =&(\Gamma_3-\Gamma_1)^2-\Gamma_2^2+2p_T'^2C^2\left[\frac{\Gamma_1\Gamma_2(\Gamma_1+\Gamma_2)v_3^2}{(\Gamma_2-\Gamma_1)^3}+\frac{\Gamma_2\Gamma_3(\Gamma_2+\Gamma_3)v_1^2}{(\Gamma_2-\Gamma_3)^3}\right]\\
&+\frac{p_T'(\Gamma_1\Gamma_2\Gamma_3+2C^2v_2^2\Gamma_1\Gamma_3)}{\sqrt{\Gamma_1\Gamma_2\Gamma_3+C^2\left(\Gamma_2\Gamma_3v_1^2+\Gamma_1\Gamma_3v_2^2+\Gamma_1\Gamma_2v_3^2\right)}}\\
(\log\Gamma_3)^{\cdot\cdot} =&(\Gamma_1-\Gamma_2)^2-\Gamma_3^2+2p_T'^2C^2\left[\frac{\Gamma_1\Gamma_3(\Gamma_1+\Gamma_3)v_2^2}{(\Gamma_3-\Gamma_1)^3}+\frac{\Gamma_3\Gamma_2(\Gamma_3+\Gamma_2)v_1^2}{(\Gamma_3-\Gamma_2)^3}\right]\\
&+\frac{p_T'(\Gamma_1\Gamma_2\Gamma_3+2C^2v_3^2\Gamma_1\Gamma_2)}{\sqrt{\Gamma_1\Gamma_2\Gamma_3+C^2\left(\Gamma_2\Gamma_3v_1^2+\Gamma_1\Gamma_3v_2^2+\Gamma_1\Gamma_2v_3^2\right)}}\,.
\end{aligned} \tag{3.313}$$

where we have introduced $p_T' := 12p_T$ for brevity. We use the diffeomorphism constraints to eliminate $\vec{\omega}$ from the geodesic equation (3.307). This yields

$$\partial_t \vec{v} = \frac{NC}{\mathrm{e}^{3\alpha}}\ \vec{v} \times \left(\left[\frac{\mathrm{e}^{\alpha} b^{-1}}{\sqrt{1 + C^2 \mathrm{e}^{-2\alpha} \vec{v}^T b^{-1} \vec{v}}} - p_T \ \mathrm{diag}\left(\frac{1}{I_1}, \frac{1}{I_2}, \frac{1}{I_3} \right) \right] \vec{v} \right) . \tag{3.314}$$

If expressed in the gauge $N = \mathrm{e}^{3\alpha}$ it can conveniently be written as

$$\begin{aligned} \dot{\vec{v}} =& C\vec{v} \times (M\vec{v}) \quad \text{where} \quad M \in \mathbb{R}^{3\times 3} \quad \text{is given by} \\ M =& \frac{\mathrm{diag}\,(\Gamma_2\Gamma_3,\ \Gamma_1\Gamma_3,\ \Gamma_1\Gamma_2)}{\sqrt{\Gamma_1\Gamma_2\Gamma_3 + C^2\left(\Gamma_2\Gamma_3 v_1^2 + \Gamma_1\Gamma_3 v_2^2 + \Gamma_1\Gamma_2 v_3^2\right)}} \\ &+ p_T' \mathrm{diag}\left(\frac{\Gamma_2\Gamma_3}{[\Gamma_2 - \Gamma_3]^2}, \frac{\Gamma_1\Gamma_3}{[\Gamma_3 - \Gamma_1]^2}, \frac{\Gamma_1\Gamma_2}{[\Gamma_1 - \Gamma_2]^2} \right) . \end{aligned} \tag{3.315}$$

Together with the constraint $v_1^2 + v_2^2 + v_3^2 = 1$ this is all we need for the numerical integration. Note that we have eliminated all dependence on the Euler angles and their momenta from the equations of motion (3.313,3.315). After giving arbitrary initial conditions the time dependence of the Euler angles can be obtained by integrating the equations

$$\begin{pmatrix} \dot{\theta} \\ \dot{\phi} \\ \dot{\psi} \end{pmatrix} = p_T C \begin{pmatrix} \sin(\psi)/\sin(\phi) & -\cos(\psi)/\sin(\phi) & 0 \\ \cos(\psi) & \sin(\psi) & 0 \\ -\cos(\psi)\sin(\psi)/\sin(\phi) & \cos^2(\psi)/\sin(\phi) & 1 \end{pmatrix} \begin{pmatrix} v_1/I_1 \\ v_2/I_2 \\ v_3/I_3 \end{pmatrix} . \tag{3.316}$$

The time evolution of the dust time T is obtained by integrating the equation

$$\dot{T} = \mathrm{e}^{3\alpha}\sqrt{1 + u_i u^i} = \sqrt{\Gamma_1\Gamma_2\Gamma_3 + C^2\left(\Gamma_2\Gamma_3 v_1^2 + \Gamma_1\Gamma_3 v_2^2 + \Gamma_1\Gamma_2 v_3^2\right)} . \tag{3.317}$$

The lifetime of the universe in terms of the dust proper time is expected to be finite.

Non-tumbling case

Before a further discussion of the general case let us have a short glance at the more simple non-tumbling case. This case is obtained if we choose for example the initial conditions $v_1 = 0 = v_2$ and $v_3 = 1$. The geodesic equation (3.315) implies now that the velocities stay constant in time. This implies $\ell_1 \equiv 0 \equiv \ell_2$ and $\ell_3 \equiv p_\psi \equiv p_T C$. Furthermore, we set $\theta = \pi/2$, $\phi = 0$ initially. With this choice only ψ stays dynamical. The potential contains now in addition to the curvature induced potential only one exponentially steep rotation wall and one centrifugal wall. The centrifugal wall is singular and hence prevents the universe point from crossing the line $\beta_- = 0$. The rotation wall becomes irrelevant in the approach towards the singularity. The time dependence of the remaining Euler angle $\psi(t)$ is obtained by integrating the equation $\dot{\psi} = \frac{p_\psi}{I_3}$. From this expression it is clear that the angle only changes significantly during bounces from the centrifugal wall. The calculations of Belinskii, Khalatnikov and Ryan [132], furthermore, suggest that the Euler angles assume constant values while the universe approaches the singularity. We shall check this claim using the numerical methods. Plots are shown on the next page in Figure 3.19.

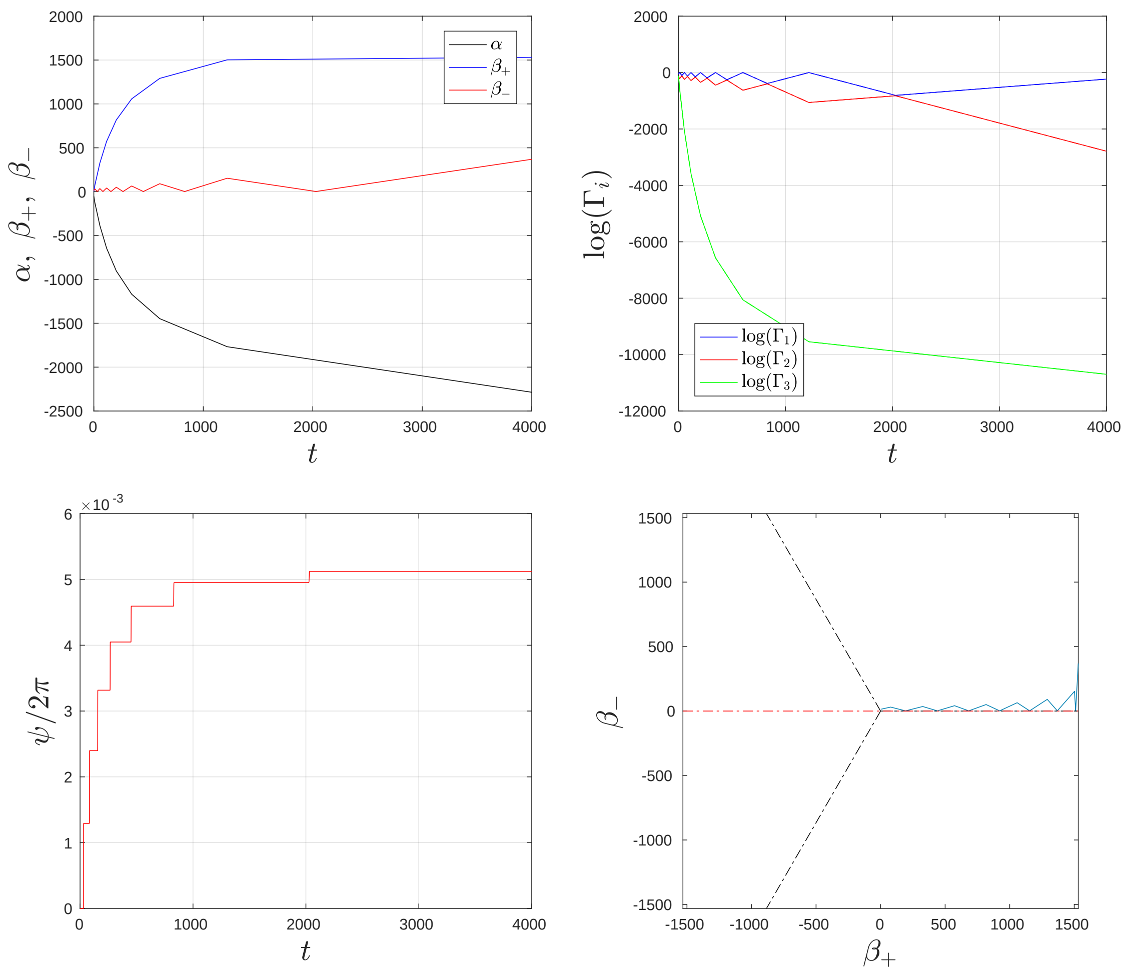


Figure 3.19: Plots of a numerical solution of equations 3.313 for the non tumbling case ($v_3 = 1$, $v_1 \equiv 0 \equiv v_2$). All plots belong to the same solution ($p_T = 1/2$, $p_\psi = 100$). We chose the initial conditions such that we obtain bounces between the curvature wall and the centrifugal wall. The Euler angle ψ changes significantly only during bounces of the universe point from the centrifugal wall. Furthermore, it appears to assume a constant value as t grows.

General case

The potential for the general case is depicted in figure 3.18. In contrast to the non-tumbling case the centrifugal walls are not static and change in a complicated manner dictated by the geodesic equation (3.315). Note that the centrifugal walls can in principle be crossed by the universe point. This is clear since we can set up the initial conditions such that we obtain this case. We can integrate the equations of motion together with the geodesic equation to obtain a numerical solution to the system. We set up initial conditions at $t = 0$. From here we evolve the solution backwards (figure 3.20) in time towards the rebounce and forwards in time towards the final singularity (figure 3.21). We remark that the validity of the numerical method broke down at some time $t \approx 1.8 \times 10^6$. This was indicated by the fact that the expression in (3.287) stopped to be close to unity during Kasner epochs. We view this as a sign that the numerical method we employ is too naive to deal with the problem in its full complexity. For the regime we are interested in, however, the method seems to be sufficient. We provide plots of the two ratios Γ_2/Γ_1, Γ_3/Γ_2 and the velocities $\vec{v}$ in order to provide a check of the approximation we will perform later on. In addition we plotted the dust time T in figure 3.20. The plot indicates that the dust time assumes constant values as $t \to \pm\infty$ and changes most significantly close to the rebounce as expected.

The simulation plotted in Fig. 3.20 and 3.21 were performed for the tumbling case, that is, the v_i are all chosen to be non-zero initially.

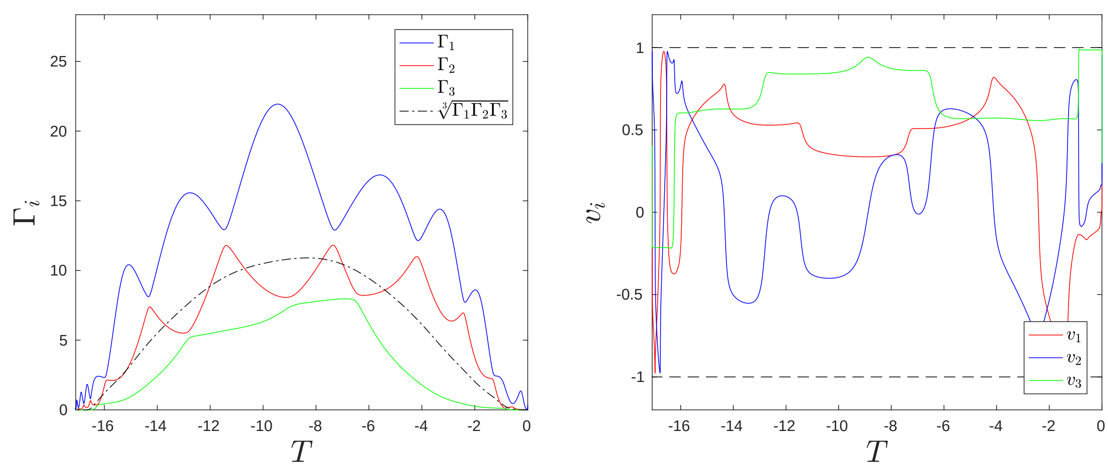


Figure 3.20: The plots show a numerical solution of the dust filled Bianchi IX universe. We chose to plot the solution against the dust proper time which allows to resolve the oscillations close to the rebounce.

Special classes of solutions

Before a discussion of the asymptotic regime close to the singularity, we comment on particular classes of solutions: One class of solutions is obtained if we choose, for example, the initial conditions $v_1 = 0 = v_2$ and $v_3 = 1$. The geodesic equation (3.315) implies now that the velocities stay constant in time. This implies that at all times $\ell_1 = 0 = \ell_2$ and $\ell_3 = p_\psi = p_T C$. This class of solutions is known as the non-tumbling case. Furthermore, there are classes of solutions which are rotating versions of the Taub solution. These solutions should be divided into two sub classes: one class that oscillates between the centrifugal walls and the curvature potential and one class that runs through the valley straight into the singularity. We set

$$v_1 = v_2 = \frac{1}{2}\,, v_3 = 0 \quad \text{and} \quad \beta_- = 0. \tag{3.318}$$

For the Γ_i variables it means that $\Gamma_1 = \mathrm{e}^{2\alpha}\mathrm{e}^{2\beta_+} = \Gamma_2$ and $\Gamma_3 = \mathrm{e}^{2\alpha}\mathrm{e}^{-4\beta_+}$. With this choice we obtain $I_3 = 0$ and $3I_1 = 3I_2 = \sinh^2(3\beta_+)$. Most importantly the geodesic equation (3.315) is trivially satisfied, that is, $v_1 = v_2 = 1/2$ and $v_3 = 0$ for all times.

Such as in the case of Bianchi I no isotropic expansion is possible without the addition of matter. The dust filled closed Friedmann universe is obtained by setting both anisotropy factors $\beta_\pm$, their velocities and the dust velocities u_i to zero (or alternatively simply by putting $C = 0$). The three curvature then reduces to ${}^{(3)}R = \frac{3\mathrm{e}^{-2\alpha}}{2}$. This corresponds to a FLRW line element with $k = 3/2$. The Hamiltonian constraint becomes the second Friedmann equation

$$\dot{\alpha}^2 = N^2\left(a_m^3 \mathrm{e}^{-3\alpha} - \frac{1}{4}\mathrm{e}^{-2\alpha}\right)\,, \tag{3.319}$$

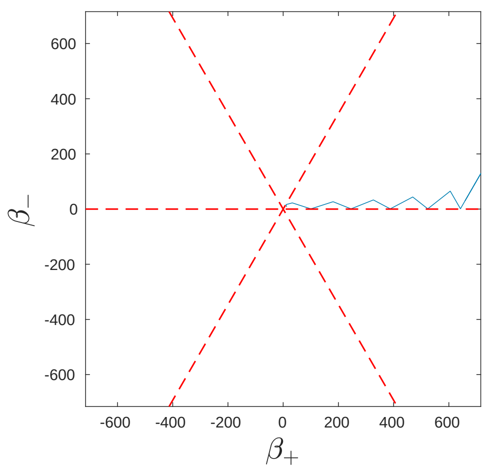
where $a_m = 2p_T$. The solution in the conformal gauge $N = a = \mathrm{e}^\alpha$ reads

$$a(t) = 4a_m^3 \sin^2\left(\frac{t - t_0}{4}\right)\,, \tag{3.320}$$

where t_0 is an arbitrary constant.

The asymptotic regime close to the singularity

A numerical solution to the equations of motion for the general case is plotted in figure 3.21. We regards this part of this solution to be not quite in the asymptotic regime but rather at the transition into the asymptotic regime.



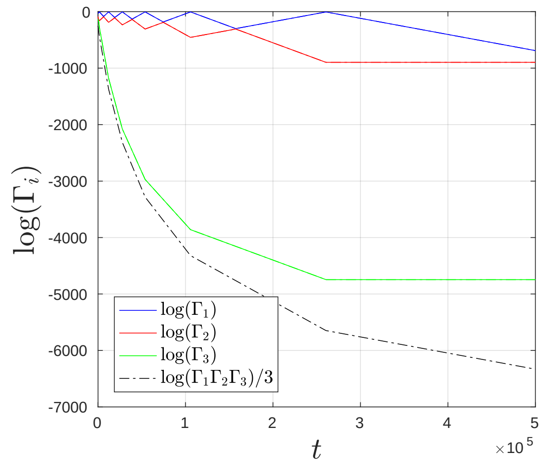


Figure 3.21: The plots show a numerical solution; a typical Kasner epoch in which the universe point bounces around between the curvature and the centrifugal walls of the potential.

In order to simplify the dynamics of the general case, BKL made two assumptions based on qualitative considerations of the equations of motion. The first assumption states that anisotropy of space grows without bound. This means that the solution enters the regime

$$\Gamma_1 \gg \Gamma_2 \gg \Gamma_3. \tag{3.321}$$

The ordering of indices is irrelevant. In fact there are six possible orderings of indices which each correspond to the universe point being constrained to one of the six regions bounded by the rotation and centrifugal walls sketched in Fig. 3.18. The region $\Gamma_1 > \Gamma_2 > \Gamma_3$ corresponds to the right region above the line $\beta_- = 0$ in figure 3.18. More precisely, the inequality (3.321) means that

$$\Gamma_2/\Gamma_1 \to 0 \quad \text{and} \quad \Gamma_3/\Gamma_2 \to 0\ . \tag{3.322}$$

Our numerical simulations support the validity of this assumption (see the plot of the ratios Γ_2/Γ_1 and Γ_3/Γ_2 in Fig. 3.22).

The second assumption made by BKL states that the Euler angles assume constant values:

$$(\theta, \phi, \psi) \to (\theta_0, \phi_0, \psi_0)\ , \tag{3.323}$$

that is, the rotation of the principal axes stops for all practical purposes and the metric becomes *effectively* diagonal. The analysis of BKL [131] supports the consistency of making both assumptions at the same time. Similar heuristic considerations can possibly be applied to other Bianchi models as well [31]. In the dust model under consideration, this assumption is equivalent to the statement that the dust velocities $\vec{v}$ assume constant values $\vec{v} \to \vec{v}^{(0)}$. Our numerical results indicate that this is in fact true (see Fig. 3.22).

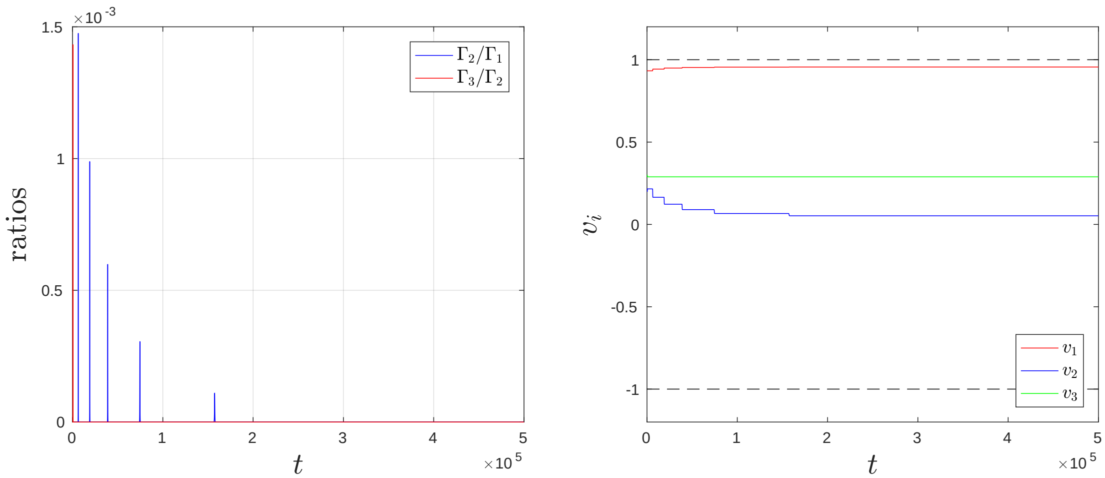


Figure 3.22: The plots show the relevant ratios of the Γ_i variables and the dust velocities v_i obtained from the numerical solution plotted in 3.21.

BKL then arrive at the simplified effective set of equations. Let us now carry out the approximation and apply it to our equations of motion. The kinetic term stays untouched during the approximation. The first step in the approximation is to ignore the rotational potential. In view of the strong inequality (3.321), we approximate the curvature potential via

$$\Gamma_1^2 + \Gamma_2^2 + \Gamma_3^2 - 2(\Gamma_1\Gamma_2 + \Gamma_3\Gamma_1 + \Gamma_2\Gamma_3) \approx \Gamma_1^2 \ . \tag{3.324}$$

Furthermore, we approximate the centrifugal potential by

$$\frac{\ell_1^2}{I_1} + \frac{\ell_2^2}{I_2} + \frac{\ell_3^2}{I_3} \approx 12C^2 p_T^2 \left[\frac{\Gamma_3}{\Gamma_2}\left(v_1^{(0)}\right)^2 + \frac{\Gamma_2}{\Gamma_1}\left(v_3^{(0)}\right)^2\right] \ . \tag{3.325}$$

Note that one centrifugal wall was ignored completely. Having Fig. 3.18 in mind, this approximation is well motivated since only two of the centrifugal walls are expected to have a significant influence on the dynamics of the universe point. After defining the new variables

$$a \equiv \Gamma_1 \ , \quad b \equiv 2p_T'^2 C^2 \left(v_3^{(0)}\right)^2 \Gamma_2, \quad c \equiv 4p_T'^4 C^4 \left(v_1^{(0)} v_3^{(0)}\right)^2 \Gamma_3, \tag{3.326}$$

we arrive at a simplified Hamiltonian constraint and equations of motion,

$$\begin{aligned} (\log a)^{\cdot}(\log b)^{\cdot} + (\log a)^{\cdot}(\log c)^{\cdot} + (\log b)^{\cdot}(\log c)^{\cdot} &= a^2 + b/a + c/b, \\ (\log a)^{\cdot\cdot} = b/a - a^2, \quad (\log b)^{\cdot\cdot} = a^2 - b/a + c/b, \quad (\log c)^{\cdot\cdot} &= a^2 - c/b, \end{aligned} \tag{3.327}$$

which coincides with the asymptotic form of equations obtained in [131]. Equations (3.327) can now be treated by the numerical methods which we have used in the previous sections. One must ensure that initial conditions are chosen such that the simulation starts close to the asymptotic regime (3.321).

The numerical simulations indicate that the non-diagonal Bianchi IX solutions, with tilted dust, evolve into the regime where $\Gamma_1 \gg \Gamma_2 \gg \Gamma_3$ and $v_i \approx const.$ The results motivate us to formulate the conjecture:

Given a tumbling solution to the general Bianchi IX model filled with pressure less tilted matter, there exists $t_0 \in \mathbb{R}$ such that the solution is well approximated by a solution to the asymptotic equations of motion for all times $t > t_0$ describing the vicinity of the singularity.

To make the notion of "approximation" mathematically more precise, a suitable measure of the "distance" on the set of solutions is needed. For this purpose, we propose to use the following simple measure:

$$\Delta(t) \equiv \sqrt{\left(\log\Gamma_1(t) - \log\bar{a}(t)\right)^2 + \left(\log\Gamma_2(t) - \log\bar{b}(t)\right)^2 + \left(\log\Gamma_3(t) - \log\bar{c}(t)\right)^2}, \quad (3.328)$$

where $\{\Gamma_1, \Gamma_2, \Gamma_3\}$ denotes the numerical solution to the exact equations of motion (3.313)–(3.315), and

$$a = \bar{a}\ , \quad b = 2p_T'^2 C^2 \left(v_3^{(0)}\right)^2 \bar{b}\ , \quad c = 4p_T'^4 C^4 \left(v_1^{(0)} v_3^{(0)}\right)^2 \bar{c} \quad (3.329)$$

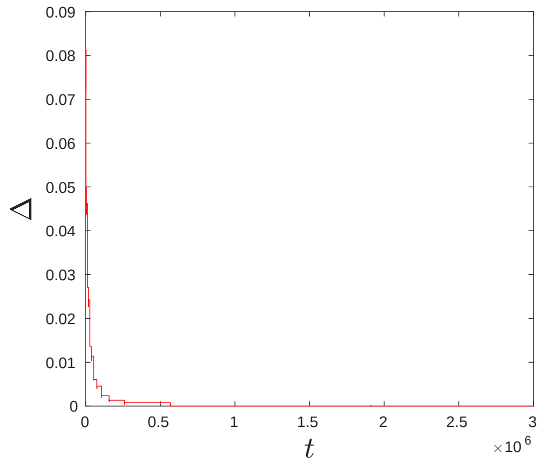
denote the numerical solution to the asymptotic equations of motion (3.327).

We have evolved the exact system of equations from $t = 0$ forward in time until $t = 3\times 10^6$. There we used the same initial conditions as the ones we used to obtain the solution shown in Fig. 3.21. We then took the final state at $t = 3\times 10^6$ as an initial condition for the asymptotic system of equations and evolved it backwards in time towards the re-bounce until $t = -980$.

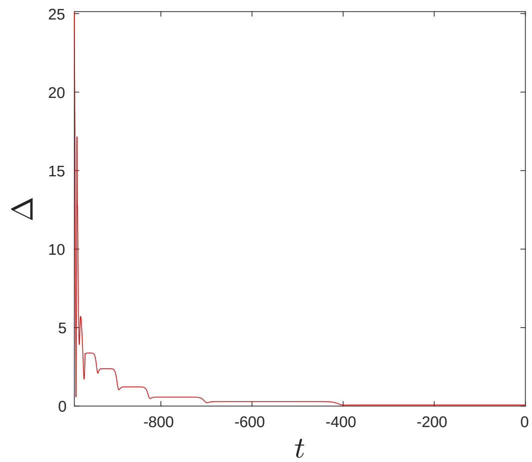
Fig. 3.23 presents the measure (3.328) as a function of time. We can see fast decrease of Δ with increasing time (evolution towards the singularity) and fast increase of Δ with decreasing time (evolution away from the singularity).

Our numerical simulations give strong support to the conjecture concerning the asymptotic dynamics of the general Bianchi IX spacetime put forward long ago by Belinski, Khalatnikov, and Ryan [131].

The approximation discussed in this section were used for a discussion of the singularity avoidance within the framework of affine coherent states quantization [97]. It might also be interesting to do the same within the Wheeler-DeWitt framework. One might, however, argue that the same considerations as in section 3.4.4 can be applied here as well.



(a)



(b)

Figure 3.23: The difference between the exact and the asymptotic solutions: (a) evolution towards the singularity, (b) evolution away from the singularity towards the rebounce.

Temporal evolution of curvature invariants in the general dust filled Bianchi IX universe

In the following we consider the Kretschamnn scalar for the general Bianchi IX model filled with dust. The calculation and the resulting expression of the Kretschmann scalar are rather involved and can be found in the Appendix C.3. The final expression is readily manipulated for a numerical evaluation.

We focus now again on the asymptotic regime close to the singularity. According to the phrase "matter does not matter" we expect the matter terms in the Kretschmann scalar to be negligible in the asymptotic regime, that is, the Weyl part should dominate over the Ricci part.

During Kasner epochs (i.e. between two successive bounces in the asymptotic regime) we expect the most relevant term to be the term in the first two lines of (C.43) right after the equals sign. We therefore assume now that the Kretschmann scalar can be approximated by

$$
\begin{aligned}
R_{\mu\nu\lambda\sigma}R^{\mu\nu\lambda\sigma} \approx \frac{1}{N^4} \Big(& \left[(\log\Gamma_1)^{\cdot}(\log\Gamma_2)^{\cdot}\right]^2 + \left[(\log\Gamma_1)^{\cdot}(\log\Gamma_3)^{\cdot}\right]^2 + \left[(\log\Gamma_2)^{\cdot}(\log\Gamma_3)^{\cdot}\right]^2 \\
& +(\log\Gamma_1)^{\cdot}(\log\Gamma_2)^{\cdot}(\log\Gamma_3)^{\cdot}\left[(\log\Gamma_1)^{\cdot}+(\log\Gamma_2)^{\cdot}+(\log\Gamma_3)^{\cdot}\right]\Big) \ .
\end{aligned}
\tag{3.330}
$$

This claim is confirmed by our numerical simulations. We remark that this term corresponds exactly to the Weyl squared scalar of the Bianchi I model. The Weyl tensor of the Bianchi I model has only an electric part, and the magnetic part vanishes (in the quasi-Gaussian gauge).

During Kasner epochs the time evolution can be parameterized using the Lifshitz - Khalatnikov parameter u following the considerations in [131]. Doing so and using the assumption (3.330) we obtain that the Hubble-normalized Kretschmann scalar can be approximated by

$$R_{\mu\nu\lambda\sigma}R^{\mu\nu\lambda\sigma}/|K^i{}_i|^4 \approx \frac{16u^2(1+u)^2}{(1+u+u^2)^3} \qquad \text{during Kasner epochs.} \tag{3.331}$$

Consequently the Kretschmann scalar blows up like the expansion $K^i{}_i$ to the power 4 during Kasner eras. In order to understand the temporal evolution of the Kretschmann scalar over the course of one epoch we have plotted the expression on the right hand side of (3.331) as a function of u in Fig. 3.24. It is important that the function has a maximum in $u = 1$. [6]

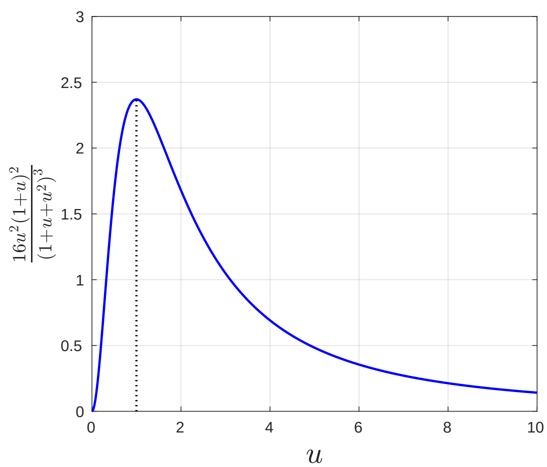


Figure 3.24: The plot shows the function on the right hand side of equation (3.331).

BKL refer to bounces from the curvature potential as *transformations of the first kind* while they call bounces from centrifugal walls *transformations of the second kind*. Transformations of the first kind change the Lifshitz-Khalatnikov parameter according to $u \xrightarrow{1} u - 1$. Transformations of the second kind interchange the values of the velocities according to $(\log \Gamma_1)^\cdot \xrightarrow{2} (\log \Gamma_2)^\cdot$, $(\log \Gamma_2)^\cdot \xrightarrow{2} (\log \Gamma_1)^\cdot$ and leave the value of u unchanged, i.e. $u \xrightarrow{2} u$. It follows that $\xrightarrow{1}$ changes the value of the Hubble normalized Kretschmann scalar (3.331) while $\xrightarrow{2}$ does not. According to the analysis in [131] a typical Kasner era can be expressed as a sequence of n Kasner epochs which starts with an epoch that has a maximum u-value larger than 1 when evolving towards the singularity. The value of u decreases with each transformation of the first kind and ends with the epoch for which u becomes smaller than

[6]This maximum implies an upper bound for the Hubble normalized Kretschmann scalar during Kasner eras given by 64/27.

1 for the first time, e.g.

$$1 < u_1 = u_{\max} \xrightarrow{1} u_2 \xrightarrow{2} u_3 \xrightarrow{1} u_4 \xrightarrow{2} u_5 \xrightarrow{1} \ \ldots \ \xrightarrow{2} u_{n-1} \xrightarrow{1} u_n = u_{\min} < 1 \ . \tag{3.332}$$

It should be remarked at this point that the u-map was found to be asymptotically exact for particular cases (for a collection of rigorous results concerning the u-map see [49, 119]). A solution of the discrete mixmaster map and a detailed study of its chaotic nature for the vacuum Bianchi IX case can be found in [133].

We are now in the position to provide a picture of the behavior of the Kretschmann scalar over the course of one Kasner era: According to the formula (3.331) plotted in Fig. 3.24 and the u-map (3.332) we expect the Hubble normalized Kretschmann scalar to increase its value with each transformation of the first kind before it hits the value $u_{\min} < 1$ for which it decreases again. This is apart from the behavior in the vicinity of the bounces precisely what we observe in the numerically evaluated Hubble normalized scalar plotted in Fig. 3.21.

Consequently during Kasner epochs, $R_{\mu\nu\lambda\sigma}R^{\mu\nu\lambda\sigma}$ increases like the expansion to the power four. Over the course of a single Kasner era the value of the Hubble normalized Kretschmann scalar increases until it drops down to a finite value when it ends. This process will repeat itself infinitely often with the beginning of the next Kasner era until the system approaches the singularity.

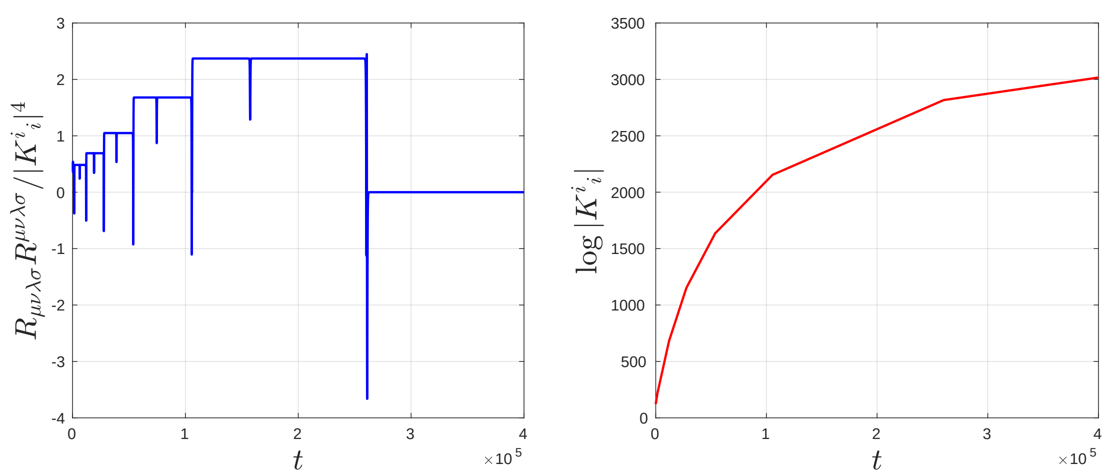


Figure 3.25: The plots show the temporal evolution of the Hubble normalized Kretschmann scalar obtained from the numerical solution plotted in 3.21.

Chapter 4

Conclusion and outlook

Conformal covariance in minisuperspace requires a rethinking about the criteria for singularity avoidance. We proposed three criteria which are compatible with the conformal covariance and applied them to specific models. The mechanism by which the singularity is resolved is mostly the same in all models. The spreading of wave packets leads to a decreasing amplitude. As a result singularities can in principle be avoided by all three criteria. Spreading of wave packets can occur if the dimension of minisuperspace is sufficiently large ($d \geq 3$) and if the approach towards the singularity is AVTD. The prototype of a model with such features is the Bianchi type I universe which we extensively studied in this thesis. The criteria for singularity avoidance not only predicted an avoidance of the initial singularity but also an avoidance of the late stages of the universe due to the spreading of the wave packets in the vacuum case. We found that matter can in principle stabilize wave packets in the late stages of the universe. We have also studied the Bianchi I model with a minimally coupled electromagnetic field where we found that the situation was similar to the vacuum case. In contrast to scalar fields, electromagnetic fields apparently do not enhance the spreading of wave packets. Indeed the effect of electromagnetic fields is negligible in the asymptotic regime close to the singularity. We expect these results to be representative for other types of models. This could be seen in the case of the Kantowski-Sachs and the Bianchi II model where the approach towards the singularity was AVTD as well. The situation, however, is not so clear when the approach to the singularity is not AVTD. This is, for example, the case for the vacuum Bianchi type VIII and IX models. One might nevertheless expect a spreading of wave packets based on the fact that between two consecutive bounces from the curvature potential the dynamics of these models are Kasner–like. The numerical results in [130] support this conjecture. It would, nevertheless, be desirable to have a more rigorous result at hand. Furthermore, it should also be interesting to investigate how decoherence affects the spreading of wave packets.

In this thesis we only considered minisuperspace models within Einstein's theory and we have restricted ourselves to the discussion of minimally coupled matter fields. It is desirable to extend the discussion to minisuperspace models with non-minimally coupled matter fields or models that result from applying the symmetry reduction to alternative theories of gravity [134] as for example the Brans-Dicke theory. Furthermore, we mostly studied Big Bang type singularities in this thesis. One might extend this work to more exotic types of singularities such as the Big Brake and Big Rip in anisotropic models. The latter type was already studied in [T3]. The authors found that the singularity was only avoided by criterion 2.

Furthermore, it would be exciting to study minisuperspace models and their quantization within the Einstein-Cartan theory or more generally within the Poincaré gauge theories with minimally coupled Fermion fields [135]. We can expect here that we would have to deal with quite different structures in the constraint equations than the ones discussed in this thesis.

An interesting next step would be to investigate singularity avoidance within midisuperspace models. Candidates for an examination are for example the LTB spacetime or more generally the silent universe model. Apart from these it would also be interesting to explore singularity avoidance in Gowdy models [69] and gravitational wave spacetimes. The Gowdy spacetimes are particularly appealing as they display BKL behavior when approaching the singularity [70]. One might also discuss the validity of the minisuperspace approximation within the midisuperspace models (e.g. Friedmann in LTB or homogeneous models within the Gowdy spacetimes [69]).

Moreover, we initiated an investigation of the factor ordering problem. The factor ordering is deeply connected with the other problems of Quantum Cosmology and in particular it appears to have some deep connection with the problem of time. Our discussion of the generalized setup in section 2.1.5 and 2.2.7 revealed some interesting structures which can be found in minisuperspace models and seem to lie at the interface between foliation theory and conformal differential geometry. Singularity avoidance also strongly depends on the factor ordering ambiguities. This issue is not exclusive to the Wheeler-DeWitt approach but was also argued to be relevant in [13, 85, 93]. The factor ordering problem also prevented us from investigating singularity avoidance in the case of non-diagonal Bianchi models (e.g. Bianchi I and II). A big part of the factor ordering problem is the question of the conformal weight of the wave function. In particular our criteria for singularity avoidance are partially not applicable if the conformal weight of the wave function is unknown. For the above mentioned reasons I believe that it is worthwhile to investigate further into this direction. It appears that the factor ordering problem in Wheeler-DeWitt Quantum Cosmology can be approached in a systematic way. One of the main motivations to study Quantum Cosmology is to provide us with toy models. The final goal, however, is to gain insights into full theory, possibly by applying what one learned from the toy models. Thus one of the main questions is how to convert the idea of conformal ordering to the full Wheeler-DeWitt equation and if this idea can harmonize with any of the regularization approaches.

Appendix A

Partial differential equations

A.1 Existence of solutions to hyperbolic partial differential equations

Consider an initial value problem in $d = 1 + n$ dimensions of the form

$$\begin{cases} \left[M^{\mu\nu}\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\nu} + a^\mu \frac{\partial}{\partial x^\mu} + b\right]\Phi = 0\ , \quad \{x^\mu\} = (x^0 = t, \boldsymbol{x} = \{x^i\}) \in \mathbb{R}_+ \times \mathbb{R}^n \\ (\Phi, \partial_\alpha \Phi)\mid_{t=0} = (f, g) \end{cases} . \tag{A.1}$$

where $\{M^{\mu\nu}\}$ is a real symmetric $d \times d$ matrix with the properties that $M^{00} < 0$ and $\{M^{ij}\}$ is positive definite. Theorem 8.6 in Ringströms book [136] can be specialized to this situation. It implies the global existence and uniqueness of solutions $\Phi \in C^\infty(\mathbb{R}^d, \mathbb{R})$ provided that $M^{\mu\nu}$, a^μ and b are smooth functions $\mathbb{R}^d \to \mathbb{R}$ and f and g are smooth functions $\mathbb{R}^n \to \mathbb{R}$. The theorem is thus applicable to a wide class of minisuperspace Wheeler-DeWitt equations.

A.2 Frobenius theorem

We formulate here a very simple version of the Frobenius theorem suited for the application to PDE systems. See [75] for a geometric formulation and generalizations of the theorem.

Let $\boldsymbol{f}_i(x) = {f_i}^A(x)\partial_A$ be $r < n$ linearly independent vector fields on $\mathbb{R}^n$ such that the coefficients are at least $C^1(\mathbb{R}^n, \mathbb{R})$. Consider the system of partial differential equations

$${f_i}^A(x)\partial_A u(x) = 0\ . \tag{A.2}$$

where $u \in C^2(\mathbb{R}^n, \mathbb{R})$. One seeks for a set of solutions $u_1, \ldots, u_{n-r}$ such that the differentials

$\mathrm{d}u_1, \ldots, \mathrm{d}u_{n-r}$ are linearly independent. The theorem states that such solutions exist locally if and only if

$$[\boldsymbol{f}_i, \boldsymbol{f}_j]u = C_{ij}^k \boldsymbol{f}_k u \ , \tag{A.3}$$

where C_{ij}^k are functions of x.

In the following let us consider a generalized system of equations of the form

$$\boldsymbol{L}_i u(x) = f_i{}^A(x)(\partial_A + \lambda_A(x))u(x) = 0 \ . \tag{A.4}$$

We suppose in the following that $\boldsymbol{f}_i(x)$ satisfies (A.3). Furthermore, the differential form $\boldsymbol{\lambda} := \lambda_A \mathrm{d}x^A$ is closed. It follows now that

$$[\boldsymbol{L}_i, \boldsymbol{L}_j]u = C_{ij}^k \boldsymbol{L}_k u \ , \tag{A.5}$$

Moreover, the Poincaré lemma implies that there exists a function Φ such that $\lambda_A = \partial_A \Phi$. Now set $\bar{u} := \mathrm{e}^{\Phi} u$ and we obtain from (A.2) that $\bar{u}$ satisfies the following PDE system

$$f_i{}^A(x)\partial_A \bar{u}(x) = 0 \ , \tag{A.6}$$

to which we can readily apply the Frobenius theorem.

A.3 Local decay rate estimate for the classical wave equation

Let Φ be a solution to the classical wave equation in $d = 1 + n$ dimensions

$$\begin{cases} \left[\frac{\partial^2}{\partial t^2} - \sum_{i=1}^{n} \frac{\partial^2}{\partial (x^i)^2}\right] \Phi = 0 \ , \quad \{x^\mu\} = (t, \boldsymbol{x} = \{x^i\}) \in \mathbb{R}_+ \times \mathbb{R}^n \\ (\Phi, \partial_\alpha \Phi) \mid_{t=0} = (f, g) \end{cases} , \tag{A.7}$$

where f and g are any smooth functions with compact support. It is well known (see e.g. [107]) that in $d \geq 3$ dimensions there exist constants $C_{1/2} > 0$ such that

$$|\Phi(t, \boldsymbol{x})| \leq C_1 |t|^{-\frac{d-2}{2}} \ , \tag{A.8}$$

$$|\partial_\mu \Phi(t, \boldsymbol{x})| \leq C_2 |t|^{-\frac{d-2}{2}} \ . \tag{A.9}$$

The positive constants $C_{1/2}$ are determined from certain Sobolev norms of f and g. Their precise form is irrelevant for our discussion but can be found in [107].

Appendix B

Conformal geometry

Let $(\mathcal{M}, \mathrm{d}\mathcal{S}^2)$ be a pseudo-Riemannian manifold with metric signature $(-,+,+,\ldots)$. A Weyl or conformal rescaling of the metric is the transformation

$$\mathrm{d}\mathcal{S}^2 \to \mathrm{d}\widetilde{\mathcal{S}}^2 = \Omega^2 \mathrm{d}\mathcal{S}^2 \ , \tag{B.1}$$

where $\Omega : \mathcal{M} \to \mathbb{R}_+$. Weyl rescalings define an equivalence relation. The resulting equivalence class $[\mathrm{d}\mathcal{S}^2]$ is referred to as conformal metric and we shall refer to $(\mathcal{M}, [\mathrm{d}\mathcal{S}^2])$ as a conformal manifold. Length and volume are not a well defined concept on such a manifold without imposing additional structures. Since angles are preserved by Weyl rescalings, however, the light cone structure is also preserved.

Particular interest lies on scale covariant tensors (or more generally tensor densities), i.e. all tensors $\mathcal{T}$ that transform as

$$\mathcal{T} \to \widetilde{\mathcal{T}} = \Omega^k \mathcal{T} \quad \text{for some } k \in \mathbb{R} \ , \tag{B.2}$$

under the transformation (B.1). We call k the conformal weight of the tensor $\boldsymbol{\mathcal{T}}$ and denote it by $k = w(\mathcal{T})$. By definition $w(\mathrm{d}\mathcal{S}^2) = 2$. The most popular conformally invariant tensor is certainly the Weyl tensor $\mathcal{W}^A{}_{BCD}$ with $w(\mathcal{W}^A{}_{BCD}) = 0$. The Weyl squared scalar $\mathcal{W}^2 := \mathcal{W}^{ABCD}\mathcal{W}_{ABCD}$ is conformally covariant with $w(\mathcal{W}^2) = -4$.

B.1 Transformation laws

Now let $\mathcal{M}$ be parametrized by the coordinates q^A. Let us pick a representative of the conformal metric $\mathrm{d}\mathcal{S}^2 \in [\mathrm{d}\mathcal{S}^2]$. The components of the Levi-Civita connection compatible with $\mathrm{d}\mathcal{S}^2$ transform according to

$$\Gamma^B_{AC} \mapsto \widetilde{\Gamma}^B_{AC} = \Gamma^B_{AC} + \left(\delta^B_A \partial_C + \delta^B_C \partial_A - \mathcal{G}_{AC}\mathcal{G}^{BD}\partial_D\right) \log \Omega \; . \tag{B.3}$$

From this one can derive the transformation laws for the Riemannian curvatures. Formulas for the Riemann tensor are quite involved but can be found in [137]. The Ricci scalar transforms like

$$\mathcal{R} \mapsto \widetilde{\mathcal{R}} = \Omega^{-2}\left[\mathcal{R} - 2(d-1)\frac{\Box\Omega}{\Omega} - (d-1)(d-4)\mathcal{G}^{AB}\frac{\partial_A\Omega\partial_B\Omega}{\Omega^2}\right] \; . \tag{B.4}$$

For a conformally covariant differential form $\boldsymbol{\omega}$ of degree $\deg(\boldsymbol{\omega})$ and with conformal weight $w(\boldsymbol{\omega})$ it holds that

$$w(\star\boldsymbol{\omega}) = w(\boldsymbol{\omega}) + d - 2\deg(\boldsymbol{\omega}) \; . \tag{B.5}$$

B.2 Yamabe problem

The Yamabe problem [138] is an important problem in conformal differential geometry. It was partially solved with the following result: *Given a compact manifold $\mathcal{M}$ with dimension $d \geq 3$ equipped with a conformal equivalence class of Riemannian metrics $[\mathrm{d}\mathcal{S}^2]$ there exists a gauge $\mathrm{d}\mathcal{S}^2 \in [\mathrm{d}\mathcal{S}^2]$ in which the Ricci curvature scalar is constant.* The non-compact and Lorentzian cases, however, remain to be some of the major open problems in the field of conformal differential geometry.

B.3 Weylian geometry

A conformal manifold lacks the notion of a scale. Consequently there is no conformally invariant notion of parallel transport of tensor fields. However, the introduction of an additional structure, namely, the so-called Weyl vector allows for the construction of a conformally invariant connection. This, furthermore, allows for the definition of conformally covariant curvature tensors and conformally covariant differentation. The articles [139, 140] served as guidelines for this section of the appendix. The paper [139] offers historical perspective and [140] gives a formulation within the language of exterior calculus.

Weyl metric

A *Weylian manifold* $(\mathcal{M}, [\mathrm{d}\mathcal{S}^2, \boldsymbol{\varphi}])$ consists of a manifold equipped with a *Weylian metric* $[\mathrm{d}\mathcal{S}^2, \varphi]$, i.e. an equivalence class of pairs, where $\mathrm{d}\mathcal{S}^2 = \mathcal{G}_{AB}\mathrm{d}q^A \otimes \mathrm{d}q^B$ is in our case a

Lorentzian metric and $\boldsymbol{\varphi} = \varphi_A \mathrm{d}q^A$ is called the *Weyl one-form* (or often simply Weyl vector). The equivalence relation between pairs is defined via

$$(\mathrm{d}\mathcal{S}^2, \boldsymbol{\varphi}) \sim (\mathrm{d}\widetilde{\mathcal{S}}^2, \widetilde{\boldsymbol{\varphi}}) \quad :\Leftrightarrow \quad \exists\, \Omega : \mathcal{M} \to \mathbb{R}_+ \ : \quad (i) \quad \mathrm{d}\widetilde{\mathcal{S}}^2 = \Omega^2 \mathrm{d}\mathcal{S} \quad (ii) \quad \widetilde{\boldsymbol{\varphi}} = \boldsymbol{\varphi} - \mathrm{d}\log\Omega \ . \tag{B.6}$$

The transformation (i) is called conformal rescaling and (ii) is called a scale gauge transformation. Together they form what is called a *Weyl transformation* in this context.[1] If $\boldsymbol{\varphi}$ is closed we speak of an *integrable Weyl structure* and if $\boldsymbol{\varphi}$ is exact the Weyl structure is referred to as trivial. With some abuse of terminology we shall refer to choosing a representative $(\mathrm{d}\mathcal{S}^2, \boldsymbol{\varphi}) \in [\mathrm{d}\mathcal{S}^2, \boldsymbol{\varphi}]$ as fixing the gauge.

The conformal connection and the scale covariant derivative

Recall that our main interest lies in conformally covariant tensor fields. In particular, we want to differentiate such fields without spoiling the conformal symmetry. In order to do so we define the (torsion–free and linear) conformal connection Γ via its components

$$\Gamma^i{}_{jk} := {}_{\mathcal{G}}\Gamma^i_{jk} + \delta^i_j \varphi_k + \delta^i_k \varphi_j - \mathcal{G}_{jk}\varphi^i \ , \tag{B.7}$$

where ${}_{\mathcal{G}}\Gamma^i{}_{jk}$ are the Christoffel symbols of the Levi-Civita connection compatible with $\mathrm{d}\mathcal{S}^2$. We will use in this section the left subscript ${}_{\mathcal{G}}(\ .\ )$ to indicate that an object is a Riemannian object constructed in a particular gauge. The *conformal connection* is constructed in such a way that under a Weyl transformation

$$\Gamma^A_{BC} \mapsto \widetilde{\Gamma}^A_{BC} = \Gamma^A_{BC} \ , \tag{B.8}$$

that is, the *conformal connection* is invariant under Weyl transformations. For later convenience we also introduce the tensor $\mathcal{C}^{AD}_{BC} := \delta^A_B \delta^D_C + \delta^A_C \delta^D_B - \mathcal{G}_{BC}\mathcal{G}^{AD}$. We can then define

$$\Gamma^A_{BC} := {}_{\mathcal{G}}\Gamma^A_{BC} + \mathcal{C}^{AD}_{BC}\varphi_D \ . \tag{B.9}$$

The scale covariant derivative of a tensor field $\boldsymbol{\mathcal{T}}$ is then defined by

$$\mathcal{D}\boldsymbol{\mathcal{T}} := \nabla\boldsymbol{\mathcal{T}} + w(\boldsymbol{\mathcal{T}})\varphi \otimes \boldsymbol{\mathcal{T}} \ , \tag{B.10}$$

---

[1]Note that in the main body of the thesis we sloppily refer to both conformal rescalings and Weyl transformations as conformal transformations.

where ∇ is the covariant derivative defined by the conformal connection Γ. By construction we now have that for a tensor field $\boldsymbol{\mathcal{T}}$ of type $\binom{r}{s}$ the tensor field $\mathcal{D}\boldsymbol{\mathcal{T}}$ is of type $\binom{r}{s+1}$ and $w(\mathcal{D}\boldsymbol{\mathcal{T}}) = w(\boldsymbol{\mathcal{T}})$. The components of a vector field for example are differentiated as

$$\mathcal{D}_A \mathcal{T}^B = \partial_A \mathcal{T}^B + \Gamma^B_{AC}\mathcal{T}^C + w(\boldsymbol{\mathcal{T}})\varphi_A \mathcal{T}^B \ . \tag{B.11}$$

The divergence of a vector field is consequently given by

$$\mathcal{D}_A \mathcal{T}^A = {}_{\mathcal{G}}\nabla_A \mathcal{T}^A + [d + w(\boldsymbol{\mathcal{T}})]\varphi_A \mathcal{T}^A \ . \tag{B.12}$$

Since the left hand side of this equation is conformally covariant can conclude that the divergence ${}_{\mathcal{G}}\nabla_A \mathcal{T}^A$ is conformally covariant if and only if $w(\boldsymbol{\mathcal{T}}) = -d$. Moreover, the scale covariant exterior derivative acting on differential forms is

$$\mathcal{D}\Phi := \mathrm{d}\Phi + w(\Phi)\boldsymbol{\varphi} \wedge \Phi \ . \tag{B.13}$$

Most importantly it holds that $\mathcal{D}\left(\mathrm{d}\mathcal{S}^2\right) = 0$ or equivalently $\mathcal{D}_C \mathcal{G}_{AB} = 0$. One says that the conformal connection is weakly compatible with the metric. The conventions here lead to a non-metricity $\mathcal{Q}_{CAB} := -\nabla_C \mathcal{G}_{AB} = 2\varphi_C \mathcal{G}_{AB}$.

Conformal curvatures

Now let $\boldsymbol{v} = v^A \partial_A$ be a vector field of arbitrary weight. We can define the conformal curvature tensor via

$$\left[\mathcal{D}_B, \mathcal{D}_A\right] v^C =: \mathcal{R}^C{}_{DAB} v^D \ . \tag{B.14}$$

It can be expressed in terms of the conformal connection:

$$\mathcal{R}^C{}_{DAB} = \partial_A \Gamma^C_{DB} - \partial_B \Gamma^C_{DA} + \Gamma^E_{DB}\Gamma^C_{EA} - \Gamma^C_{BE}\Gamma^E_{DA} \ . \tag{B.15}$$

Other curvature tensors can now be defined such as in Riemannian geometry, for example

$$\mathcal{R}_{AB} := \mathcal{R}^C{}_{ACB} \quad \text{and} \quad \mathcal{R} := \mathcal{R}^A{}_A \ . \tag{B.16}$$

They have the following properties:

- The curvature tensors are conformally covariant. In particular $w(\mathcal{R}^C{}_{DAB}) = 0$, $w(\mathcal{R}_{AB}) = 0$ and $w(\mathcal{R}) = -2$.
- $\mathcal{R}^C{}_{DAB} = -\mathcal{R}^C{}_{DAB}$.

- The first Bianchi identity $\mathcal{R}^C{}_{[DAB]} = 0$ holds. This is a consequence of the absence of torsion.
- The second Bianchi identity $\nabla_{[A}\mathcal{R}^C{}_{BD]E} = 0$ holds.
- $\mathcal{R}_{ABCD} + \mathcal{R}_{BACD} = -\mathcal{F}_{CD}\ \mathcal{G}_{AB}$ and thus $\mathcal{R}_{AB} - \mathcal{R}_{BA} = 2\mathcal{R}_{[AB]} = -\frac{d}{2}\mathcal{F}_{AB}$. This is a consequence of the non-metricity of the Weylian connection. The conformally invariant curvature tensor $\mathcal{F}_{AB} := \partial_A\varphi_B - \partial_B\varphi_A$ is an analogue of the electromagnetic field strength tensor. $\mathcal{F}_{AB}$ vanishes if and only if $\boldsymbol{\varphi}$ is closed, i.e. the Weyl structure is integrable.

Denoting now the curvatures of the Riemannian manifold equipped with the metric $\mathcal{G}_{AB}$ by ${}_{\mathcal{G}}\mathcal{R}^C{}_{ABD}$ and so on we obtain the following relations

$$\mathcal{R}^C{}_{DAB} = {}_{\mathcal{G}}\mathcal{R}^C{}_{DAB} + 2\ {}_{\mathcal{G}}\nabla_{[A}\left(\mathcal{C}^{CG}_{B]D}\varphi_G\right) + \left(\mathcal{C}^{EG}_{DB}\mathcal{C}^{CF}_{EA} - \mathcal{C}^{CF}_{BE}\mathcal{C}^{EF}_{DA}\right)\varphi_F\varphi_G\ , \tag{B.17}$$

$$\mathcal{R}_{AB} = {}_{\mathcal{G}}\mathcal{R}_{AB} - (d-1)\mathcal{F}_{AB} - \mathcal{G}_{AB}\ {}_{\mathcal{G}}\nabla_C\varphi^C + (d-2)\left(\varphi_A\varphi_B - {}_{\mathcal{G}}\nabla_B\varphi_A - \mathcal{G}_{BD}\varphi^C\varphi_C\right)\ , \tag{B.18}$$

$$\mathcal{R} = {}_{\mathcal{G}}\mathcal{R} - 2(d-1)\ {}_{\mathcal{G}}\nabla_A\varphi^A - (d-2)(d-1)\varphi^A\varphi_A\ . \tag{B.19}$$

Trivial Weyl structure: Let Φ be a is strictly positive conformally covariant scalar of conformal weight $k \neq 0$. We can then define a Weyl 1-form via

$$\boldsymbol{\varphi} := -\frac{1}{k}\mathrm{d}\log\Phi\ . \tag{B.20}$$

The resulting Weylian metric is referred to as trivial since we can gauge the Weyl vector away. This can be seen from the following: We can find a conformal transformation such that $\widetilde{\Phi} = \Omega^k\Phi = 1$ by setting $\Omega = \Phi^{-1/k}$. This implies that

$$(\Phi^{-2/k}\mathrm{d}\mathcal{S}^2, 0) \in [\mathrm{d}\mathcal{S}^2, \varphi]\ . \tag{B.21}$$

In this gauge the conformal connection is metric compatible and the curvatures are equal to the Riemannian curvatures. In this sense Weylian geometry can be regarded as a generalization of Riemannian geometry. One usually refers to the gauge (B.21) as the *Riemann gauge*.

The operator $\mathcal{D}^2$ and the Yamabe operator

Consider first the Laplace-Beltrami type operator

$$\mathcal{D}^2\Psi := \mathcal{D}^A\mathcal{D}_A\Psi\ , \tag{B.22}$$

where Ψ is a scalar field of weight $w(\Psi) = k$. Since it maps conformally covariant scalar fields of weight $w(\Psi)$ to conformally covariant scalar fields of weight $w(\mathcal{D}^2\Psi) = w(\Psi) - 2$ one says that the operator $\mathcal{D}^2$ has conformal bi-weight $(w(\Psi)-2, w(\Psi))$. We can express the operator in terms of the Weyl 1-form as

$$\mathcal{D}^2\Psi = \left[{}_{\mathcal{G}}\Box + (2k+d-2)(\varphi^A\partial_A + k\varphi^A\varphi_A) + k\left({}_{\mathcal{G}}\nabla_A\varphi^A - k\varphi^A\varphi_A\right)\right]\Psi \ , \tag{B.23}$$

where ${}_{\mathcal{G}}\Box := \frac{1}{\sqrt{-\mathcal{G}}}\partial_A\left(\sqrt{-\mathcal{G}}\mathcal{G}^{AB}\partial_B\right)$ is the usual Laplace-Beltrami operator on the Riemannian manifold $(\mathcal{M}, \mathrm{d}\mathcal{S}^2)$. Using equation (B.19) we can eliminate ${}_{\mathcal{G}}\nabla_A\varphi^A$ from the equation and obtain

$$\mathcal{D}^2\Psi = \left[{}_{\mathcal{G}}\Box + (2k+d-2)\left(\varphi^A\partial_A + \frac{k}{2}\varphi^A\varphi_A\right) + \frac{k}{2(d-1)}\left({}_{\mathcal{G}}\mathcal{R} - \mathcal{R}\right)\right]\Psi \ . \tag{B.24}$$

It now follows that when restricting ourselves to the weight $k = \frac{2-d}{2}$ we obtain

$$\left[\mathcal{D}^2 - \xi\mathcal{R}\right]\Psi = \left[{}_{\mathcal{G}}\Box - \xi\ {}_{\mathcal{G}}\mathcal{R}\right]\Psi \ , \tag{B.25}$$

where $\xi = \frac{d-2}{4(d-1)}$. Hence $\mathcal{D}^2 - \xi\mathcal{R}$ coincides with the conformal Yamabe operator acting on scalar fields Ψ of weight $w(\Psi) = -\frac{d-2}{2}$. The expression (B.25) is completely independent of the Weyl 1-form. Since it maps scalars of conformal weight $-\frac{d-2}{2}$ to scalars of conformal weight $-\frac{d+2}{2}$ the operator $\mathcal{D}^2 - \xi\mathcal{R}$ has conformal bi-weight $\left(-\frac{d+2}{2}, -\frac{d-2}{2}\right)$.

Appendix C

Auxiliary calculations

C.1 Dirac consistency of naive conformal ordering

In this part of the appendix we provide auxiliary calculations for section 2.2.7. Recall that $K_i^{AB} = \nabla^{(A} A_i{}^{B)} + \lambda_i \mathcal{G}^{AB}$. Furthermore, it helps to keep in mind that

$$\bar{P}_A{}^B B_B{}^i = 0 \ , \quad A_i{}^B \bar{P}_B{}^A = 0 \ , \quad \text{and} \quad \nabla_A P_B{}^C = -\nabla_A \bar{P}_B{}^C \ . \tag{C.1}$$

The commutator $\left[\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_i\right]$ splits into the following parts

$$\left[\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_i\right] \Psi = \mathrm{i} \left(\frac{1}{2} \left[\Box, A_i{}^A \partial_A\right] + \frac{w(\Psi)}{2} \left[\Box, \lambda_i\right] - \frac{\xi_d}{2} \left[\mathcal{R}, A_i{}^A \partial_A\right] - \left[\mathcal{V}, A_i{}^A \partial_A\right] \right) \Psi \ . \tag{C.2}$$

The commutators that appear on the right hand side of the expression can be written as

$$\begin{aligned}
\left[\Box, A_i{}^A \partial_A\right] &= 2\nabla^{(A} A_i{}^{B)} \nabla_A \partial_B + \left(\Box A_i{}^A + A_i{}^B \mathcal{R}_B{}^A\right) \partial_A \\
\left[\Box, \lambda_i\right] &= \Box \lambda_i + 2\mathcal{G}^{AB} \left(\partial_A \lambda_i\right) \partial_B \\
\left[\mathcal{V}, A_i{}^A \partial_A\right] &= -A_i{}^A \partial_A \mathcal{V} = -2\lambda_i \mathcal{V} \\
\left[\mathcal{R}, A_i{}^A \partial_A\right] &= -A_i{}^A \partial_A \mathcal{R} \ .
\end{aligned} \tag{C.3}$$

It holds that

$$\nabla^{(A} A_i{}^{B)} \nabla_A \partial_B \Psi = -\lambda_i \Box \Psi + K_i^{AB} \nabla_A \partial_B \Psi \ , \tag{C.4}$$

Recall that the K_i^{AB} are conformally covariant with weight $w(K_i{}^{AB}) = -2$. Recall also that for the closure of the classical constraint algebra we required that

$$K_i^{AB} \bar{P}_A{}^C \bar{P}_B{}^D = 0 \ . \tag{C.5}$$

This implies that we can rewrite (C.4) by using that

$$K_i^{AB}\nabla_A\partial_B\Psi = K_i^{CD}\left(P_C{}^A + 2\bar{P}_C{}^A\right)B_D{}^j A_j{}^B\nabla_A\partial_B\Psi \ . \tag{C.6}$$

A careful inspection of the commutator (C.2) and a comparison with equation (2.209) then yields the three equations according to the strategy for the computation that we lined out in section 2.2.7 :

- 1^{st} equation
$$Z_i^{jA} = -K_i^{CD}B_D{}^j\left(P_C{}^A + 2\bar{P}_C{}^A\right) \ . \tag{C.7}$$
This equation followed from the inspection of the terms in front of the operator $\nabla_A\partial_B$. Note that the above expression yields that $w(Z_i^{jA}) = -2$ as expected.

- 2^{nd} equation
$$\left[Z_i^{jA}\nabla_A + z_i^j\right]A_j{}^B + w(\Psi)\lambda_j Z_i^{jB} = -\frac{1}{2}\left(\Box A_i{}^B + A_i{}^B\mathcal{R}_B{}^A + 2w(\Psi)\mathcal{G}^{BA}\partial_A\lambda_i\right) \ . \tag{C.8}$$
This equation follows from an inspection of the terms in front of the operator ∂_A. We will split the equation into two equations: One by projecting it with $P_B{}^A$ and one by projecting it with $\bar{P}_B{}^A$.

- 3^{rd} equation
$$w(\Psi)\left(Z_i^{jA}\partial_A + z_i^j\right)\lambda_j = -\frac{w(\psi)}{2}\Box\lambda_i - \xi_d\left(A_i{}^A\partial_A - \lambda_i\right)\mathcal{R} \ . \tag{C.9}$$
This equation followed from an inspection of the remaining scalar part.

We consider the 2^{nd} equation (C.8) and contract it with $B_B{}^j$ (this is equivalent to a projection with $P_B{}^A$). The resulting equation can be solved for the scalars z_i^j as anticipated. We obtain

$$z_i^j = -\left[\frac{1}{2}\left(\Box A_i{}^B + A_i{}^A\mathcal{R}_A{}^B + 2w(\Psi)\nabla^B\lambda_i\right) + Z_i^{kA}\nabla_A A_k{}^B + w(\Psi)Z_i^{kB}\lambda_k\right]B_B{}^j \ . \tag{C.10}$$

Let us try to bring this expression into the form (2.208). We first note that

$$\begin{aligned} 2\nabla_A K_i^{AB} &= \Box A_i{}^B + A_i^A\mathcal{R}_A{}^B + \nabla^B\nabla_A A_i{}^A + 2\mathcal{G}^{BA}\partial_A\lambda_i \\ \text{and}\quad \nabla_A A_i{}^A &= K_i - d\lambda_i \quad \text{where}\quad K_i := G_{AB}K_i^{AB} \ . \end{aligned} \tag{C.11}$$

Hence we can replace the following term

$$\Box A_i{}^B + A_i{}^A \mathcal{R}_A{}^B + 2w(\Psi)\nabla^B \lambda_i = 2\nabla_A K_i^{AB} - \nabla^B K_i \ . \tag{C.12}$$

This yields that

$$z_i^j = \left[-\nabla_A K_i^{AB} + \frac{1}{2}\nabla^B K_i - Z_i^{kA} \nabla_A A_k{}^B - w(\Psi) Z_i^{kB} \lambda_k \right] B_B{}^j \ . \tag{C.13}$$

We note that $w(K_i) = 0$. Thus the scalars $(\nabla^B K_i) B_B{}^j$ are conformally covariant with $w(\nabla^B K_i) = -2$ and we will not manipulate this term any further. The divergence of Z_i^{jA} can be written as

$$\nabla_A Z_i^{jA} = -2(\nabla_A K_i^{AD}) B_D{}^j - 2K_i^{AD} \nabla_{(A} B_{D)}{}^j + \nabla_A (A_k{}^A K_i^{kj}) \ , \tag{C.14}$$

where we defined the scalars $K_i^{jk} := K_i^{CD} B_D{}^j B_C{}^k$ for brevity. Solving for $-(\nabla_A K_i^{AD}) B_D{}^j$ yields

$$-(\nabla_A K_i^{AD}) B_D{}^j = \frac{1}{2}\nabla_A Z_i^{jA} + K_i^{AD} \nabla_{(A} B_{D)}{}^j - \frac{1}{2}\nabla_A (A_k{}^A K_i^{kj}) \ . \tag{C.15}$$

Furthermore, we note that

$$Z_i^{kB} \lambda_k B_B{}^j = -K_i^{jk} \lambda_k \ . \tag{C.16}$$

We can now write

$$\begin{aligned} z_i^j =& \frac{1}{2}\nabla_A Z_i^{jA} + \frac{1}{2}(\nabla^A K_i) B_A{}^j - \left[\frac{1}{2}\nabla_A (K_i^{jk} A_k{}^A) - w(\Psi) K_i^{jk} \lambda_k \right] \\ & - Z_i^{kA} (\nabla_A A_k{}^B) B_B{}^j + K_i^{AD} \nabla_{(A} B_{D)}{}^j \ . \end{aligned} \tag{C.17}$$

Now note that the term inside the brackets, that is,

$$\frac{1}{2}\nabla_A (A_k{}^A K_i^{kj}) - w(\Psi) K_i^{jk} \lambda_k \tag{C.18}$$

is conformally covariant with weight -2. The first term in the second row of (C.17) can be written as

$$Z_i^{kA} (\nabla_A A_k{}^B) B_B{}^j = K_i^{AB} \nabla_{(A} B_{B)}{}^j - Z_i^{k[A} A_k{}^{B]} \nabla_{[A} B_{B]}{}^j \ . \tag{C.19}$$

Finally we can write

$$z_i^j = \frac{1}{2}\nabla_A Z_i^{jA} + \frac{1}{2}(\nabla^A K_i) B_A{}^j - \left[\frac{1}{2}\nabla_A (K_i^{jk} A_k{}^A) - w(\Psi) K_i^{jk} \lambda_k \right] + Z_i^{kA} A_k{}^B \nabla_{[A} B_{B]}{}^j \ . \tag{C.20}$$

Also the last term is now manifestly conformally covariant with weight -2. It can also be written as

$$\begin{aligned} Z_i^{k[A} A_k{}^{B]} \nabla_{[A} B_{B]}{}^j =& -2K_i^{AC} B_C{}^k A_k{}^B \nabla_{[A} B_{B]}{}^j \\ =& - K_i^{AC} B_C{}^k B_B{}^j \nabla_A A_k{}^B + K_i^{jk} \left(K_k - d\lambda_k \right) \ . \end{aligned} \tag{C.21}$$

In the following we shall attempt to bring the consistency conditions into a form that is manifestly conformally covariant and invariant under transformations of the shift. Let us now contract the second equation with $\bar{P}_B{}^C$. We obtain

$$\left(Z_i^{jA} \nabla_A A_j{}^B + w(\Psi) \lambda_j Z_i^{jB} \right) \bar{P}_B{}^C = -\frac{1}{2} \left(\Box A_i{}^B + A_i{}^B \mathcal{R}_B{}^A + 2w(\Psi) \nabla^B \lambda_i \right) \bar{P}_B{}^C \tag{C.22}$$

By Using equation (C.12) we get

$$\left(Z_i^{jA} \nabla_A A_j{}^B + w(\Psi) \lambda_j Z_i^{jB} + \nabla_A K_i^{AB} - \frac{1}{2} \nabla^B K_i \right) \bar{P}_B{}^C = 0 \ . \tag{C.23}$$

Now note that

$$\begin{aligned} Z_i^{jA} \left(\nabla_A A_j{}^B \right) \bar{P}_B{}^C &= -K_i^{CD} \left(\delta_C^A + \bar{P}_C{}^A \right) \left(\nabla_A P_D{}^B \right) \bar{P}_B{}^C \\ Z_i^{jB} \bar{P}_B{}^C &= -2K_i^{BD} B_D{}^j \bar{P}_B{}^C \ . \end{aligned} \tag{C.24}$$

Therefore the condition becomes

$$\left(\nabla_A K_i^{AB} - K_i^{CD} \left(\delta_C^A + \bar{P}_C{}^A \right) \left(\nabla_A P_D{}^B \right) - 2w(\Psi) K_i^{BA} \lambda_A - \frac{1}{2} \nabla^B K_i \right) \bar{P}_B{}^C = 0 \ . \tag{C.25}$$

Which can be written as

$$\left(\nabla_A K_i^{AB} - K_i^{CD} \bar{P}_C{}^A \left(\nabla_A P_D{}^B \right) - K_i^{AD} \left(\nabla_A P_D{}^B \right) - 2w(\Psi) K_i^{BA} \lambda_A - \frac{1}{2} \nabla^B K_i \right) \bar{P}_B{}^C = 0 \ . \tag{C.26}$$

Now consider

$$0 = \nabla_B \left(K_i^{CD} \bar{P}_C{}^A \bar{P}_D{}^B \right) = \left[\nabla_D K_i^{CD} - \nabla_B \left(K_i^{CD} P_D{}^B \right) \right] \bar{P}_C{}^A + K_i^{CD} \bar{P}_D{}^B \nabla_B \bar{P}_C{}^A \ . \tag{C.27}$$

We can rewrite the last term by noticing that

$$K_i^{CD} \bar{P}_D{}^B = K_i^{AD} \bar{P}_D{}^B P_A{}^C \quad \text{and} \quad 0 = \nabla_B (P_C{}^D \bar{P}_D{}^A) = \nabla_B (P_C{}^E) \bar{P}_D{}^A + P_C{}^D \nabla_B \bar{P}_D{}^A \ . \tag{C.28}$$

It follows than that

$$\left[\nabla_D K_i^{CD} - \nabla_B \left(K_i^{CD} P_D{}^B\right) - K_i^{ED} \bar{P}_D{}^B \nabla_B P_E{}^C\right] \bar{P}_C{}^A = 0 \ . \tag{C.29}$$

Using this we can rewrite the condition to become

$$\left[\nabla_A \left(K_i^{BD} P_D{}^A\right) - K_i^{AD} \nabla_A P_D{}^B - 2w(\Psi) K_i^{BA} \lambda_A - \frac{1}{2} \nabla^B K_i\right] \bar{P}_B{}^C = 0 \ . \tag{C.30}$$

This can be written as

$$\left[2\nabla_A \left(K_i^{D[A} P_D{}^{B]}\right) + 2w(\Psi) K_i^{BA} \lambda_A + \frac{1}{2} \nabla^B K_i\right] \bar{P}_B{}^C = 0 \ , \tag{C.31}$$

or alternatively as

$$\bar{P}^C{}_B \left[\nabla_A - 2w(\Psi)\lambda_A\right] \left(K_i^{D[A} P_D{}^{B]} + \frac{1}{4} \mathcal{G}^{AB} K_i\right) = 0 \ . \tag{C.32}$$

We can now convince ourselves that this condition is conformally covariant and that the condition is covariant under the transformation $A_i{}^A \mapsto \widetilde{A}_i{}^A = L_i{}^j A_j{}^A$. In other words: The tensor

$$O_i^C := \bar{P}^C{}_B \left[\nabla_A - 2w(\Psi)\lambda_A\right] \left(K_i^{D[A} P_D{}^{B]} + \frac{1}{4} \mathcal{G}^{AB} K_i\right) \tag{C.33}$$

is conformally covariant with weight $w(O_i^C) = -2$. A lengthy calculation shows that it transforms as $O_i^A \mapsto \widetilde{O}_i^A = L_i{}^j O_j^A$ as $A_i{}^A \mapsto \widetilde{A}_i{}^A = L_i{}^j A_j{}^A$. This implies that the tensor $O_B^A := B_B{}^i O_i^A$ is invariant under the transformation $A_i{}^A \mapsto \widetilde{A}_i{}^A = L_i{}^j A_j{}^A$. Moreover, it is traceless $O_A^A = 0$. In principle one should also be able to manipulate the third condition in such a way that becomes manifestly covariant. The hope was that this process also makes the conditions more transparent. This was not justified in the case of the first condition and we decide to stop the computation at this point.

C.2 Weyl squared scalar for diagonal Bianchi II

With the help of some computer algebra we obtain

$$\begin{aligned}C_{\mu\nu\lambda\sigma}C^{\mu\nu\lambda\sigma} =& \frac{4}{3}\Bigg(-\frac{18\dot{N}\left(\dot{\alpha}\left(\dot{\beta}_+^2+\dot{\beta}_-^2\right)-2\dot{\beta}_+^3+\dot{\beta}_+\left(\ddot{\beta}_++6\dot{\beta}_-^2\right)+\dot{\beta}_-\ddot{\beta}_-\right)}{N^5} \\ & -\frac{6\dot{N}e^{-2(\alpha(t)+4\beta_+)}\dot{\beta}_+}{N^3}+\frac{9\dot{N}^2\left(\dot{\beta}_+^2+\dot{\beta}_-^2\right)}{N^6} \\ & +\frac{3e^{-2(\alpha(t)+4\beta_+)}\left(2\dot{\alpha}\dot{\beta}_++2\ddot{\beta}_+-31\dot{\beta}_+^2+\dot{\beta}_-^2\right)}{N^2} \\ & +\frac{1}{N^4}\left(9\left(\dot{\alpha}^2\left(\dot{\beta}_+^2+\dot{\beta}_-^2\right)+2\dot{\alpha}\left(-2\dot{\beta}_+^3+\dot{\beta}_+\left(\ddot{\beta}_++6\dot{\beta}_-^2\right)+\dot{\beta}_-\ddot{\beta}_-\right)\right.\right. \\ & \left.\left.+4\ddot{\beta}_+\dot{\beta}_-^2+\ddot{\beta}_+^2+8\dot{\beta}_+\dot{\beta}_-\ddot{\beta}_-+4\dot{\beta}_+^4+\dot{\beta}_+^2\left(8\dot{\beta}_-^2-4\ddot{\beta}_+\right)+\ddot{\beta}_-^2+4\dot{\beta}_-^4\right)\right) \\ & +e^{-4(\alpha(t)+4\beta_+)}\Bigg)\ .\end{aligned} \tag{C.34}$$

For the vacuum solution discussed in section 3.3 we obtain

$$\begin{aligned}C_{\mu\nu\lambda\sigma}C^{\mu\nu\lambda\sigma} =& \frac{1}{18}\operatorname{sech}^6\left(2\sqrt{3}t\sqrt{p_T^2-p_Y^2}\right) \\ & \times\Bigg(-9e^{-4\sqrt{3}(C_T-p_Tt)}\left(\left(41p_T^2-40p_Y^2\right)\cosh\left(4\sqrt{3}t\sqrt{p_T^2-p_Y^2}\right)+p_T^2\right) \\ & \times\cosh^4\left(2\sqrt{3}t\sqrt{p_T^2-p_Y^2}\right) \\ & +9e^{-8\sqrt{3}(C_T-p_Tt)}\Bigg(-4p_T\sqrt{(p_T-p_Y)(p_T+p_Y)}\sinh\left(4\sqrt{3}t\sqrt{p_T^2-p_Y^2}\right) \\ & \times\Bigg(18\left(-7p_T^4+(p_T-p_Y)(p_T+p_Y)\left(p_T^2+28p_Y^2\right)\cosh\left(4\sqrt{3}t\sqrt{p_T^2-p_Y^2}\right)\right. \\ & \left.+43p_T^2p_Y^2-36p_Y^4\right)-7e^{4\sqrt{3}(C_T-p_Tt)}\cosh^4\left(2\sqrt{3}t\sqrt{p_T^2-p_Y^2}\right)\Bigg) \\ & +9(p_T-p_Y)(p_T+p_Y)\left(95p_T^4-228p_T^2p_Y^2+352p_Y^4\right) \\ & -36\left(7p_T^6-39p_T^4p_Y^2-16p_T^2p_Y^4+48p_Y^6\right)\cosh\left(4\sqrt{3}t\sqrt{p_T^2-p_Y^2}\right) \\ & +9\left(5p_T^6+95p_T^4p_Y^2-132p_T^2p_Y^4+32p_Y^6\right)\cosh\left(8\sqrt{3}t\sqrt{p_T^2-p_Y^2}\right)\Bigg) \\ & +\frac{2\cosh^8\left(2\sqrt{3}t\sqrt{p_T^2-p_Y^2}\right)}{p_T^2-p_Y^2}\Bigg)\ .\end{aligned} \tag{C.35}$$

C.3 Calculation of the Bianchi IX Kretschmann scalar

In this part of the appendix we compute the Kretschmann scalar for the dust filled Bianchi IX universe. The calculations can also be found in [T4]. The Kretschmann scalar can be decomposed according to (2.82). For our purposes it is convenient to make use of the constraints and the equations of motion to simplify the expressions such that they are suited for a numerical evaluation. We will do so throughout the calculation in this section and bring our expression into a form that is ready for a numerical evaluation. This means that all expressions should only involve the variables $\log\Gamma_i$, $(\log\Gamma_i)^{\cdot}$ and v_i as well as the constant parameters $p_T' \equiv 12p_T$ and C. Furthermore, we shall use the quasi-Gaussian gauge $N^i = 0$ while keeping the lapse N unspecified. We now proceed by calculating the terms on the right-hand side of equation (2.82).

From the Einstein field equations $R_{\mu\nu} - \frac{1}{2}Rg_{\mu\nu} = \kappa T_{\mu\nu} = \kappa\rho u_\mu u_\nu$ it follows that we can write

$$R_{\mu\nu}R^{\mu\nu} = \kappa^2 T_{\mu\nu}T^{\mu\nu} = \kappa^2\rho^2 \quad \text{and} \quad R = -\kappa T^{\mu}{}_{\mu} = \kappa\rho \ . \tag{C.36}$$

Recall that in the model under consideration

$$\rho = \frac{p_T \mathrm{e}^{-3\alpha}}{\sqrt{1 + h^{ij}u_i u_j}} = \frac{p_T}{\sqrt{\Gamma_1\Gamma_2\Gamma_3 + C^2\left(\Gamma_2\Gamma_3 v_1^2 + \Gamma_1\Gamma_3 v_2^2 + \Gamma_1\Gamma_2 v_3^2\right)}} \ . \tag{C.37}$$

We conclude that the Ricci part $2R_{\mu\nu}R^{\mu\nu} - \frac{1}{3}R^2$ of the Kretschmann scalar blows up as

$$\left[\Gamma_1\Gamma_2\Gamma_3 + C^2\left(\Gamma_2\Gamma_3 v_1^2 + \Gamma_1\Gamma_3 v_2^2 + \Gamma_1\Gamma_2 v_3^2\right)\right]^{-1} \tag{C.38}$$

when approaching the singularity. The calculation of the Weyl part of the Kretschmann scalar, however, is less trivial. The 3+1 split allows for a decomposition of the Weyl tensor into electric and magnetic part (see e.g. [129]) according to

$$\begin{aligned} &C_{\mu\nu\lambda\sigma}C^{\mu\nu\lambda\sigma} = 8\left(E_{ij}E^{ij} - B_{ij}B^{ij}\right) \quad \text{where} \\ &E_{ij} = K_{ij}K_k{}^k - K_i{}^k K_{jk} + {}^{(3)}R_{ij} - \frac{\kappa}{2}\left[S_{ij} + \frac{1}{3}h_{ij}\left(4\epsilon - S^i{}_i\right)\right] \ , \\ &B_{ij} = \epsilon_{ikl}\left[D^k K_j{}^l - \frac{\kappa}{2}\delta^k_j j^l\right] \ , \end{aligned} \tag{C.39}$$

with ϵ_{ikl} being the Levi-Civita tensor. The other objects involved in the decomposition are explained below. Now let $P^\mu_\nu = \delta^\mu_\nu + n^\mu n_\nu$ denote the projector onto spatial hypersurfaces orthogonal to the normal vector $\{n^\mu\} = (1/N, 0, 0, 0)$, that is $P^\mu_i = \delta^\mu_i$, $P^\mu_0 = 0$. D_i denotes the 3 dimensional covariant derivative on these hypersurfaces. The quantities involved in equation (C.39) are

$$\begin{aligned}\epsilon &= n^\mu n^\nu T_{\mu\nu} = \rho(1+u^i u_i)\ , \\ S_{ij} &= P^\mu_i P^\nu_j T_{\mu\nu} = \rho u_i u_j\ , \\ j^i &= -P^{i\mu} n^\nu T_{\mu\nu} = p_T u^i/\sqrt{h}\ ,\end{aligned} \tag{C.40}$$

where ϵ, S_{ij} and j^i are the energy density, the shear density and the momentum density as measured by Eulerian observers (observers with four velocity n^μ).

A direct calculation yields

$$\begin{aligned}4N^2\Gamma_1\Gamma_2\Gamma_3 B_{ij}B^{ij} = {} & \left(\Gamma_1^2+\Gamma_2^2+\Gamma_3^2\right)\left[\frac{\dot\Gamma_1}{\Gamma_1}+\frac{\dot\Gamma_2}{\Gamma_2}+\frac{\dot\Gamma_3}{\Gamma_3}\right]^2 \\ & + (\Gamma_1+\Gamma_2+\Gamma_3)\left(\dot\Gamma_1+\dot\Gamma_2+\dot\Gamma_3\right)\left(\frac{\dot\Gamma_1}{\Gamma_1}+\frac{\dot\Gamma_2}{\Gamma_2}+\frac{\dot\Gamma_3}{\Gamma_3}\right) \\ & + \frac{1}{4}(\Gamma_1+\Gamma_2+\Gamma_3)^2\left[\frac{\dot\Gamma_1^2}{\Gamma_1^2}+\frac{\dot\Gamma_2^2}{\Gamma_2^2}+\frac{\dot\Gamma_3^2}{\Gamma_3^2}-3\left(\frac{\dot\Gamma_1}{\Gamma_1}+\frac{\dot\Gamma_2}{\Gamma_2}+\frac{\dot\Gamma_3}{\Gamma_3}\right)^2\right] \\ & + \frac{N^2C^2p_T'^2(\Gamma_1+\Gamma_2+\Gamma_3)^2}{24\Gamma_1\Gamma_2\Gamma_3}\left[\frac{v_1^2}{I_1}+\frac{v_2^2}{I_2}+\frac{v_3^2}{I_3}\right]\ .\end{aligned} \tag{C.41}$$

Let us now turn to the computation of $E_{ij}E^{ij}$, which can be written out as

$$\begin{aligned}E_{ij}E^{ij} = {} & K^i{}_j K^j{}_k\left(K^k{}_l K^l{}_i - 2K^k{}_i K^l{}_l\right) + K^i{}_j K^j{}_i (K^l{}_l)^2 \\ & - 2\left(K^i{}_l K^{lj} - K^l{}_l K^{ij}\right)\,{}^{(3)}R_{ij} + {}^{(3)}R_{ij}{}^{(3)}R^{ij} \\ & + 6\rho\left(K^i{}_l K^{lj} - K^l{}_l K^{ij} - {}^{(3)}R^{ij}\right)u_i u_j \\ & + \rho\left(8+6u_k u^k\right)\left[K^i{}_j K^j{}_i - (K^l{}_l)^2 - {}^{(3)}R\right] \\ & + \rho^2\left[54\left(u_k u^k\right)^2 + 96\ u_k u^k + 48\right]\ .\end{aligned} \tag{C.42}$$

We now evaluate the single terms. The term in the first line of (C.42) right after the equal sign can be written as

$$
\begin{aligned}
&8N^4\left[K^i{}_jK^j{}_k\left(K^k{}_lK^l{}_i-2K^k{}_iK^l{}_l\right)+K^i{}_jK^j{}_i(K^l{}_l)^2\right]=\\
&[(\log\Gamma_1)^{\cdot}(\log\Gamma_2)^{\cdot}]^2+[(\log\Gamma_1)^{\cdot}(\log\Gamma_3)^{\cdot}]^2+[(\log\Gamma_2)^{\cdot}(\log\Gamma_3)^{\cdot}]^2\\
&+(\log\Gamma_1)^{\cdot}(\log\Gamma_2)^{\cdot}(\log\Gamma_3)^{\cdot}\left[(\log\Gamma_1)^{\cdot}+(\log\Gamma_2)^{\cdot}+(\log\Gamma_3)^{\cdot}\right]\\
&+N^4C^4{p'_T}^4\left[\frac{v_1^4}{\Gamma_1^2(\Gamma_2-\Gamma_3)^4}+\frac{v_2^4}{\Gamma_2^2(\Gamma_1-\Gamma_3)^4}+\frac{v_3^4}{\Gamma_3^2(\Gamma_1-\Gamma_2)^4}\right.\\
&+\frac{2v_1^2v_2^2}{\Gamma_1\Gamma_2\left(\Gamma_1-\Gamma_3\right)^2\left(\Gamma_2-\Gamma_3\right)^2}\\
&\left.+\frac{2v_2^2v_3^2}{\Gamma_3\Gamma_2\left(\Gamma_2-\Gamma_1\right)^2\left(\Gamma_3-\Gamma_1\right)^2}+\frac{2v_1^2v_3^2}{\Gamma_1\Gamma_3\left(\Gamma_1-\Gamma_2\right)^2\left(\Gamma_3-\Gamma_2\right)^2}\right]\\
&-\frac{N^2C^2{p'_T}^2v_1^2}{\Gamma_1(\Gamma_2-\Gamma_3)^2}\left[(\log\Gamma_1)^{\cdot}\left[(\log\Gamma_2)^{\cdot}+(\log\Gamma_3)^{\cdot}-(\log\Gamma_1)^{\cdot}\right]+2(\log\Gamma_2)^{\cdot}(\log\Gamma_3)^{\cdot}\right]\\
&-\frac{N^2C^2{p'_T}^2v_2^2}{\Gamma_2(\Gamma_1-\Gamma_3)^2}\left[(\log\Gamma_2)^{\cdot}\left[(\log\Gamma_1)^{\cdot}+(\log\Gamma_3)^{\cdot}-(\log\Gamma_2)^{\cdot}\right]+2(\log\Gamma_1)^{\cdot}(\log\Gamma_3)^{\cdot}\right]\\
&-\frac{N^2C^2{p'_T}^2v_3^2}{\Gamma_3(\Gamma_2-\Gamma_1)^2}\left[(\log\Gamma_3)^{\cdot}\left[(\log\Gamma_2)^{\cdot}+(\log\Gamma_1)^{\cdot}-(\log\Gamma_3)^{\cdot}\right]+2(\log\Gamma_2)^{\cdot}(\log\Gamma_1)^{\cdot}\right]\ .
\end{aligned}
\tag{C.43}
$$

We denote the three-dimensional Ricci tensor of the diagonal model by ${}^{(3)}\bar{R}_{ij}$. The three-dimensional Ricci tensor of the non-diagonal model can then obtained via rotation according to ${}^{(3)}R_{ij}=O_i{}^kO_j{}^l\ {}^{(3)}\bar{R}_{kl}$. The only non-vanishing components of ${}^{(3)}\bar{R}_{ij}$ are given by

$$
\begin{aligned}
{}^{(3)}\bar{R}_{11}&=1+\frac{\Gamma_1^2}{2\Gamma_2\Gamma_3}-\frac{\Gamma_2}{2\Gamma_3}-\frac{\Gamma_3}{2\Gamma_2}\\
{}^{(3)}\bar{R}_{22}&=1+\frac{\Gamma_2^2}{2\Gamma_1\Gamma_3}-\frac{\Gamma_1}{2\Gamma_3}-\frac{\Gamma_3}{2\Gamma_1}\\
{}^{(3)}\bar{R}_{33}&=1+\frac{\Gamma_3^2}{2\Gamma_1\Gamma_2}-\frac{\Gamma_1}{2\Gamma_2}-\frac{\Gamma_2}{2\Gamma_1}\ .
\end{aligned}
\tag{C.44}
$$

The first term in the second line of (C.42) reads

$$
\begin{aligned}
&-2\left(K^i{}_lK^{lj}-K^l{}_lK^{ij}\right)\ {}^{(3)}R_{ij}=\frac{\left(\Gamma_2+\Gamma_3-\Gamma_1\right)(\log\Gamma_2)^{\cdot}(\log\Gamma_3)^{\cdot}}{2N^2\Gamma_2\Gamma_3}\\
&\quad+\frac{\left(\Gamma_1+\Gamma_3-\Gamma_2\right)(\log\Gamma_1)^{\cdot}(\log\Gamma_3)^{\cdot}}{2N^2\Gamma_1\Gamma_3}+\frac{\left(\Gamma_1+\Gamma_2-\Gamma_3\right)(\log\Gamma_1)^{\cdot}(\log\Gamma_2)^{\cdot}}{2N^2\Gamma_2\Gamma_1}\\
&\quad+\frac{C^2{p'_T}^2}{2\Gamma_1\Gamma_2\Gamma_3}\left[\frac{\left(\Gamma_1-\Gamma_2-\Gamma_3\right){v_1}^2}{\left(\Gamma_2-\Gamma_3\right)^2}+\frac{\left(\Gamma_2-\Gamma_1-\Gamma_3\right){v_2}^2}{\left(\Gamma_1-\Gamma_3\right)^2}+\frac{\left(\Gamma_3-\Gamma_1-\Gamma_2\right){v_3}^2}{\left(\Gamma_1-\Gamma_2\right)^2}\right]\ .
\end{aligned}
\tag{C.45}
$$

The three-dimensional Ricci squared scalar can be written as

$$ {}^{(3)}R_{ij}{}^{(3)}R^{ij} = \frac{\left(\Gamma_1^2 - 12 I_1 \Gamma_2 \Gamma_3\right)^2 + \left(\Gamma_2^2 - 12 I_2 \Gamma_1 \Gamma_3\right)^2 + \left(\Gamma_3^2 - 12 I_3 \Gamma_1 \Gamma_2\right)^2}{4\left(\Gamma_1 \Gamma_2 \Gamma_3\right)^2} \; . \tag{C.46} $$

The term in the third line of (C.42) becomes

$$ \begin{aligned} & 6\rho\left(K^i{}_l K^{lj} - K^l{}_l K^{ij} - {}^{(3)}R^{ij}\right) u_i u_j = \\ & \frac{3\rho C^3 p_T' v_1 v_2 v_3}{N\sqrt{\Gamma_1\Gamma_2\Gamma_3}} \left[\frac{(\log\Gamma_1)^{\cdot}}{\Gamma_3 - \Gamma_2} + \frac{(\log\Gamma_2)^{\cdot}}{\Gamma_1 - \Gamma_3} + \frac{(\log\Gamma_3)^{\cdot}}{\Gamma_2 - \Gamma_1}\right] \\ & + \frac{3\rho C^4 {p_T'}^2}{2}\left[\frac{(\Gamma_2-\Gamma_3)^2 v_2 v_3}{\Gamma_2\Gamma_3(\Gamma_1-\Gamma_2)^2(\Gamma_1-\Gamma_3)^2}\right. \\ & \left. + \frac{(\Gamma_1-\Gamma_3)^2 v_1 v_3}{\Gamma_1\Gamma_3(\Gamma_2-\Gamma_3)^2(\Gamma_2-\Gamma_1)^2} + \frac{(\Gamma_1-\Gamma_2)^2 v_1 v_2}{\Gamma_1\Gamma_2(\Gamma_3-\Gamma_1)^2(\Gamma_3-\Gamma_2)^2}\right] \\ & + \frac{3\rho C^2}{\Gamma_1\Gamma_2\Gamma_3}\left[\left((\Gamma_2-\Gamma_3)^2 - \Gamma_1^2 - \frac{\Gamma_1\Gamma_2\Gamma_3}{2N^2}(\log\Gamma_1)^{\cdot}\left[(\log\Gamma_2)^{\cdot} + (\log\Gamma_3)^{\cdot}\right]\right)\frac{v_1^2}{\Gamma_1}\right. \\ & + \left((\Gamma_1-\Gamma_3)^2 - \Gamma_2^2 - \frac{\Gamma_1\Gamma_2\Gamma_3}{2N^2}(\log\Gamma_2)^{\cdot}\left[(\log\Gamma_1)^{\cdot} + (\log\Gamma_3)^{\cdot}\right]\right)\frac{v_2^2}{\Gamma_2} \\ & \left. + \left((\Gamma_1-\Gamma_2)^2 - \Gamma_3^2 - \frac{\Gamma_1\Gamma_2\Gamma_3}{2N^2}(\log\Gamma_3)^{\cdot}\left[(\log\Gamma_1)^{\cdot} + (\log\Gamma_2)^{\cdot}\right]\right)\frac{v_3^2}{\Gamma_3}\right] \end{aligned} \tag{C.47} $$

We can use the Hamiltonian constraint equation to simplify

$$ K^i{}_j K^j{}_i - (K^l{}_l)^2 - {}^{(3)}R = -p_T'\sqrt{\frac{1+u_i u^i}{\Gamma_1\Gamma_2\Gamma_3}} \; . \tag{C.48} $$

We therefore obtain a simple expression for the term in the fourth line of (C.42). Since we have direct numerical access to the quantities in the fourth and fifth line of (C.42), we will not manipulate them further.

It is well known that the Weyl squared scalar vanishes for the Friedmann models. The dust filled closed Friedmann universe is included in the model under consideration as the particular case for which $\Gamma_1 = \Gamma_2 = \Gamma_3$ and $C = 0$. As a consistency check of our calculation we convinced ourselves that the Weyl squared scalar vanishes for these restrictions. We found that $B_{ij}B^{ij}$ and $E_{ij}E^{ij}$ vanish separately and hence $C_{\mu\nu\lambda\sigma}C^{\mu\nu\lambda\sigma} = 0$ as expected.

Bibliography

[1] S. M. Carroll, *Spacetime and Geometry: An Introduction to General Relativity*, (Cambridge University Press , Cambridge, 2019).

[2] P. J. E. Peebles, *Principles of Physical Cosmology*, (Princeton University Press, Princeton, 1993).

[3] S. Hawking and R. Penrose, *The Nature of Space and Time,* (Princeton University Press, Princeton, 1996).

[4] S. W. Hawking and G. F. R. Ellis, *The Large Scale Structure of Space-Time,* (Cambridge University Press, Cambridge, 1973).

[5] B. S. DeWitt, *Quantum Theory of Gravity. I. The Canonical Theory,* Phys. Rev. 160, 1113 (1967).

[6] B. S. DeWitt, *Quantum Theory of Gravity. II. The Manifestly Covariant Theory,* Phys. Rev. 162, 1195 (1967).

[7] B. S. DeWitt, *Quantum Theory of Gravity. III. Applications of the Covariant Theory,* Phys. Rev. 162, 1239 (1967).

[8] J. Wheeler, in: *Relativity, Groups and Topology,* edited by C. DeWitt and B. DeWitt (Gordon and Breach, New York, 1964).

[9] P. W. Higgs, *Integration of Secondary Constraints in Quantized General Relativity,* Phys. Rev. Lett. 3, 66 (1959).

[10] C. Kiefer, *Quantum Gravity.* Third edition (Oxford University Press, Oxford, 2012).

[11] J. C. Feng, *Volume average regularization for the Wheeler-DeWitt equation,* Phys. Rev. D 98, 026024 (2018). arXiv:1802.08576 [gr-qc].

[12] T. Thiemann, *Modern Canonical Quantum General Relativity.* Third edition (Cambridge University Press, 2017).

[13] M. Bojowald, *Critical evaluation of common claims in loop quantum cosmology*, invited contribution to Special Issue "Quantum Models for Cosmology". arXiv:2002.05703[gr-qc].

[14] E. Kasner, *Geometrical Theorems on Einstein's Cosmological Equations.* Am. J. Math. 43, 217 (1921).

[15] J. Ehlers, P. Geren and R. K. Sachs, *Isotropic Solutions of the Einstein–Liouville Equations.* J. Math. Phys. 9, 1344 (1968).

[16] R. M. Wald, *Asymptotic behavior of homogeneous cosmological models in the presence of a positive cosmological constant,* Phys. Rev. D 28, 2118 (1983).

[17] C. Misner, in: *Magic without Magic: John Archibald Wheeler,* edited by J. Klauder (Freeman, San Francisco, 1972).

[18] G. F. R. Ellis and H. Van Elst, *Cosmological models (Cargèse lectures 1998).* NATO Adv.Study Inst. Ser. C. Math. Phys. Sci. 541:1-116, (1999). arXiv:gr-qc/9812046.

[19] K. V. Kuchař and M. P. Ryan, *Is minisuperpspace quantization valid?: Taub in mixmaster,* Phys. Rev. D 40, 3982 (1989).

[20] C. Kiefer, *Continuous measurement of minisuperspace variables by higher multipoles,* Class. Quant. Grav. 4, 1369 (1987).

[21] J. J. Halliwell, *Decoherence in Quantum Cosmology,* Phys. Rev. D 39, 2912 (1989).

[22] D. Brizuela, C. Kiefer and M. Krämer, *Quantum-gravitational effects on gauge-invariant scalar and tensor perturbations during inflation: The de Sitter case.* Phys. Rev. D 93, 104035 (2016). arXiv:1511.05545 .

[23] D. Brizuela, C. Kiefer and M. Krämer, *Quantum-gravitational effects on gauge-invariant scalar and tensor perturbations during inflation: The slow-roll approximation.* Phys. Rev. D 94, 123527 (2016). arXiv:1611.02932 [gr-qc].

[24] M. P. Dąbrowski, C. Kiefer and B. Sandhoefer, *Quantum phantom cosmology,* Phys. Rev. D 74, 044022 (2006). arXiv:hep-th/0605229

[25] M. Bouhmadi-López, C. Kiefer and P. Martín-Moruno, *Phantom singularities and their quantum fate: general relativity and beyond,* Gen. Relativ. Gravit. 51, 135 (2019), arXiv:1904.01836 [gr-qc].

[26] M. Bouhmadi-Lopez, C. Kiefer, B. Sandhoefer and P. V. Moniz, *On the quantum fate of singularities in a dark-energy dominated universe,* Phys. Rev. D 79, 124035 (2009). arXiv:0905.2421 [gr-qc].

[27] A. Yu. Kamenshchik, C. Kiefer and B. Sandhoefer, *Quantum cosmology with big-brake singularity,* Phys. Rev. D 76, 064032 (2019). arXiv:0705.1688 [gr-qc].

[28] V.A. Belinskii, I.M. Khalatnikov and E.M. Lifshitz, *A general solution of the Einstein equations with a time singularity,*. Adv. Phys. 31, 639 (1982).

[29] A. Krasiński et al., *The Bianchi Classification in the Schücking-Behr Approach.* Gen. Rel. Gravit. 35 3, 475 (2002).

[30] R. T. Jantzen, *The dynamical degrees of freedom in spatially homogeneous cosmology*, Comm. Math. Phys. 64, 211 (1979).

[31] R. T. Jantzen, *Spatially homogeneous dynamics: a unified picture*, arXiv:gr-qc/0102035. Originally published in the Proceedings of the International School Enrico Fermi, Course LXXXVI (1982) on *Gamov Cosmology*, edited by R. Ruffini and F. Melchiorri (North Holland, Amsterdam, 1987), pp. 61–147.

[32] A. Ashtekar and J. Samuel, *Bianchi cosmologies: The role of spatial topology*, Class. Quant. Grav. 8, 2191 (1991).

[33] O. Coussaert and M. Henneaux, *Bianchi cosmological models and gauge symmetries,* Class. Quant. Grav. 10, 1607 (1993). arXiv:gr-qc/9301001

[34] R. T. Jantzen and C. Uggla, *The kinematical role of automorphisms in the orthonormal frame approach to Bianchi Cosmology*, J. Math. Phys. 40, 353 (1999).

[35] T. Christodoulakis, G. Kofinas and G. O. Papadopoulus, *Automorphism Inducing Diffeomorphisms, Invariant Characterization of Homogeneous 3-Spaces and Hamiltonian Dynamics of Bianchi Cosmologies*, Commun. Math. Phys. 226, 377 (2002). arXiv:gr-qc/0107050

[36] M.A.H. MacCallum, *Cosmological models from a geometric point of view.* Cargèse Lectures in Physics 6, ed. E. Schatzman, pages 61-174. Gordon and Breach, New York (1973). arXiv:2001.11387 [gr-qc].

[37] T. Christodoulakis, G. Kofinas, E. Korfiatis, G. O. Papadopoulos and A. Paschos, *Time-Dependent Automorphism Inducing Diffeomorphisms In Vacuum Bianchi Cosmologies*

And The Complete Closed Form Solutions For Type II and V, J. Math. Phys. 42, 3580 (2001). arXiv:gr-qc/0008050

[38] T. Christodoulakis, *Lectures on Quantum Cosmology.* Lect. Notes Phys. 592, 318 (2002) arXiv:gr-qc/0109059

[39] L. Bianchi, *Sugli spazii a tre dimensioni che ammettono un gruppo continuo di movimenti. (On the spaces of three dimensions that admit a continuous group of movements.)* Soc. Ital. Sci. Mem. di Mat. 11, 267 (1898).

[40] J. Plebański and A. Krasiński, *An Introduction to General Relativity and Cosmology.* (Cambridge University Press, Cambridge , 2010.)

[41] G. F. R. Ellis and M. A. H. MacCallum, *A class of homogeneous cosmological models.* Comm. Math. Phys. 12 2, 108 (1969).

[42] C. W. Misner, *Mixmaster Universe*, Phys. Rev. Letters 22, 1071 (1969).

[43] C. W. Misner, *Quantum Cosmology*, Phys. Rev. 186, 1071 (1969).

[44] M. P. Ryan, *Hamiltonian Cosmology*, Lecture Notes in Physics, Vol. 13. (Springer–Verlag, Berlin, 1979.)

[45] M. P. Ryan and L. C. Shepley, *Homogeneous Relativistic Cosmologies*, (Princeton University Press, Princeton, 1973.)

[46] M.P. Ryan, *Qualitative Cosmology: Diagrammatic Solutions for Bianchi Type IX Universes with Expansion, Rotation, and Shear. I. The Symmetric Case.* Ann. Physics 65, 506 (1971).

[47] M.P. Ryan, *Qualitative Cosmology: Diagrammatic Solutions for Bianchi Type IX Universes with Expansion, Rotation, and Shear. II. The General Case.* Ann. Physics 68, 541 (1971).

[48] J.M. Heinzle, C. Uggla and N. Rohr, *The cosmological billiard attractor*, Adv. Theor. Math. Phys. 13, 075016 (2009). arXiv:gr-qc/0702141

[49] C. Uggla, *Spacetime singularities: recent developments.* Int. J. Mod. Phys. D 22, 1330002 (2013). arXiv:1306.6527 [gr-qc]

[50] J. Wainwright and G.F.R Ellis (Eds.), *Dynamical Systems in Cosmology.* (Cambridge University Press, Cambridge, 1997).

[51] T. Christodoulakis, G. Kofinas and E. C. Vagenas, *Simultaneous Hamiltonian Treatment of Class A Spacetimes and Reduction of Degrees of Freedom at the Quantum Level*. Grav. Cosmol. 8, 213 (2002). arXiv:gr-qc/9407042

[52] J. M. M. Senovilla, *Singularity Theorems and Their Consequences*. Gen. Rel. Grav. 30, 701 (1998). arXiv:1801.04912 [gr-qc]

[53] C. B. Collins and G. F. R. Ellis, *Singularities in Bianchi Cosmologies*. Phys. Rep. 56, 65 (1979).

[54] J. R. Oppenheimer and H. Snyder, *On Continued Gravitational Contraction*. Phys. Rev. 56, 455 (1939).

[55] J. D. Barrow and S. Hervik , *The Weyl tensor in spatially homogeneous cosmological models*. Class. Quant. Grav. 19, 155 (2002). arXiv:gr-qc/0206061

[56] M. P. Dąbrowski, *Are singularities the limits of cosmology?* arXiv:1407.4851 [gr-qc].

[57] F. J. Tipler, *Singularities in conformally flat spacetimes*, Phys. Lett. A 64, 8 (1977).

[58] A. Królak, *Towards the proof of the cosmic censorship hypothesis*, Class. Quant. Grav. 3, 267 (1986).

[59] X-f. Lin and R.M. Wald, *Proof of the closed-universe-recollapse conjecture for general Bianchi type-IX cosmologies*. Phys. Rev. D 41, 2444 (1990).

[60] J. D. Barrow, G. J. Galloway and F. J. Tipler, *The closed-universe recollapse conjecture*. Mon. Notices Royal Astron. Soc. 223 4, 835 (1986).

[61] L. Fernández-Jambrina, *Grand Rip and Grand Bang/Crunch cosmological singularities*. Phys. Rev. D 90, 064014 (2014). arXiv:1408.6997 [gr-qc]

[62] *Springer Handbook of Spacetime*, edited by A. Ashtekar and V. Petkov (Springer-Verlag, 2014).

[63] P. S. Joshi, in: [62], pp. 409–436. arXiv:1311.0449v1 [gr-qc].

[64] B. K. Berger, in: [62], pp. 437–460.

[65] V. Belinski, *On the Cosmological Singularity*. Int. J. Mod. Phys. D 20, 1907 (2014). arXiv:1404.3864 [gr-qc]

[66] V. A. Belinski, I. M. Khalatnikov and E. M. Lifshitz, *Oscillatory Approach to a Singular Point in the Relativistic Cosmology.* Adv. Phys. 19, 525 (1970).

[67] D. Garfinkle, *Numerical Simulations of Generic Singularities.* Phys. Rev. Letters 93, 16. (2004). arXiv:gr-qc/0312117

[68] A. J. S. Hamilton, *Inflation followed by BKL collapse inside accreting, rotating black holes*, Phys. Rev. D 96, 084041 (2017). arXiv:1703.01921 [gr-qc]

[69] R. H. Gowdy, *Vacuum spacetimes with two-parameter isometry groups and compact invariant hypersurfaces: Topologies and boundary conditions*, Ann. Phys. (N.Y.) 83, 203 (1974).

[70] V. Moncrief and J. Isenberg, *Asymptotic behavior of the gravitational field and the nature of singularities in Gowdy spacetimes.* Ann. Phys. (N.Y.) 199, 84 (1990).

[71] B. F. Schutz, *Perfect Fluids in General Relativity: Velocity Potentials and a Variational Principle.* Phys. Rev. D 2, 2762 (1970).

[72] B. F. Schutz, *Hamiltonian Theory of a Relativistic Perfect Fluid.* Phys. Rev. D 4, 3559 (1971).

[73] J. D. Brown and K. V. Kuchar, *Dust as a Standard of Space and Time in Canonical Quantum Gravity.* Phys. Rev. D 51, 5600 (1995). arXiv:gr-qc/9409001.

[74] K. Sundermeyer, *Constrained Dynamics.* (Springer Verlag, Berlin, 1982.)

[75] J. M. Lee, *Introduction to Smooth Manifolds.* (Springer, 2012.)

[76] M. Asaoka, Aziz El Kacimi Alaoui, S. Hurder and K. Richardson, *Foliations: Dynamics, Geometry and Topology.* (Birkhäuser, 2014).

[77] E. Schrödinger, *Quantisierung als Eigenwertproblem.* Ann. Phys. (Berlin) 79, 8 (1926) and 81, 8 (1926).

[78] J. J. Halliwell, *Introductory Lectures on Quantum Cosmology (1990).* First published in Proceedings of the 1990 Jerusalem Winter School on Quantum Cosmology and Baby Universes, edited by S. Coleman, J. B. Hartle, T. Piran and S. Weinberg (World Scientific, Singapore, 1991). arXiv:0909.2566 [gr-qc]

[79] S. W. Hawking and D. N. Page, *Operator Ordering and the Flatness of the Universe.* Nucl. Phys. B 264, 185 (1986).

[80] G. Calcagni, *Classical and Quantum Cosmology.* (Springer-Verlag, 2017).

[81] D. L. Wiltshire, *An introduction to quantum cosmology.* Published in "Cosmology: the Physics of the Universe", eds B. Robson, N. Visvanathan and W.S. Woolcock (World Scientific, Singapore, 1996) pp 473-531 arXiv:gr-qc/0101003

[82] K. Kuchař, *Time and interpretations of quantum gravity,* in 'Proceedings of the 4th Canadian Conference on General Relativity and Relativistic Astrophysics' (ed. G. Kunstatter, D. Vincent, and J. Williams), pp. 211-314. World Scientific, Singapore (1992).

[83] S. J. Robles-Pérez, *Quantum Cosmology of a conformal multiverse,* Phys. Rev. D 96, 063511 (2017). arXiv:1706.06023 [gr-qc]

[84] A. Vilenkin, *Interpretation of the Wave Function of the Universe.* Phys. Rev. D 39, 1116 (1989).

[85] T. Demaerel and W. Struyve, *Elimination of cosmological singularities in quantum cosmology by suitable operator orderings.* Phys. Rev. D 100, 046008 (2019) arXiv:1904.13220 [gr-qc].

[86] A. Ashtekar and P. Singh, *Loop Quantum Cosmology: A Status Report.* Class. Quant. Grav. 28, 065005.28: 213001, (2011) arXiv:1108.0893 [gr-qc].

[87] E. Wilson-Ewing, *The loop quantum cosmology bounce as a Kasner transition.* Class. Quant. Grav. 35, (2018) 065005. arXiv:1711.10943 [gr-qc].

[88] A. Ashtekar, T. Pawlowski and P. Singh, *Quantum Nature of the Big Bang.* Phys. Rev. Lett. 96, 141301 (2006). arXiv:gr-qc/0602086.

[89] A. Ashtekar, T. Pawlowski and P. Singh, *Quantum Nature of the Big Bang: An Analytical and Numerical Investigation.* Phys. Rev. D 73, 124038 (2006). arXiv:gr-qc/0604013.

[90] M. Bojowald and J. Mielczarek, *Some implications of signature-change in cosmological models of loop quantum gravity* . JCAP 08, (2015) 052. arXiv:1503.09154 [gr-qc].

[91] N. Pinto-Neto, *The Bohm Interpretation of Quantum Cosmology.* Found.Phys.35:577-603,(2005) arXiv:gr-qc/0410117.

[92] P.H. Hájíček and C. Kiefer, *Singularity avoidance by collapsing shells in quantum gravity* Int. J. Mod. Phys. D10, 775(2001) arXiv:gr-qc/0107102

[93] T. Schmitz and C. Kiefer, *Singularity avoidance for collapsing quantum dust in the Lemaître-Tolman-Bondi model.* Phys. Rev. D 99, 126010 (2019). arXiv:1904.13220 [gr-qc].

[94] T. Schmitz, *Towards a quantum Oppenheimer-Snyder model.* Phys. Rev. D 101, 026016 (2020). arXiv:1912.08175[gr-qc].

[95] D. Malafarina, *Classical collapse to black holes and quantum bounces: A review.* Universe 2017, 3(2), 48. arXiv:1703.04138 [gr-qc]

[96] H. Bergeron, E. Czuchry, J. Gazeau, P. Małkiewicz and W. Piechocki, *Singularity avoidance in a quantum model of the Mixmaster universe.* Phys. Rev. D 92, 124018 (2015) arXiv:1501.07871 [gr-qc]

[97] A. Góźdź, W. Piechocki and G. Plewa, *Quantum Belinski-Khalatnikov-Lifshitz scenario*, Eur. Phys. J. C 79 (2019) 45. arXiv:1807.07434 [gr-qc]

[98] P. Małkiewicz, *Multiple choices of time in quantum cosmology.* Class. Quant. Grav. 32 (2015) 135004 arXiv:1407.3457 [gr-qc]

[99] L. Chataignier, *On the Construction of Quantum Dirac Observables and the Emergence of WKB Time.* arXiv:1910.02998 [gr-qc].

[100] A. Alonso-Serrano, M. Bojowald and D. Brizuela, *Quantum approach to a Bianchi I singularity.* arXiv:2001.11488 [gr-qc].

[101] J. B. Hartle and S. W. Hawking, *Wave function of the Universe.* Phys. Rev. D 28, 12 (1983).

[102] A. Vilenkin, *Quantum cosmology and the initial state of the Universe.* Phys. Rev. D 37, 888 (1988).

[103] J. Louko and T. Vachaspati, *On the Vilenkin boundary condition proposal in anisotropic universes.* Phys. Lett. B 223, 1 (1989).

[104] C. Kiefer, *Wave packets in minisuperspace.* Phys. Rev. D 38, 1761 (1988).

[105] J.M. Lee, *Riemannian manifolds: An Introduction to curvature.* (Springer, 1997).

[106] T. Frankel, *The Geometry of Physics.* Third edition (Cambridge University Press, Cambridge, 2012.)

[107] S. Klainerman, *Global existence for nonlinear wave equations.* Comm. Pure Appl. Math. 33 (1980).

[108] G. Heckmann and E. Schücking, in *Gravitation: An Introduction to Current Research*, edited by L. Witten (Wiley, 1962)

[109] M. P. Ryan, S. M. Waller and L. C. Shepley, *Bianchi Type Electromagnetic Cosmology – Type I Hamiltonian*, Astrophys. J. 254, 425 (1982).

[110] L. P. Hughston and K. C. Jacobs, *Homogeneous electromagnetic and massive-vector-meson fields in Bianchi cosmologies.* Astrophys. J. 160, (1970).

[111] M. Abramowitz and I. Stegun , *Handbook of Mathematical Functions.* (Dover Publications, New York, 1965.)

[112] R. Kantowski and R. K. Sachs, *Some Spatially Homogeneous Anisotropic Relativistic Cosmological Models.* J. Math. Phys. 7, 443 (1966).

[113] H.D. Conradi, *Quantum Cosmology of Kantowski-Sachs like models.* Class. Quant. Grav. 12, 2423 (1995). arXiv:gr-qc/9412049

[114] J. Langer and F. Hanák *Wave packets for the quantum Kantowski-Sachs universe.* Czech. J. Phys. 50, 697 (2000).

[115] B.C. Xanthopoulos and T. Zannias, *Kantowski-Sachs metrics with source: A massless scalar field.* J. Math. Phys. 33, 1415 (1992).

[116] B.C. Xanthopoulos and T. Zannias, *Kantowski-Sachs metrics with source: A conformally invariant scalar field.* J. Math. Phys. 33, 1420 (1992).

[117] A. I. Janis, E. T. Newman and J. Winicour, *Reality of the Schwarzschild Singularity.* Phys. Rev. Letter 20, 878 (1968).

[118] M. Wyman, *Static spherically symmetric scalar fields in general relativity.* Phys. Rev. D 24, 839 (1981).

[119] J.M. Heinzle and C. Uggla, *Mixmaster: Fact and Belief.* Class. Quant. Grav. 26, 293 (2011). arXiv:0901.0776 [gr-qc]

[120] V. Belinski and M. Henneaux, *The Cosmological Singularity.* (Cambridge University Press, Cambridge, 2017.)

[121] N.J. Cornish and J.J. Levin, *The mixmaster universe: A chaotic Farey tale*. Phys. Rev. D 55, 7489 (1997). arXiv:gr-qc/9612066

[122] H. Ringström, *Curvature blow up in Bianchi VIII and IX vacuum spacetimes.* Class. Quant. Grav. 17, 713 (2000). arXiv:gr-qc/9911115

[123] T. Damour and P. Spindel, *Quantum Einstein-Dirac Bianchi Universes.* Phys. Rev. D, 83, 123520 (2011). arXiv:1103.2927 [gr-qc]

[124] A. Kheyfets, W.A. Miller and R. Vaulin, *Quantum geometrodynamics of the Bianchi IX cosmological model.* Class. Quant. Grav. 23, 4333 (2006). arXiv:gr-qc/0512040

[125] J.D. Brown and K.V. Kuchař, *Dust as a Standard of Space and Time in Canonical Quantum Gravity.* Int. J. Mod. Phys. D 51, 5600 (1995). arXiv:gr-qc/9409001

[126] L.F. Shampine and M.W. Reichelt, *The MATLAB ODE Suite.* SIAM Journal on Scientific Computing 18 (1997).

[127] B.K. Berger, *Numerical study of initially expanding mixmaster universes*, Class. Quant. Grav. 7 (1990).

[128] D. Hobill *et al.*, *The Mixmaster cosmology as a dynamical system*, Class. Quant. Grav. 8 (1991).

[129] M. Alcubierre, *Introduction to 3+1 Numerical Relativity* . (Oxford University Press, Oxford, 2008.)

[130] M. Koehn, *Relativistic Wavepackets in Classically Chaotic Quantum Cosmological Billiards.* Physical Review, D85, 063501 (2012). arXiv:1107.6023 [gr-qc]

[131] V.A. Belinskii, I.M. Khalatnikov, and M.P. Ryan, *The oscillatory regime near the singularity in Bianchi-type IX universes*, Preprint **469** (1971), Landau Institute for Theoretical Physics, Moscow (unpublished); published as sections 1 and 2 in [132].

[132] M.P. Ryan, *The Oscillatory Regime Near the Singularity in Bianchi-Type IX Universes.* Ann. Physics 70, 301. (1972).

[133] L. P. Chernoff and V. N. Barrow, *The model of mixmaster universe with arbitrarily moving matter*, J. Exp. Theor. Phys. **34**, 1 (1972).

[134] S. Capozziello and V. Faraoni, *Beyond Einstein Gravity*, (Springer, 2011).

[135] M. Blagojević and F. W. Hehl, *Gauge Theories of Gravitation*, (Imperial College Press, London, 2013).

[136] H. Ringström, *The Cauchy Problem in General Relativity* , (European Mathematical Society, 2009).

[137] M. P. Dabrowski, J. Garecki and D. B. Blaschke, *Conformal transformations and conformal invariance in gravitation.* Annalen Phys. (Berlin) 18 (2009), 13. arXiv:0806.2683 [gr-qc]

[138] J. M. Lee and T. H. Parker, *The Yamabe Problem.* Bull. Am. Math. Soc. 17, 37 (1987).

[139] E. Scholz, *Weyl geometry in late 20th century physics.* arXiv:1111.3220v1[math.HO]

[140] J. T. Wheeler, *Weyl geometry.* (2017) Gen. Relativ. Gravit. (2018) 50:80. arXiv:1801.03178 [gr-qc]

Acknowledgments

First of all, I would like to thank my supervisor Prof. Dr. Claus Kiefer for providing to me the opportunity to work on this interesting topic. I am grateful for generous financial support and for giving me the freedom to pursue my research interests.

I would also like to thank Prof. Dr. Alexander Altland for acting as a second reviewer of this thesis. Furthermore, I am grateful to Prof. Dr. Andreas Eckart for being the head of the committee and to Dr. Rochus Klesse for agreeing to keep the minutes during the final examination.

I thank Prof. Dr. Włodzimierz Piechocki for initiating our collaboration and for organizing my visits to the nuclear physics institute in Warsaw. I am thankful to the German Academic Exchange Service DAAD and to the Ministry of Science and Higher Education in Poland MNiSW for financially supporting this endeavor.

It was pleasure to work together with Dennis Piontek on the quantum cosmology of the Bianchi I model. Furthermore, I would also like to thank Tatevik Vardanyan for joining forces with me when working on the diagonalization of the Bianchi II metric.

I express my gratitude to the PhD students of the Cologne gravity group Branislav Nicolic, Tim Schmitz, Leonardo Chataignier and YiFan Wang. I am not only greatly indebted for all the stimulating and inspiring discussions but also for the cheerful times during the lunch breaks and outside of the office hours. The same holds of course for all the Master Students that joined the group during my time as a PhD student: Anirudh Gundhi, David Wichmann, Patrick Wong, Dennis Piontek, Mario Montero, Dimitrios Gkiatas, Tatevik Vardanyan, Anton Krieger, Alexander Hermanns, Sebastian Arenas, Christina Koliofoti, Ali Lezeik and Sandeep Suresh. I am thankful to Lorenz Mayer and Nick Nußbaum for intense discussions and pointing out some relevant literature. I would also like to thank Dr. Anne Franzen for answering questions related to the decay rate estimates and Prof. Dr. Friedrich W. Hehl for his critical attitude and for pointing out helpful references. I also thank my long-time office mates Ori Alberton and Federico Tonelli for creating and maintaining an excellent working environment.

In particular I would like to thank Prof. Dr. Claus Kiefer, Branislav Nikolic, Tim Schmitz, Leonardo Chataignier, Tatevik Vardanyan, Alexander Hermanns, Christina Koliofoti, Ali Lezeik and Sandeep Suresh for helping me with the proof reading of this thesis.

Last but not least I thank Julia Loskill for all the love and support during the final days before submitting this thesis.

Erklärung

Hiermit versichere ich an Eides statt, dass ich die vorliegende Dissertation selbstständig und ohne die Benutzung anderer als der angegebenen Hilfsmittel und Literatur angefertigt habe. Alle Stellen, die wörtlich oder sinngemäß aus veröffentlichten und nicht veröffentlichten Werken dem Wortlaut oder dem Sinn nach entnommen wurden, sind als solche kenntlich gemacht. Ich versichere an Eides statt, dass diese Dissertation noch keiner anderen Fakultät oder Universität zur Prüfung vorgelegen hat; dass sie - abgesehen von unten angegebenen Teilpublikationen und eingebundenen Artikeln und Manuskripten - noch nicht veröffentlicht worden ist sowie, dass ich eine Veröffentlichung der Dissertation vor Abschluss der Promotion nicht ohne Genehmigung des Promotionsausschusses vornehmen werde. Die Bestimmungen dieser Ordnung sind mir bekannt. Darüber hinaus erkläre ich hiermit, dass ich die Ordnung zur Sicherung guter wissenschaftlicher Praxis und zum Umgang mit wissenschaftlichem Fehlverhalten der Universität zu Köln gelesen und sie bei der Durchführung der Dissertation zugrundeliegenden Arbeiten und der schriftlich verfassten Dissertation beachtet habe und verpflichte mich hiermit, die dort genannten Vorgaben bei allen wissenschaftlichen Tätigkeiten zu beachten und umzusetzen. Ich versichere, dass die eingereichte elektronische Fassung der eingereichten Druckfassung vollständig entspricht.

Köln, den ________________ ______________________________

Nick Kwidzinski

Teilpublikationen

[T1] Nick Kwidzinski, Daniele Malafarina, Jan Ostrowski,
Włodzimierz Piechocki and Tim Schmitz,
Hamiltonian formulation of dust cloud collapse,
accepted for publication in Phys. Rev. D.
arXiv:2001.01903 [gr-qc]

[T2] Claus Kiefer and Nick Kwidzinski,
Singularity avoidance in anisotropic quantum cosmology,
J. Phys.: Conf. Ser. 1275 (2019) 012011.

[T3] Claus Kiefer, Nick Kwidzinski und Dennis Piontek,
Singularity avoidance in Bianchi I quantum cosmology,
Eur. Phys. J. C (2019) 79:686.
arXiv:1903.04391 [gr-qc]

[T4] Nick Kwidzinski und Włodzimierz Piechocki,
Curvature invariants for the Bianchi IX spacetime filled with tilted dust,
Eur. Phys. J. C (2019) 79:199.
arXiv:1901.01790 [gr-qc]

[T5] Ewa Czuchry, Nick Kwidzinski und Włodzimierz Piechocki,
Comparing the dynamics of diagonal and general Bianchi IX spacetime,
Eur. Phys. J. C (2019) 79:173 .
arXiv:1409.2206 [gr-qc]

[T6] Claus Kiefer, Nick Kwidzinski und Włodzimierz Piechocki,
On the dynamics of the general Bianchi IX spacetime near the singularity,
Eur. Phys. J. C (2018) 78:691.
arXiv:1807.06261 [gr-qc]

Lebenslauf

Kontakt	Nick Kwidzinski Instititut für Theoretische Physik Universität zu Köln Zülpicher Str. 77 50937 Köln
Persönliches	geboren 27.01.1988 in Unna Staatsangehörigkeit: deutsch
Ausbildung	
Promotion in Theoretischer Physik	Universität zu Köln, (seit Oktober 2016 bis voraussichtlich Juni 2020) Titel: Quantum Fate of Singularities in Anisotropic Cosmological Models Betreuer: Prof. Dr. Claus Kiefer
M.Sc. in Physik	Universität zu Köln, (2016) Titel: Classical and quantum cosmology of Born-Infeld type models Betreuer: Prof. Dr. Claus Kiefer
B.Sc. in Physik	Universität zu Köln, (2014) Titel: Bewegungsgleichungen in Systemen gekoppelter harmonischer Oszillatoren Betreuer: Prof. Dr. Ralf Bulla
Abitur	Ernst-Barlach-Gymnasium in Unna (2007)