Abstract

A canonical transformation is performed on the phase space of a number of homogeneous cosmologies to simplify the form of the scalar (or, Hamiltonian) constraint. Using the new canonical coordinates, it is then easy to obtain explicit expressions of Dirac observables, i.e. phase space functions which commute weakly with the constraint. This, in turn, enables us to carry out a general quantization program to completion. We are also able to address the issue of time through “deparametrization” and discuss physical questions such as the fate of initial singularities in the quantum theory. We find that they persist in the quantum theory inspite of the fact that the evolution is implemented by a 1-parameter family of unitary transformations. Finally, certain of these models admit conditional symmetries which are explicit already prior to the canonical transformation. These can be used to pass to quantum theory following an independent avenue. The two quantum theories –based, respectively, on Dirac observables in the new canonical variables and conditional symmetries in the original ADM variables– are compared and shown to be equivalent.

1 Introduction

Quantum general relativity has a number of peculiar features which are not encountered in quantum theories of non-gravitational interactions: presence of “dynamical” constraints; diffeomorphism invariance and the consequent absence of a background geometry; nonlinearities which make the structure of the effective configuration space topologically complicated; the absence of suitable symmetries to single out the vacuum and select the Hermitian scalar product; and, the difficulty of interpreting the resulting mathematical framework in simple physical terms. Over the past six years, a nonperturbative approach has been developed to address these issues systematically (see, e.g. [1, 2, 3]). In particular, there now exists [4, 5] a general quantization program which is adapted to the peculiarities of general relativity. Unfortunately, however, for the full, untruncated theory, several steps of the program are yet to be completed.

It is therefore desirable to apply the program to simpler, truncated models (see e.g. [4, 5]) both to test its viability and to gain insight into the type of techniques that will be needed in the full theory. One such model is provided by 3-dimensional general relativity.
This model has taught us several interesting lessons, both conceptual and technical (see chapter 17 in [1]). The purpose of this paper is to continue investigations in the same spirit by examining a class of “solvable” spatially homogeneous cosmologies. These are homogeneous cosmologies which admit additional symmetries. In the classical theory, the presence of these symmetries enables one to integrate the field equations completely. We will see that their presence also simplifies the task of quantization: We will be able to carry out the general program of [1, 4] to completion. Furthermore, these models will enable us to explore certain aspects of the program which could not be analysed in 3-dimensional general relativity.

The key simplification that allows one to complete the quantization program is the following: in these models one can perform a canonical transformation on the classical phase space to drastically simplify the expression of the scalar (also known as the Hamiltonian) constraint of geometrodynamics. In the new canonical variables, the potential term in the scalar constraint *disappears entirely!* Furthermore, the supermetric in the kinetic term is *flat*. The only remnant of the potential term of the usual ADM variables is in the ranges of permissible values of the new canonical coordinates, i.e., in the global topology of the constraint surface. Now, in full general relativity, one can again significantly simplify the form of the constraints by performing (quite different) canonical transformations which too, in particular, remove the potential term from the scalar constraint (see e.g. [8, 9]). Although the origins and the forms of these canonical transformations are quite different from the one used in this paper, there is nonetheless some qualitative similarity between the situations. One can exploit it to gain some insight into the full theory.

In particular, it is of considerable interest to understand the effect of such canonical transformations on quantization. Are the quantum theories based on the old and the new canonical coordinates—or, more precisely, on polarizations of the phase space naturally adapted to the old and the new canonical coordinates—equivalent? In full general relativity, one cannot answer the question at the present stage since the quantization program remains incomplete in both old and new variables: in the older ADM variables no solution to the quantum constraint is known while in the newer connection variables [8, 10], although a family of solutions *is* known, the Hilbert space structure on the space of these solutions is yet to be determined. For some of the models under consideration, on the other hand, both programs can be completed so that a comparison is possible.

The overall situation can be summarized as follows. First, by exploiting the simplicity of the form of the scalar constraint in the new variables, one can obtain the general solution to its quantum version. Furthermore, one can find a complete set of Dirac observables — functions on phase space whose Poisson brackets with the constraint vanish weakly. Now, in the quantization program of [1, 4], one selects the inner product on physical states—i.e. on solutions to quantum constraints—by demanding that the real Dirac observables be promoted to self-adjoint operators in the quantum theory. In all the models under consideration, this strategy works and provides us with a distinguished ⋆-representation of the algebra of Dirac observables. Second, in the traditional ADM variables, some of these models also admit what are known as conditional symmetries [10]. These are 1-parameter families of diffeomorphisms on the effective configuration space whose action commutes with the quantum scalar constraint, i.e., the Wheeler-DeWitt operator. Thus,
if we pass to the quantum theory using the traditional quantization method, we acquire 1-parameter symmetry groups acting on the space of physical states. By requiring that this action be unitary, one can uniquely “Hilbertize” the space of physical states thereby achieving the goal of quantum geometrodynamics [11]. This second procedure relies on the existence of symmetries on the effective configuration space of the model; unlike in the strategy followed using new variables, there is no need to isolate a complete set of Dirac observables. It is therefore not clear a priori that the two quantum theories –based on the new and the old canonical variables– would be equivalent. We will show that they in fact are, although some of the issues that arise are subtle and require care. This analysis illustrates the type of issues that are likely to arise when we explore the effect of the canonical transformation [8] on quantization of the full theory.

The completion of the various steps in the program provides us with a Hilbert space of physical states and a complete set of physical observables. Yet, the theory remains difficult to interpret physically because one is left with what is often called a “frozen formalism” in which nothing happens. This comes about because in the classical theory, dynamics is generated by a constraint. To illustrate this point, let us consider a free (relativistic) particle of mass $m$ in Minkowski space. In the classical Hamiltonian description, configuration space is the 4-dimensional Minkowski space, phase space is the cotangent bundle over it, and dynamics is governed by the constraint $P \cdot P + m^2 = 0$. To quantize the system it is simplest to work in the momentum representation. The physical states are then square-integrable functions on the (future) mass shell. These are all annihilated by the quantum constraint. There is no notion of time or of evolution; nothing happens. The picture we obtain by carrying out the quantization program for the spatially homogeneous models under consideration is completely analogous. Recall however, that in the case of the relativistic particle, one can cast the quantum theory in another form in which dynamics does appear. One can simply consider the position representation and rewrite the quantum constraint as the (positive frequency component of the) Klein Gordon equation. The wave function is then seen to evolve in time: the quantum constraint equation simply reduces to the evolution equation for quantum states. It turns out that the simplicity of the homogeneous models under consideration enables us to treat the issue of time in a completely analogous fashion. More precisely, we will be able to deparametrize [12, 1] the theory explicitly and show that in the quantum theory, the scalar constraint reduces to a Schrödinger evolution equation. This in turn will enable us to analyse how various physically interesting observables evolve in time. In particular, we will be able to explore the fate of singularities in the quantum theory. More generally, this framework will enable us to interpret the mathematical framework of the quantum theory in direct physical terms.

The plan of the paper is as follows. Section 2 is devoted to preliminaries. We recall general facts about homogeneous cosmologies and single out the models to be discussed in detail. In section 3, we present the canonical transformation which removes the potential term from the scalar constraint. In section 4 we carry out the quantization program using the new canonical variables. We discuss the physical interpretation of the resulting mathematical structure in section 5. In section 6, we pursue quantization in the old canonical variables (with the potential term in the expression of the scalar constraint) via the al-
ternate strategy of using conditional symmetries. While the resulting quantum theory is difficult to interpret because of the lack of (explicit expressions of) Dirac observables, it is mathematically complete from the traditional viewpoint. We conclude section 6 by comparing this mathematical framework with that developed in section 4. In section 7 we summarize both the overall picture and the lessons that can be drawn from this analysis.

The paper thus contains several related but distinct results. Readers familiar with the basic facts of spatially homogeneous models can proceed directly to the summary at the end of section 2. Readers whose primary interest lies in the technical and conceptual problems of quantization rather than in Bianchi models can skip section 2 and most of section 3 and proceed directly to the summary of the Hamiltonian structure presented in the last paragraph of section 3. Finally, readers whose primary interest lies in the issue of time and dynamics in (canonical) quantum gravity and who are familiar with the Hamiltonian structure of the Bianchi I model can proceed directly to section 5.

2 Mathematical Preliminaries

In this paper, we will consider diagonal, spatially homogeneous models which admit intrinsic, multiply transitive symmetry groups. For completeness, in this section we will specify the meaning of various terms appearing in the definition of this class and place this class in the general context of spatially homogeneous space-times. However, this material is not needed directly in the main part of the paper.

A spacetime is said to be spatially homogeneous if it admits a foliation by space-like sub-manifolds such that the isometry group of the 4-metric acts on each leaf transitively. If the action of the isometry group is multiply transitive and if there is no subgroup whose action is simply transitive, the spacetime is of Kantowski-Sachs type. If on the other hand, the isometry group admits a (not necessarily proper) subgroup which acts simply transitively on each leaf, the spacetime is said to be of Bianchi type. In this case, one focuses on the subgroup –which is necessarily 3-dimensional– and further classifies space-times using the properties of the corresponding Lie algebras. If the trace $C_{ba}$ of structure constants $C_{ac}$ of the Lie algebra vanishes, the space-time belongs to Bianchi Class A while if it does not vanish, it belongs to Bianchi class B $[13]$.

A spatially homogeneous 4-metric is said to be diagonal if it can be written in the form:

$$ds^2 = -(N(t))^2 dt^2 + \sum_{a=1}^{3} g_{aa}(t)(\omega^a)^2 ,$$

where $N(t)$ is the lapse function and $\omega^a$ is a basis of spatial 1-forms which are left invariant by the action of the isometry group. One can always change the time-coordinate $t$ to proper-time so that the coefficient of the first term is simply $-1$. The diagonal models are then characterized by the three components $g_{aa}$ which are functions only of time. A key issue, however, is whether the diagonal form of the metric is compatible with the vacuum field equations. This is the case for models for which the vector (or, the diffeomorphism) constraint is identically satisfied and only the scalar (or, the Hamiltonian) constraint remains to be imposed. In this paper, we will restrict ourselves to this class of models.
since they admit a Hamiltonian formulation, which is the point of departure for canonical quantization. In the case of Kantowski-Sachs metrics and the class A models, the vector constraint is identically satisfied; they belong to the class under consideration. For class B models, on the other hand, compatibility with field equations is not automatic: It is only restricted versions of type III, V and VI models (in which only two of the three metric coefficients are independent) that are both diagonal and satisfy the vector constraint identically. To summarize: the class of diagonal models compatible with the vacuum field equations consists of class A Bianchi models, in which the minisuperspaces will be 3-dimensional; Kantowski-Sachs models in which they will be 2-dimensional (since two of the $g_{aa}$ are always equal in these models) and certain class B Bianchi models in which they will be again 2-dimensional. Thus these models have either 2 or 1 true degree of freedom.

Misner [14] has introduced a very useful parametrization of the diagonal spatial metric:

$$g_{aa} = e^{2\beta^a},$$

$$\begin{pmatrix} \beta^1 \\ \beta^2 \\ \beta^3 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1/\sqrt{3} \\ 1 & 1 & -1/\sqrt{3} \\ 1 & -2 & 0 \end{pmatrix} \begin{pmatrix} \beta^0 \\ \beta^+ \\ \beta^- \end{pmatrix}. \quad (2)$$

We will see that the further restrictions we have to impose to arrive at the class of models which are of interest in this paper can be expressed concisely in terms of the parameters $(\beta^0, \beta^+, \beta^-)$.

Before discussing these restrictions, however, let us explore class A models in a little more detail. Since the trace of the structure constants vanishes for these models, they can be expressed entirely in terms of a symmetric, second rank matrix $n_{ab}$ [15]:

$$C^{abc}_{,d} = \varepsilon^{mbc} n^{ma}, \quad (3)$$

where $\varepsilon_{mbc}$ is the completely anti-symmetric symbol. The signature of $n^{ma}$ can then be used to divide the class A models into various types: If $n^{ab}$ vanishes identically, we have Bianchi type I; if it has signature $(0, 0, +)$, we have type II; signature $(+, -, 0)$ corresponds to type VI; $(+, +, 0)$ corresponds to VII; $(+, +, -)$ to type VIII; and, $(+, +, +)$ to type IX.

For Bianchi class B models, the trace $C^{a}_{ba} =: a_b$ does not vanish and implies a decomposition of the structure constants of the form:

$$C^{a}_{bc} = \varepsilon_{mbc} n^{ma} + a_b \delta^{a}{}_{c}, \quad (4)$$

where $n^{ab}$ is again symmetric but now satisfies the constraint $n^{ab} a_b = 0$. The models are now classified by the signature of $n^{ab}$ and –if the zero-eigenvector $a_b$ of $n^{ab}$ is non-degenerate– in addition by the value of the constant $h$ defined via:

$$a_m a_n = \frac{h}{2} \varepsilon_{mab} \varepsilon_{ncd} n^{ac} n^{bd}. \quad (5)$$

For type V metrics $n^{ab}$ vanishes. For type III metrics, $n^{ab}$ has signature $(+, -, 0)$ and $h$ equals $-1$. We shall not specify values of these parameters for the remaining class B models because we will not need them.
We can now continue the specification of conditions to arrive at the class of space-times of interest in this paper. The next restriction is to multiply transitive diagonal models. The Kantowski-Sachs models obviously belong to this class. Among Bianchi types, the condition of multiple transitivity leads to a further restriction since a generic Bianchi model is only simply transitive. In these models, if an additional Killing vector exists, it is always a rotation and these space-times are referred to in the literature as locally rotationally symmetric (LRS) models. In each of the Bianchi types I, II, VII0, VIII and IX, one can obtain a LRS model simply by setting the Misner parameter to zero. (Thus, among class A models, only type VI0 fails to admit a multiply transitive sub-family.) It turns out, however, that the family of LRS type VII0 models coincides with the family of LRS type I models. Therefore, we need only consider LRS families associated with types I, II, VIII and IX. Finally there is a family of models admitting a multiply transitive symmetry group among the class B space-times. This family consists of the LRS type III models and the isotropic type V models. The LRS type III models are obtained by setting $\beta^-$ equal to zero while the isotropic type V models are obtained by setting both $\beta^\pm$ to zero.

In this paper, however, we consider models which are somewhat more general than the diagonal multiply transitive ones: we need the multiple transitivity to hold only intrinsically. In the Kantowski-Sachs case, this loosening of the restriction makes no difference. In the Bianchi models, however, it does: we require the additional symmetry to be a Killing field only of the 3-metric intrinsic to the homogeneous slices and not necessarily of the full 4-metric. Clearly, all multiply transitive models are also intrinsically multiply transitive. However, we now acquire additional models: diagonal Bianchi types I and II without any further restrictions and diagonal type V models with the restriction that $\beta^+$ is set to zero in order to make the vector constraint vanish identically. Types I and II belong to class A while V belongs to class B. The minisuperspaces are 3-dimensional in types I and II and 2-dimensional in type V.

To summarize then, the diagonal, intrinsically multiply transitive (DIMT) models are the following: Bianchi types I and II; sub-families of Bianchi types III, VIII and IX defined by $\beta^- = 0$; Kantowski-Sachs space-times; and Bianchi type V models with $\beta^+ = 0$. For Bianchi types I and II, the minisuperspaces are 3-dimensional, parametrized by $\beta^0, \beta^+$ and $\beta^-$ in the Misner scheme; for Bianchi type V, the 2-dimensional minisuperspace is parametrized by $\beta^0$ and $\beta^-$; and, for all the remaining models—which are diagonal, multiply transitive (DMT)– the minisuperspaces are 2-dimensional, parametrized by $\beta^0$ and $\beta^+$. In the remainder of this paper, we restrict ourselves to these models. Thus, when we speak of type VIII or type IX, for example, unless otherwise specified, we will mean LRS type VIII and LRS type IX.

By exploiting the additional symmetries, one can explicitly solve the vacuum equations in all DIMT models. For details and especially for explicit expressions for the invariant 1-forms $\omega^a$ (defined in (1)) for all of these models, see [16, 13, 18].
3 Canonical Transformations

This section is divided into three parts. In the first, we introduce the general framework. In the Misner variables, the scalar constraint has the familiar form of a sum of a kinetic term and a potential term. The idea is to perform a canonical transformation so that—when expressed in terms of the new canonical variables—the potential term disappears entirely. This is achieved in the second and the third sub-sections. The resulting Hamiltonian description is remarkably simple and serves as the point of departure for quantization in the next section.

3.1 Hamiltonian framework

One can use the ADM procedure [7, 15] to arrive at the Hamiltonian formulation of all DMT models. The configuration spaces can be labelled by the Misner parameters—collectively denoted as $\beta^A$ in what follows—which take values in $(-\infty, \infty)$; the spaces are topologically trivial. (The index $A$ will take values $0, +, -$ in type I and II models, $0, -$ in type V and $0, +$ in the remaining (i.e., DMT) models.) Following the terminology commonly used, we will refer to them as minisuperspaces. The phase spaces are cotangent bundles over these configuration spaces. We will denote the momenta conjugate to $\beta_A$ by $p_A$. Thus, the fundamental Poisson bracket relations are $\{\beta^A, p_B\} = \delta^A_B$.

As noted above, in all these models, the vector constraints are automatically satisfied and one is left only with the scalar constraint. To simplify calculations, one usually chooses the “Taub time gauge”, i.e., one chooses the lapse function $N_T = 12 \exp 3\beta_0$ [19]. (This time gauge is also known as Misner’s supertime gauge [14].) To discuss the structure of the resulting constraint function, it is convenient to treat the type V models separately. With the Taub gauge choice the scalar constraint for the type V models takes the form [18]:

$$C_T \equiv C_0 + C_- = 0,$$
$$C_0 = -\frac{1}{2}p_0^2 + k_0 e^{4\beta_0}, \quad C_- = \frac{1}{2}p_-^2,$$

where $k_0 = 72$. For the remaining models we have [15, 20]:

$$C_T = \frac{1}{2} \eta^{AB} p_A p_B + U_T = 0,$$
$$U_T = k_0 e^{2(2\beta_0 - \beta^+)} + k_+ e^{4(\beta_0 - 2\beta^+)},$$

where $\eta^{AB}$ is $\text{diag}(-1, 1, 1)$ for type I and II models and $\text{diag}(-1, 1)$ for the remaining (i.e. DMT) models; and the values of the constants $k_0$, $k_+$ and $k_-$ (defined below) characterizing the different models are given in the following table:
Finally, for the non-type V models, it is convenient to make a linear point transformation to cast the scalar constraint in a form that will be particularly useful. Set

\[( \bar{\beta}_0, \bar{\beta}^+, \bar{\beta}^- ) = \frac{1}{\sqrt{3}} (2\beta^0 - \beta^+, -\beta^0 + 2\beta^+, \sqrt{3}\beta^- ) . \] (8)

Then, the scalar constraint can be re-expressed as:

\[ C_T \equiv C_0 + C_+ + C_- = 0 , \]

where

\[ C_0 = -\frac{1}{2}\bar{p}_0^2 + k_0 e^{2\sqrt{3}\beta^0} , \quad C_+ = \frac{1}{2}\bar{p}_+^2 + k_+ e^{-4\sqrt{3}\beta^+} , \quad C_- = \frac{1}{2}k_-\bar{p}_-^2 . \] (9)

Thus, the scalar constraint for all DIMT models is separable, a fact which underlies the “solvability” of these models. This property will enable us in the next two sub-sections to perform the canonical transformation which will drastically simplify the form of the constraint.

### 3.2 Cases with non-positive \( k_0 \)

When \( k_0 \) is non-positive, the constraint is a sum of terms of the form:

\[ C^{(1)} = \epsilon \frac{1}{2} (\bar{p}_A^2 + a_A^2 e^{2d_A\bar{\beta}^A} ) , \] (10)

with no sum over \( A \). The constant coefficients \( a_A, d_A \) are given by: \( a_- = 0; a_A^2 = 2\vert k_A \vert \) for \( A = 0, +; d_0 = \sqrt{3} \) and \( d_+ = -2\sqrt{3} \). Finally, \( \epsilon \) takes the values \( \pm 1 \). We now want to define new coordinates \( \bar{\beta}^A \) and momenta \( \bar{p}_A \) so that terms \( C^{(1)} \) in (10) take the form \( C^{(1)} = \epsilon \frac{1}{2}\bar{p}_A^2 \) so that the potential term disappears completely. Clearly, if \( a_A = 0 \), the corresponding term in the expression of the scalar constraint is already of the desired form whence we can and will simply set \( \bar{\beta}^A = \beta^A \) and \( \bar{p}_A = \bar{p}_A \); no canonical transformation is needed in that \((\bar{\beta}^A, \bar{p}_A)\) plane. Therefore, in this and the next sub-section, we will consider in detail only those cases in which \( a_A \neq 0 \), and assume, without loss of generality, that \( a_A \) is positive.

The required canonical transformation is easy to obtain. Let us begin by setting

\[ \bar{p}_A = \sqrt{\bar{p}_A^2 + a_A^2 e^{2d_A\bar{\beta}^A}} . \] (11)

Note that by definition, \( \bar{p}_A > 0 \). To find the corresponding canonically conjugate \( \bar{\beta}^A \), we have to solve an elementary differential equation. The result is:

\[ \bar{\beta}^A = \frac{1}{d_A} \left( \ln [-\bar{p}_A + \sqrt{\bar{p}_A^2 + a_A^2 e^{2d_A\bar{\beta}^A}}] - \ln [a_A e^{d_A\bar{\beta}^A}] \right) . \] (12)
Thus (11) and (12) together define a canonical transformation which yields a $C^{(1)}$ of the desired form. The inverse of this canonical transformation is given by

$$a_A e^{d_A \beta^A} = \bar{p}_A / \cosh(d_A \tilde{\beta}^A), \quad \bar{p}_A = -\tilde{p}_A \tanh(d_A \tilde{\beta}^A),$$

from which we can see that the canonical transformation is globally defined on the phase space, since $(\bar{\beta}^A, \bar{p}_A)$ take all values.

Note that $C_+$ is always of the form $C^{(1)}$, with $\epsilon = 1$. Thus the above canonical transformation (11, 12) leads to the desired form for this term, $C_+ = \frac{1}{2} \tilde{p}_+^2$, and a non-holonomic constraint $\tilde{p}_+ > 0$. This last constraint is important since it is now the only remnant of the potential term in the barred variables.

As far as $C_0$ is concerned, in type I and II models, we can simply set $\tilde{\beta}^0 = \tilde{\beta}^0$ and $\tilde{p}_0 = \tilde{p}_0$, since $k_0$ --and hence $a_0$-- vanishes in these cases. As the description stands, there is no restriction on the sign of $\tilde{p}_0$ and hence of $\tilde{p}_0$. However, if we flip the sign, the dynamical trajectories in the phase space --and hence space-time geometries they define-- remain unaltered. What changes is the sign of the affine parameter along the trajectories in the phase space, or equivalently, the convention regarding future versus past evolution in the physical space-time picture. Keeping both signs is therefore redundant. In order to make the Hamiltonian description parallel to the textbook discussion of the relativistic particle, we will choose $\tilde{p}_0 \geq 0$.

When $k_0 < 0$, i.e. for the KS and the LRS type IX models, $C_0$ is again of the form $C^{(1)}$, with $\epsilon = -1$. For these cases, it follows from (11) that we again have $\tilde{p}_0 > 0$. This leads to the form $C_0 = -\frac{1}{2} \tilde{p}_0^2$ and the restriction $\tilde{p}_0 > 0$. Thus we have shown that one can use the canonical transformation (11, 12) to transform the constraint (for all DIMT models except type V, and LRS types III and VIII, which we will discuss below) to the form

$$C_T = \frac{1}{2} \eta^{AB} \tilde{p}_A \tilde{p}_B = 0 .$$

(14)

Thus, as was desired, now the constraint contains only a kinetic piece quadratic in momenta; the potential term has been eliminated. Furthermore, the metric defined by the kinetic term is just the flat Minkowski metric! Thus, locally in phase space, the dynamics of any of these models is the same as that of any other and is furthermore indistinguishable from that of a massless, relativistic, free particle in a two or three dimensional Minkowski space. The canonical transformation has essentially enabled us to pass to the “action angle type” variables appropriate to each model.

However, in each of these models, the information in the potential terms is now essentially coded in the global structure of the phase space. Due to the presence of the non-holonomic constraints on the $\tilde{p}_A$, one can no longer consider them as momenta. However, in the $(\tilde{\beta}^A, \tilde{p}_A)$ coordinates, the phase space still has the structure of a cotangent bundle over the space coordinatized by $\{\tilde{p}_A\}$. It is therefore convenient to regard the $\tilde{p}_A$ as the configuration variables and the $\tilde{\beta}^A$ as the corresponding momenta. The holonomic as well as the non-holonomic constraints restrict only the configuration variables $\tilde{p}_A$. The restricted manifolds are given by:

\[\text{Even if one ignores this redundancy and keeps both signs of } \tilde{p}_0 \text{ in the classical theory, the requirement that one restrict oneself to an irreducible representation of the algebra of Dirac observables forces one to choose one or the other sign in quantum theory.}\]
• Bianchi type I: Future (+) light cone in 3 dimensions ($3L^+$).

• LRS type I: Future light cone in 2 dimensions ($2L^+$), obtained by setting $\beta^- = \tilde{\beta}^- = 0$ in $3L^+$.

• Bianchi type II: Right ($R$) half of the future light cone in 3 dimensions ($3L^+_R$); since only the right half of $3L^+$ is allowed due to the additional non-holonomic constraint $\tilde{p}_+ > 0$.

• LRS type II: Right half of the future light cone in 2 dimensions ($2L^+_R$), obtained by setting $\tilde{\beta}^- = 0$ in $3L^+_R$. (Note that this is just half the real line.)

• KS: Future light cone in 2 dimensions, $2L^+$, as for LRS type I.

• LRS type IX: Right half of the future light cone in 2 dimensions $2L^+_R$, as for LRS type II.

3.3 Cases with positive $k_0$

The constant $k_0$ is positive in the following models: type V, LRS types III and VIII. In these cases, the part $C_0$ of the scalar constraint is of the form:

$$C^{(2)} = -\frac{1}{2}(\tilde{p}_0^2 - a_0^2 e^{2d_0\tilde{\beta}^0}) ,$$

where $a_0^2 = 2k_0$ in all cases, $d_0 = 2$ in type V, and, $d_0 = \sqrt{3}$ in the remaining cases. Therefore, the canonical transformations which cast $C_0$ in the form $C_0 = -\frac{1}{2}\tilde{p}_0^2$ are now:

$$\tilde{p}_0 = \sqrt{\tilde{p}_0^2 - a_0^2 e^{2d_0\tilde{\beta}^0}} ,$$

$$\tilde{\beta}^0 = \frac{1}{d_0} \left( \ln[\tilde{p}_0 - \sqrt{\tilde{p}_0^2 - a_0^2 e^{2d_0\tilde{\beta}^0}}] - \ln[a_0 e^{d_0\tilde{\beta}^0}] \right) ,$$

and the inverse transformation assumes the form:

$$a_0 e^{d_0\tilde{\beta}^0} = \tilde{p}_0/\sinh(d_0\tilde{\beta}^0) , \quad \tilde{p}_0 = \tilde{p}_0 \coth(d_0\tilde{\beta}^0) .$$

Note that there are regions of the phase space in which $\tilde{p}_0^2 - a_0^2 e^{2d_0\tilde{\beta}^0}$ is negative. In these regions the new “coordinate” $\tilde{p}_0$, e.g., is imaginary. However, there exists a neighborhood of the constraint surface in which $\tilde{p}_0^2 - a_0^2 e^{2d_0\tilde{\beta}^0}$ is everywhere positive, and thus $\tilde{p}_0$ is real. Furthermore, because of the simple form of the constraint, without loss of generality, in the quantization procedure we will be able to restrict ourselves to this neighborhood. Finally, on the constraint surface, there is an additional non-holonomic constraint $\tilde{p}_0 \geq 0$.

In all these cases –types V, LRS III and LRS VIII models– $C_+$ and $C_-$, when not already in the desired form $+\frac{1}{2}\tilde{p}_0^2$, continue to be of the form $C^{(1)}$ whence the canonical

\(^{2}\)Strictly speaking, the origin should be excluded for the KS models. However, since the presence or absence of the solitary boundary point makes only a trivial difference in the quantum theories under consideration, we will no longer draw a distinction.
transformations in the \((\tilde{\beta}^+, \tilde{p}^+)\) and \((\tilde{\beta}^-, \tilde{p}^-)\) planes are the same as those given in the previous subsection (equations 11, 12). As before, the tilde coordinates continue to exhibit the phase space as a cotangent bundle and the natural configuration space is coordinatized by the \(\{\tilde{p}_A\}\). The constraints again restrict only the configuration space. We are led to the following list:

- type V: Future light cone in 2 dimensions, \(2\mathcal{L}^+\), as for LRS type I.
- LRS type III: Future light cone in 2 dimensions, \(2\mathcal{L}^+\), as for LRS type I.
- LRS type VIII: Right half of the future light cone in 2 dimensions, \(2\mathcal{L}^+_R\), as for LRS type II.

To summarize\(^3\), the phase space dynamics for all the DIMT models has been reduced to that of a massless relativistic particle moving in (3 or 2-dimensional) Minkowski space where, however, the momenta \(\tilde{p}_A\) of the particle –which are our new configuration variables– are subject to the non-holonomic constraint \(\tilde{p}_0 \geq 0\) and, in some models, also \(\tilde{p}_+ > 0\). Inspite of these constraints, in each of these models the phase space (as well as the reduced phase space) still has the structure of a cotangent bundle over the new configuration space, spanned by the \(\tilde{p}_A\).

4 Quantization

This section is divided into three parts. In the first, we outline the general strategy, in the second, we carry out the quantization program systematically in the case of the type II model, and, in the third we briefly discuss the type I model. Since these two models are the prototypes for the rest, other DIMT models can be treated in a completely analogous fashion; they will not be discussed further.

4.1 Outline

We now want to exploit the simplicity of the scalar constraint in the tilde canonical variables to carry out quantization.

There exist two standard procedures for quantization of systems with first class constraints: the reduced phase space method and the Dirac procedure of imposing operator constraints to select the physical states. In all the models considered in this paper, if we use \(\tilde{p}_A\) as the configuration variables, the constraints are independent of momenta. Hence, quantization via the reduced phase space method leads to the same result as quantization via Dirac’s operator constraint method. Since our primary interest stems from the

\(^3\)We have restricted ourselves to vacuum space-times in this paper. However, one can sometimes can add sources to the DIMT models also which lead to separable constraints that can be transformed to the form \((14)\). For example, one can add a cosmological constant \(\Lambda\) to the Bianchi type I models. This leads to a potential term \(24\Lambda e^{6\beta_0}\) in the Taub time gauge; a term which is easily absorbed by a canonical transformation of the above type.
quantization program of \([1, 4]\) which is an extension of Dirac’s procedure, we will use the operator constraint method.

In broad terms, the DIMT models fall into two classes: those in which the effective configuration space is the full future null cone \(\mathcal{L}^+\) in 2 or 3 dimensional Minkowski space and those in which it is only the right half \(\mathcal{L}_R^+\) of this null cone. The mathematical structure of the models in the first class is identical to that of a free relativistic particle in 2 or 3 dimensional Minkowski space. Therefore, as far as the mathematical steps in the quantization program are concerned, one can simply mimic the textbook procedure for quantization of the relativistic particle. In models in the second class, however, certain subtle issues arise because of the presence of the non-holonomic constraints \(\tilde{p}_+ > 0\). Therefore, we will first treat this case in detail and then turn briefly to models in the first class. For concreteness, we will use the type II and type I models as representatives of the two classes.

4.2 The type II model

Let us follow the quantization program of \([1, 4]\) step by step to bring out the assumptions involved. Since the model is simple enough, the final result is not surprising. However, in order to compare and contrast this result with the one obtained in section 6, it is important to note the procedure carefully. Also, in several other cases, treated elsewhere \([1, 5]\), the final result is not at all obvious from the start and can in fact be quite surprising. In such cases, it becomes critical to adhere to the program systematically.

To begin with, as in the Dirac approach to quantization of constrained systems, let us ignore the scalar constraint. The phase space is then topologically \(R^6\) coordinatized by \((\tilde{\beta}^A, \tilde{p}_A)\), where \(\tilde{p}_+\) and \(\tilde{p}_0\) range over \((0, \infty)\) and all other coordinates range over \((-\infty, \infty)\). It is natural to choose the \(\tilde{p}_A\) as the configuration variables and the \(\tilde{\beta}^A\) as the conjugate momenta. Let us denote the configuration space by \(\mathcal{C}\). In the passage to quantum theory, let us first consider the topological vector space \(\mathcal{V}\) spanned by distributions \(\Psi\) over the space \(\mathcal{C}\). This will be the initial space of quantum states, prior to the imposition of constraints. Given a smooth function \(f(\tilde{p})\) on \(\mathcal{C}\) we define a configuration operator \(\hat{f}\) on \(\mathcal{V}\) and given a complete, smooth vector field \(v\) on \(\mathcal{C}\), we define a momentum operator \(\hat{v}\) on \(\mathcal{V}\) as follows:

\[
(\hat{f} \circ \Psi)(\tilde{p}) := f(\tilde{p}) \cdot \Psi(\tilde{p}) \quad (\hat{v} \circ \Psi)(\tilde{p}) := i\hbar(\mathcal{L}_v + \frac{1}{2}(\text{Div}\tilde{\mu}v))\Psi(\tilde{p}).
\]

Here, \(\tilde{\mu}\) is an arbitrary volume element (i.e., a nonvanishing 3-form) on \(\mathcal{C}\) (to be fixed later) and the divergence of the vector field \(v\) with respect to \(\tilde{\mu}\) is defined by: \((\text{Div}\tilde{\mu}v) \cdot \tilde{\mu} := \mathcal{L}_v\tilde{\mu}\). The operators are defined in such a way that their commutators are precisely \(i\hbar\) times the Poisson brackets between their classical analogs. Note that \(\mathcal{V}\) is not equipped with the structure of a Hilbert space. One can, if one is so inclined, introduce an inner product and make \(\mathcal{V}\) into a Hilbert space. However, typically, most solutions to constraints are not normalizable with respect to such an inner product and the resulting Hilbert space structure has no physical significance.

Our next task is to solve the quantum constraint equations \(\dot{C}_T \circ \Psi = 0\), thereby singling
out the physical states. Since the scalar constraint function,

$$C_T = \frac{1}{2}(-\tilde{p}_0^2 + \tilde{p}_+^2 + \tilde{p}_-^2)$$  \hspace{1cm} (19)$$

is a smooth function of $\tilde{p}_A$ alone, this task is easy to accomplish. Physical states lie in the vector space of solutions to the quantum constraint equation, which is spanned by states of the form:

$$\Psi_{sol}(\tilde{p}) = \delta(\tilde{p}_0 - \sqrt{\tilde{p}_+^2 + \tilde{p}_-^2}) \cdot \psi(\tilde{p})$$ \hspace{1cm} (20)$$

where (as before) $\Psi_{sol}$ is a 3-dimensional distribution on $\mathbb{C}$ and $\psi$ is a 2-dimensional distribution on $L^+_{\mathbb{R}}$. (That is, we have to smear $\Psi_{sol}$ by a test field on the 3-dimensional space $\mathbb{C}$ while we have to smear $\psi$ by a test field on the right half of the 2-dimensional future light cone $L^+_{\mathbb{R}}$ in $\mathbb{C}$. Note that since $\tilde{p}_0 \in (0, \infty)$, the non-holonomic constraints are also satisfied.) Denote the space of these solutions by $V_{sol}$. Since the distribution $\delta(\tilde{p}_0 - \sqrt{\tilde{p}_+^2 + \tilde{p}_-^2})$ is a pre-factor common to all solutions, each state $\Psi_{sol}$ is completely characterized by the distribution $\psi$ on $L^+_{\mathbb{R}}$.

We can now consider physical –i.e., Dirac– observables. These are the operators which leave the space $V_{sol}$ of solutions invariant. Every $\hat{f}$ defined above has this property. However, since $L^+_{\mathbb{R}}$ is only 2-dimensional, two (suitably chosen) operators among these suffice to constitute a complete set of physical configuration operators. Let us choose these to be $\hat{\tilde{p}}_{\pm}$, operator analogs of $\tilde{p}_{\pm}$.

The choice of a minimal, complete set of momentum operators requires more care. Now, the corresponding vector fields $\tilde{v}$ need to satisfy four additional properties: $i$) they must be tangential to $L^+_{\mathbb{R}}$; $ii$) they should span the tangent space to $L^+_{\mathbb{R}}$; $iii$) they should be closed under the Lie bracket; and $iv$) the diffeomorphisms they generate should leave invariant the three dimensional vector space spanned by the two functions $\tilde{p}_{\pm}$ and constants. The first two of these conditions ensure that the corresponding operators $\hat{\tilde{v}}$ are well-defined and form a complete set of momentum operators while the last two conditions ensure that the vector space generated by the configuration and momentum operators (together with the identity) is closed under the commutator bracket. Consider the vector fields:

$$\tilde{v}_- = \left( \frac{\partial}{\partial \tilde{p}_-} \right) + \frac{\tilde{p}_-}{\tilde{p}_0} \left( \frac{\partial}{\partial \tilde{p}_0} \right)$$

$$\tilde{v}_+ = \tilde{p}_+ \left( \frac{\partial}{\partial \tilde{p}_+} \right) + \frac{\tilde{p}_+^2}{\tilde{p}_0} \left( \frac{\partial}{\partial \tilde{p}_0} \right)$$ \hspace{1cm} (21)$$

These vector fields span the tangent space at each point of $L^+_{\mathbb{R}}$ and are complete; in particular, on the “boundary” $\tilde{p}_+ = 0$ (which is not a part of $L^+_{\mathbb{R}}$), the coefficient of $\partial/\partial \tilde{p}_+$ vanishes. Let us denote the corresponding complete set of momentum observables by $\tilde{v}_-$ and $\tilde{v}_+$. Their action on solutions to the quantum constraint is given by:

$$\langle \tilde{v}_\pm \circ \Psi_{sol}(\tilde{p}) \rangle = i\hbar \delta(\tilde{p}_0 - \sqrt{\tilde{p}_+^2 + \tilde{p}_-^2})(\mathcal{L}_{\tilde{v}_\pm} + \frac{1}{2} \text{Div} \tilde{v}_\pm) \psi(\tilde{p})$$ \hspace{1cm} (22)$$

Since $\tilde{v}_\pm$ are tangential to $L^+_{\mathbb{R}}$ the action maps physical states to physical states. Next, a straightforward calculation shows that the vector fields $\tilde{v}_\pm$ –and hence also the corresponding operators $\hat{\tilde{v}}_{\pm}$– commute with one another. Finally, the nonvanishing commutators
between the configuration and the momentum operators are given by:

\[
[\hat{v}_-, \hat{p}_-] = i\hbar \quad \text{and} \quad [\hat{v}_+, \hat{p}_+] = i\hbar \hat{p}_+ .
\]  

(23)

Thus, our choice of vector fields \( \hat{v}_\pm \) satisfies all the four conditions required above. The complete set of Dirac observables is therefore given by \( \hat{p}_\pm \) and \( \hat{v}_\pm \) and they provide us with two “canonically conjugate” pairs.

We now come to the problem of finding an inner product. It is here that we bring in the “reality conditions”: The inner product should be such that the Dirac operators corresponding to real classical observables should be self-adjoint [1, 4]. Since the above set of four Dirac observables (together with the identity operator) is complete, i.e. since it generates the entire algebra of physical observables, it suffices to impose the reality conditions only on this set. Consequently, it follows from the results of [21] that, if there exists an inner product on an irreducible representation of the algebra of Dirac observables which makes these four Dirac observables self-adjoint, the inner product is unique. To show existence, it will suffice to simply exhibit the answer. For any two solutions \( \Psi_\text{sol} \) and \( \Phi_\text{sol} \) (see (20)), the required inner product is given by:

\[
\langle \Psi | \Phi \rangle_\text{phy} \equiv \langle \psi | \phi \rangle = \int_{\mathcal{L}_R^+} \bar{\psi} \phi \mu .
\]  

(24)

Here \( \mu \) is the measure on \( \mathcal{L}_R^+ \) (i.e. a nonvanishing 2-form) such that

\[
\mu \wedge dC_T = \bar{\mu},
\]  

(25)

where \( \bar{\mu} \) is the measure on \( \mathcal{C} \) used in the expressions of the momentum operators (22), and \( dC_T \) is a nowhere vanishing covariant normal to \( \mathcal{L}_R^+ \). Now, for any vector field \( v \) on \( \mathcal{C} \), tangential to \( \mathcal{L}_R^+ \), it is straightforward to show that \( \text{Div}_R v = \text{Div}_\mu v \), where the (2-dimensional) divergence of \( v \) on \( \mathcal{L}_R^+ \) is defined by \( (\text{Div}_\mu v) \cdot \mu := \mathcal{L}_v \mu \). Thus, it follows that the physical momentum operators (22) are self-adjoint with respect to the inner product (24). (Since we are working in a representation in which the operators \( \hat{p}_\pm \) are diagonal, these operators are self adjoint for any choice of measure on \( \mathcal{L}_R^+ \); the constraint on the measure comes only from the requirement that the momentum operators \( \hat{v}_\pm \) be self adjoint.) The physical states are those \( \Psi_\text{sol} \) which have finite norm. This condition selects, from all distributional solutions \( \Psi_\text{sol} \) to the quantum constraints, the ones for which \( \psi \) are square integrable functions on \( \mathcal{L}_R^+ \) (w.r.t. the measure \( \mu \)). The Hilbert space \( \mathcal{H} \) of physical states is simply \( L^2(\mathcal{L}_R^+, \mu) \).

Recall that there is considerable freedom in the choice of \( \mu \); it can be any nowhere vanishing measure on \( \mathcal{L}_R^+ \). Different choices of \( \mu \) lead to unitarily equivalent theories: If we were to replace \( \mu \) by \( \mu' = f^2 \mu \), then the map \( \psi \mapsto \psi' = \psi / f \) is the required unitary mapping from \( \mathcal{H} \) to \( \mathcal{H}' \). One can use this freedom to simplify the expression (22) of the momentum operators \( \hat{v}_\pm \). The simplest expression results if we choose the measure \( \mu \) with respect to which the vector fields \( \hat{v}_\pm \) are divergence-free. This condition provides a set of differential equations on \( \mu \) whose solution yields the expression

\[
\mu_0 = \frac{1}{\hat{p}^+} \, d\hat{p}^+ \wedge d\hat{p}^- ,
\]  

(26)
For simplicity, from now on, we shall use this measure.

This completes the implementation of the quantization program for the Bianchi type II model. In the final picture, the Hilbert space $\mathcal{H}_0$ of physical quantum states is given by $L^2(\mathcal{L}_+^0, \mu_0)$; a complete set of Dirac observables is given by $\tilde{p}_\pm$ and $\tilde{v}_\pm$; and, the algebra of Dirac operators is given by the relations (23). This simple picture has emerged precisely because we could cast the scalar constraint function in the simple form (19) via a canonical transformation to the $(\beta^A, \tilde{p}_A)$ variables. The issue of physical interpretation of this mathematical framework will be discussed in detail in section 5.

### 4.3 The type I model

In this subsection, we wish to consider models in which the constraint allows $\tilde{p}_A$ to belong to the full (future) null cone. This discussion will also shed light on some subtleties that underlie the choices of Dirac observables made above for the type II model.

The prototype of the models with the full light cone is provided by Bianchi type I. Let us restrict ourselves to this case. Then, the constraint in the original $(\beta^A, p_A)$ variables is already in the desired form since there is no potential term to begin with. Therefore, there is no need to carry out any canonical transformation; the tilde variables are the same as the original ones. To emphasize this point and also to distinguish this case notationally from the type II model, we will work with the original phase space coordinates $(\beta^A, p_A)$, all of which range over $(-\infty, \infty)$.

We can again follow the quantization program step by step. The first few steps are identical to those for Bianchi type II: On the vector space of distributions $\Psi$ on the new configuration space, we have a representation of the configuration and momentum operators as in (18) and the quantum constraint for the type I model is solved by states analogous to those in (20). The only technical difference is that there is only one non-holonomic constraint, namely the one which restricts $p_0$ to be positive, whence the 2-dimensional distributions $\psi$ which characterize the solutions to the quantum constraint are defined on the entire future light cone $\mathcal{L}^+$. A complete set of classical Dirac configuration observables is given by $p_\pm$. We will denote the corresponding quantum operators by $\hat{p}_\pm$.

However, for the momentum observables, there is a key difference from the type II model: Operators analogous to $\hat{v}_\pm$ will no longer suffice because now the vector fields $\tilde{v}_\pm$ span the tangent space of $\mathcal{L}^+$ only almost everywhere; they are linearly dependent on the lines $p_+ = 0$. Hence we must choose different Dirac momentum observables. Perhaps the simplest choice is to use the two boost generators:

\begin{align}
 v_+ &= p_0 \left( \frac{\partial}{\partial p_+} \right) + p_+ \left( \frac{\partial}{\partial p_0} \right), \\
 v_- &= p_0 \left( \frac{\partial}{\partial p_-} \right) + p_- \left( \frac{\partial}{\partial p_0} \right),
\end{align}

which are linearly independent everywhere on (and tangential to) $\mathcal{L}^+$. However, this set fails to be closed under the Lie bracket: the bracket of two boosts is a rotation. Thus, we
must enlarge the set of momentum observables by adding the rotation vector fields

\[ v_0 = p_+ \left( \frac{\partial}{\partial p_-} \right) - p_- \left( \frac{\partial}{\partial p_+} \right). \tag{28} \]

Denote the momentum operators by \( \hat{v}_A \). Now, if we compute the commutators between these momentum operators and the configuration ones, we find that the Lie algebra does not close unless we add to the configuration operators \( \hat{p}_0 \equiv (\hat{p}_+)^2 + (\hat{p}_-)^2 \). These six Dirac operators, \( (\hat{p}_A, \hat{v}_A) \) form a Lie algebra which is isomorphic to the Lie algebra of the Poincaré group in 3-dimensional Minkowski space: the configuration operators provide the generators of translations while the momentum operators provide the generators of Lorentz transformations. The classical Dirac observables corresponding to these six operators are real, whence the six operators have to be self adjoint in the quantum theory. Given the explicit expression of the momentum operators (18), which involves the choice of a measure on \( L^+ \), the above “reality condition” again selects the inner product (of the form (24)) uniquely. If the measure is chosen so that all three vector fields are divergence-free (to simplify the expressions of the momentum operators) we are led to the measure \( \mu'_0 = \frac{1}{\sqrt{p_0}} dp_+ \wedge dp_- \). Thus, not surprisingly, the program has led us to a description which is the same as the textbook treatment of the free relativistic particle in 3-dimensional Minkowski space. The Hilbert space is now the space \( L^2(L^+, \mu'_0) \), the space of square-integrable functions on the entire future cone \( L^+ \) in the configuration space spanned by \( p_A \), where the measure \( \mu'_0 \) is given above.

What would have happened if we had ignored the fact that \( \tilde{v}_\pm \) are not linearly independent everywhere and used the same set of Dirac observables as in the case of the Bianchi II model? Then, the Hilbert space \( L^2(L^+, \mu'_0) \) constructed here would have provided a reducible representation of the algebra of those Dirac observables. Since, for physical reasons, one must restrict oneself to an irreducible representation, we would have been led to use, as the space of physical states only “half of” \( L^2(L^+, \mu'_0) \), which would clearly have been wrong. Thus, strict completeness of Dirac observables is important for quantization. Considerable care must be exercised even in the case when completeness fails on sets of measure zero.

However, since here the effective configuration space \( L^+ \) is only 2-dimensional, there are two algebraic relations between the above six operators. We could have avoided this redundancy by choosing the Dirac observables differently: For example, we could have chosen momentun operators corresponding to the vector fields

\[
\begin{align*}
   u_+ &= \left( \frac{\partial}{\partial p_+} \right) + \frac{p_+}{p_0} \left( \frac{\partial}{\partial p_0} \right), \\
   u_- &= \left( \frac{\partial}{\partial p_-} \right) + \frac{p_-}{p_0} \left( \frac{\partial}{\partial p_0} \right).
\end{align*}
\]

These vector fields commute amongst themselves, and the Dirac operators \( (\hat{u}_\pm, \hat{\rho}_\pm) \) form two canonically conjugate pairs. With this choice, however, the quantum description would not have closely resembled the textbook treatment of a free relativistic particle.

This point is important to quantization of the full 2+1 as well as 3+1 dimensional general relativity using loop variables since these fail to be complete on sets of measure zero on the classical phase space (see, e.g., [1, 3]). In the 2+1 theory, one knows how to face the resulting difficulties. In the 3+1 theory, however, the issue is only partially understood.

\[ \text{16} \]
Similarly, in the case of the type II model, it would be wrong to ignore the global structure of the configuration space –i.e., the non-holonomic constraint $\tilde{p}_+ > 0$– and use the generators of boosts and rotations as Dirac observables. That algebra would have led us to the Hilbert space $L^2(\mathcal{L}^+, \mu_0')$ on the full future cone rather than $L^2(\mathcal{L}^+_{K}, \mu_0)$ obtained in the previous sub-section. Indeed, this difference in the global structure is the only remnant in the tilde variables $(\tilde{\beta}^A, \tilde{p}_A)$ of the potential term $U_T$ in the scalar constraint in the original ADM variables $(\beta^A, p_A)$. It is therefore crucial to keep track of it in the quantization procedure.

5 Physical Interpretation

This section is divided into 3 parts. In the first, we state the problem we wish to address and outline the general strategy (see e.g. [4]). This is implemented in detail for the simplest DIMT model –Bianchi type I– in the second part and for the the prototype of the remaining DIMT models –Bianchi type II– in the third part. The overall situation in other DIMT models is analogous to that in these two cases.

5.1 The problem

In section 4, we carried out the quantization program of [1, 4] to completion for all DIMT models. Since we were able to construct complete sets of Dirac observables, we could use the “reality conditions” to select the appropriate Hilbert space structures on the spaces of physical states. Contrary to a general belief (see, e.g., [12]), we did not have to single out time and deparametrize the system in order to arrive at this mathematical description.

Since we have access to a complete set of Dirac observables, we can pose and answer a number of physical questions. For example, we can compute the spectra of these observables; comment on their continuous versus discrete eigenvalues; evaluate their expectation values in given physical states, thereby providing probabilistic estimates for finding any given range of values on any given state; etc. These are interesting questions. However, of necessity, they all refer only to Dirac observables: the action of more general operators fails to be well-defined since they do not even leave the Hilbert space of physical states invariant.

Now, in the classical theory, dynamics is governed by the scalar constraint whence Dirac observables are, in particular, constants of motion. We therefore expect that, in quantum theory as well, questions which are formulated using only the Dirac observables introduced so far –$(\hat{\beta}_\pm, \hat{v}_\pm)$ in the type II model and $(\hat{p}_A, \hat{v}_A)$ in the type I model– will also refer to physical quantities which do not “evolve.” After all, we have a framework in which there is no notion of time and hence of evolution. Nothing “happens.” So far, there is only a timeless, frozen formalism. However, we would like to ask questions, e.g., about evolution of anisotropies, about the behavior of spacetime curvature, about the fate of classical singularities in the quantum theory. The machinery of Dirac observables at hand does not in itself suffice to even phrase such questions. Neither the anisotropies $\beta^A$ nor the curvature scalars such as $C_{abcd}C^{abcd}$ commute with the constraint; they are not expressible purely in terms of our Dirac observables. Thus, there seems to exist a quandary: while the
mathematical machinery wants us to work primarily in terms of Dirac operators, many of
the interesting physical questions refer to “dynamics” and hence, on the face of it, seem
to force us beyond Dirac observables.

There is, however, a well defined strategy that one can adopt to get out of this apparent
quandary. The idea is to isolate, prior to the imposition of the constraint, one of the
arguments of the physical wave functions as an “internal time variable” and interpret the
constraint as an evolution equation with respect to this internal time. One can then
introduce new one parameter families of Dirac operators and interpret the non-trivial
dependence on the parameter as “time evolution.” Note, however, that this “time” is
one of the configuration variables. It does not arise from a background space-time; at
a fundamental level, there is in fact no space-time whatsoever in the quantum theory.
Nonetheless this generalized notion of time appears to be sufficient to pose and answer
the dynamical questions raised above. Furthermore, it appears to suffice also for the
analysis of measurement theory since, as we will see below, one can specify exhaustive
sets of mutually exclusive alternatives on slices of constant (generalized) time in the
configuration space. To summarize, although it may seem puzzling at first, it is possible
to introduce “time evolving Dirac observables” in an appropriate sense and use them
effectively to analyse the questions of dynamics. It is this strategy that lets us get out of
the apparent quandary.

This general strategy is of course rather old (see, e.g., articles by Kuchař and Rovelli
in [23] and the references they contain) although its full power does not seem to be always
appreciated. What we wish to show in the next two subsections is: i) this strategy can
be implemented in detail in all DIMT models; and, ii) the implementation enables us to
ask and answer a number of “dynamical” questions of physical interest, including the fate
of singularities. This goes a long way towards understanding the physics in the quantum
theory of these spatially homogeneous models. Our overall conclusion is that while it is
not essential to face “the issue of time” to complete the quantization program itself, a
satisfactory treatment of this issue is necessary to extract the full physical content of the
resulting mathematical framework and that this can be achieved for all DIMT models.

5.2 The type I model

Let us begin by noting that not all mathematically equivalent representations in quantum
theory are suitable for addressing the issue of time. (For details, see, e.g., the article
by Ashtekar in [23].) For the free relativistic particle, for example, time is explicit in
the position representation; the quantum constraint equation, \( \eta^{ab} \nabla_a \nabla_b \Phi(x) = 0 \) can be
immediately interpreted as the evolution equation. In the momentum representation, by
contrast, the constraint equation \( \eta^{ab} \hat{p}_a \hat{p}_b \Phi(p) = 0 \), does not have the form of an evolution
equation at all. Not surprisingly, the situation is the same in DIMT models. This is why
the use of the momentum representation led to a frozen formalism in section 4.

In the type I model, the minimum change necessary is to consider, in the very begin-
ning, wave functions which depend not on \( p_A \) but rather on \((p_\pm, \beta^0)\). (Alternatively, we
can use the three \( \beta^A \) as arguments of the wave functions; the essential point is only that

\[\text{For a review of other approaches to the problem of time in quantum gravity see [22].}\]
the representation be diagonal in \( \beta^0 \).) Then, the quantum constraint equation becomes:

\[- i \hbar \partial_0 \Phi(p_\pm, \beta^0) = \sqrt{\hat{p}^2_+ + \hat{p}^2_-} \cdot \Phi(p_\pm, \beta^0) , \tag{29}\]

where \( \partial_0 = \partial/\partial \beta^0 \). Note that we have also incorporated the non-holonomic constraint \( p_0 \geq 0 \). (See also footnote 1.) This equation is easy to integrate:

\[\Phi(p_\pm, \beta^0) = (\exp(\frac{i}{\hbar} \sqrt{\hat{p}^2_+ + \hat{p}^2_-} \beta^0)) \cdot \phi(p_\pm) \tag{30}\]

Denote as before the space of these states by \( \mathcal{V}_\text{sol} \). Physical states will be normalizable elements of \( \mathcal{V}_\text{sol} \).

The six operators \((\hat{p}_A, \hat{v}_A)\) of section 4.3 continue to provide a complete set of Dirac observables. On the space of solutions (31), their explicit expressions reduce to: \( \hat{p}_\pm \circ \phi = p_\pm \cdot \phi; \hat{v}_0 \circ \phi = \sqrt{\hat{p}^2_+ + \hat{p}^2_-} \cdot \phi; \hat{v}_\pm \circ \phi = i \hbar \sqrt{\hat{p}^2_+ + \hat{p}^2_-} \cdot \partial_\pm \phi \); and, \( \hat{v}_0 \circ \phi = i \hbar (\partial_+ - \partial_-) \phi \), where \( \partial_\pm = \partial/\partial p_\pm \). Once again, we can use the “reality conditions” to arrive at the inner product. We begin with a general measure \( \tilde{\mu}(p_\pm, \beta^0) \) on the domain space of the solutions \( \Phi(p_\pm, \beta^0) \) to (29), write the inner product as

\[\langle \Psi(p_\pm, \beta^0) | \Phi(p_\pm, \beta^0) \rangle = \int \tilde{\mu}(p_\pm, \beta^0) \, dp_\pm \wedge dp_- \, \Psi(p_\pm, \beta^0) \Phi(p_\pm, \beta^0) , \tag{31}\]

and constrain the measure by requiring that the six Dirac observables be self-adjoint with respect to this inner product. This condition restricts the measure to have the form \( \tilde{\mu}(p_\pm, \beta^0) = \mu(\beta^0)/\sqrt{\hat{p}^2_+ + \hat{p}^2_-} \); the dependence on \( p_\pm \) is completely determined while that on \( \beta^0 \) is left unconstrained. Thus, the inner-product compatible with the reality conditions must have the form:

\[\langle \Psi(p_\pm, \beta^0) | \Phi(p_\pm, \beta^0) \rangle = \int \frac{\mu(\beta^0)}{\sqrt{\hat{p}^2_+ + \hat{p}^2_-}} (dp_\pm \wedge dp_-) \, \Psi(p_\pm, \beta^0) \, \Phi(p_\pm, \beta^0) \]

\[= K \int_{\beta^0=\text{const}} \frac{dp_+ \wedge dp_-}{\sqrt{\hat{p}^2_+ + \hat{p}^2_-}} \, \Psi(p_\pm, \beta^0) \, \Phi(p_\pm, \beta^0) \tag{32}\]

\[= K \int_{\beta^0=\text{const}} \frac{dp_+ \wedge dp_-}{\sqrt{\hat{p}^2_+ + \hat{p}^2_-}} \, \tilde{\psi}(p_\pm) \, \phi(p_\pm) , \]

where we have used the constraint equation (23) in the passage to the second step and where \( K = \int d\beta^0 \mu(\beta^0) \) is the total measure of the \( \beta^0 \) line with respect to \( \mu(\beta^0) \). Note that because of the constraint equation, the final integral is independent of the value of \( \beta^0 \) at which the integral is evaluated and has the same form as in the frozen formalism of section 4. However, we did not have to deparametrize the theory (in the sense of [12]) and slice the configuration space with \( \beta^0 = \text{const.} \) slices in order to arrive at these expressions of the inner product. We began with a general measure on the 3-dimensional domain space and used the reality conditions on Dirac observables to conclude that the inner product must have the form given above. For simplicity, from now on we will assume that \( \mu(\beta^0) \) is chosen so that the constant \( K \) is normalized to unity.
Our next task is to introduce “time dependent Dirac observables.” Let us begin with the anisotropies $\beta^A$. Clearly, as they stand, $\beta^A$ themselves are not Dirac observables since they do not commute (even weakly) with the constraint; if $\Phi$ is a physical state, $\beta^A \circ \Phi$ is not. However, using the fact that the physical states satisfy $(29)$, we can construct a one-parameter family of Dirac operators $\hat{\beta}^A(t)$, parametrized by a real parameter $t$. To see this, let us begin by noting that, because of $(29)$, every physical state $\Phi(p_\pm, \beta^0)$ is completely determined by its value on a $\beta^0 = \text{const}$ surface. Hence, we can define the operators $\hat{\beta}^A(t)$ as follows: To act on a physical state $\Phi(p_\pm, \beta^0)$, freeze it on the surface $\beta^0 = t$, act on it by the operators $\hat{\beta}^A$ and evolve the resulting function to all values of $\beta^0$ using the constraint equation $(29)$. (Here, the action of $\hat{\beta}^A$ on the “frozen” states is the obvious one: $\hat{\beta}^0 \circ \Phi(p_\pm, \beta^0 = t) = t \cdot \Phi(p_\pm, \beta^0 = t)$ and $\hat{\beta}^\pm \circ \Phi(p_\pm, \beta^0 = t) = i\hbar \partial_\pm \Phi(p_\pm, \beta^0 = t)$.) By construction, the state $\hat{\beta}^A(t) \circ \Phi$ satisfies $(29)$ and is thus again a physical state. The explicit expression of these operators is given by:

$$\hat{\beta}^A(t) \circ \Phi(p_\pm, \beta^0) := e^{i\hat{H}(\beta^0 - t)} \circ \hat{\beta}^A \circ \Phi(p_\pm, \beta^0 = t) ,$$

where we have set $\hat{H} = (1/\hbar)\sqrt{\left(\hat{P}_+^2 + \hat{P}_-^2\right)}$. It is straightforward to check explicitly that for each real number $t$, the operators $\hat{\beta}^A(t)$ commute weakly with the scalar constraint. (For details, see e.g. the analogous construction for the nonrelativistic parametrized particle in [1, §6.2].)

Note that $\hat{\beta}^0(t)$ is just a multiple of identity, $\hat{\beta}^0(t) \circ \Phi = t \Phi$, and therefore commutes with every other operator. In each classical solution, $\beta^0$ increases monotonically in time and can be taken to be an internal time parameter. The expression of $\hat{\beta}^0(t)$ therefore suggests that it is natural to interpret the parameter $t$ as a generalized time in quantum theory. The parameter $t$ of course does not refer to any specific space-time, whence the adjective “generalized.” However, on semi-classical states an approximate space-time interpretation is possible. Note finally that in the classical theory, the volume $V$ of the spatially homogeneous slice is given by $V = \exp 3\beta^0$. Therefore, in quantum theory, the 1-parameter family of Dirac observables $\hat{V}(t) := \exp 3\hat{\beta}^0(t)$ represents the “volume operator at time $t$.” Its action on physical states is $\hat{V}(t) \circ \Phi = \exp (3t) \cdot \Phi$. Thus, the volume observable increases monotonically in time also on the quantum physical sector.

As in the classical theory, the anisotropies $\beta^\pm(t)$ are the two genuine dynamical quantities. Given any two physical states $\Phi, \Psi$, one can study the dependence on the parameter $t$ of the transition amplitudes $\langle \Phi | \hat{\beta}^\pm(t) \circ \Psi \rangle$. In particular, for $\Phi = \Psi$ this tells us how the expected quantum anisotropies evolve in that state. One can similarly introduce the time dependent Dirac observables $\hat{\rho}_A(t)$. However, since $\hat{\rho}_\pm$ commute with $\hat{H}$, $\hat{\rho}_\pm(t)$ turn out not to depend on the parameter value $t$. Furthermore, from $(29)$ it follows that $\hat{\rho}_0 = (\hat{p}_+^2 + \hat{p}_-^2)^{1/2}$. Thus, as far as the momentum operators are concerned, the procedure of $(33)$ just leads us back, as one might expect, to the Dirac observables introduced in section 4.3. Given any instant $t_0$ of time, we now have a complete set of Dirac observables $(\hat{\beta}^\pm(t_0), \hat{\rho}_\pm(t_0))$. These satisfy the canonical commutation relations. However, since $\hat{\beta}^0(t_0) = t_0 \mathbf{1}$ is just a multiple of identity and $\hat{\rho}_0(t)$ is algebraically related to $\hat{\rho}_\pm$, the commutators involving $\hat{\beta}^0(t_0)$ and $\hat{\rho}_0(t)$ do not mirror the corresponding Poisson brackets on the unconstrained phase space. Finally, given a general classical observable, $F(\beta^\pm, p_\pm)$, ...
one can construct the corresponding one parameter families \( \hat{F}(\beta^\pm,p_\pm)(t) \) of Dirac operators and study their dependence on the (generalized) time parameter \( t \) as follows:

\[
(\hat{F}(\beta^A,p_A)(t) \circ \Phi)(\beta^0,p_\pm) := e^{i\hat{H}(\beta^0-t)} \circ F(\hat{\beta}^A,\hat{p}_A) \circ \Phi(p_\pm,\beta^0 = t) .
\]

In practice of course one often encounters difficult factor ordering problems in this procedure. Conceptually and technically, however, these are on the same footing as the analogous problems encountered already in non-relativistic quantum mechanics where there are no constraints and no problem of time.

Of particular interest to us is the Weyl curvature scalar \( W := C_{abcd}C^{abcd} \). This quantity diverges at the singularity which occurs at \( \beta^0 = -\infty \) in all non-flat classical solutions. What is the situation in the quantum theory? Do these singularities persist or do they get washed away due to “quantum fuzzing”? Since the time evolution of \( \Phi \) is unitary with respect to the inner product \( \langle \beta \rangle \), one might at first expect that the quantum evolution is free of singularities. To see if this is the case, let us construct the 1-parameter family of Dirac observables \( \hat{W}(t) \) and examine their dependence on the parameter \( t \). A simple calculation using (34) yields:

\[
\hat{W}(t) \circ \Phi(p_\pm,\beta^0) = \frac{1}{32\pi} e^{i\hat{H}(\beta^0-t)} e^{-12\hat{\beta}_\perp 0}(1 + \cos 3\hat{\theta}) \circ \Phi(p_\pm,\beta^0 = t) .
\]

\[
= \frac{1}{32\pi} e^{-12t\hat{\beta}^0 0}(1 + \cos 3\hat{\theta}) \circ \Phi(p_\pm,\beta^0) ,
\]

where \( \tan \hat{\theta} = (\hat{p}_- / \hat{p}_+) \) and \( \hat{p}_0^2 = (\hat{p}_-^2 + \hat{p}_+^2) \). Thus, as \( t \) tends to \(-\infty \), \( \hat{W}(t) \circ \Phi \) diverges on every normalizable state\(^7\). Alternatively, it is easy to check that \( \hat{V}(t)^4 \hat{W}(t) \) is a time independent Dirac observable. (There is no factor ordering ambiguity in this product.) From its definition, it follows trivially that as the parameter \( t \) goes to \(-\infty \), the operator \( \hat{V}(t) \) goes to zero, whence the Weyl scalar \( \hat{W}(t) \) diverges. Thus, the singularity persists inspite of the unitarity of quantum evolution. (Similar results have been obtained by Husain [24] for the Gowdy models.)

This may seem surprising at first since the mathematics of the model is the same as that of a free relativistic particle. In that case, the quantum theory is well-defined; there are no singularities. How does this difference arise? Note first that the apparent paradox exists already in the classical Hamiltonian description of the two systems; it is not quantum mechanical in origin. The difference arises because the physical interpretation associated with various mathematical symbols is different in the two cases. In particular, the analogs of anisotropies of the type I model are the position coordinates of the relativistic particle. Let us first consider the classical theory. On a generic particle trajectory, the position coordinates of the particle tend to \( \pm \infty \) as time goes to \(-\infty \). This “divergence” of course does not signal a physical pathology. Since the underlying mathematics is identical, in a generic type I solution, the anisotropies \( \beta^\pm \) also diverge as \( \beta^0 \) tends to \(-\infty \). This divergence, on the other hand, does represent a physical pathology. The spacetime geometry becomes singular whence test objects, for example, would

\(^7\)Since the set defined by \( 1 + \cos 3\theta = 0 \) is of measure zero, states with support just on this set are either indistinguishable from zero or genuinely distributional and hence not normalizable. Note also that the classical solutions corresponding to initial data in this set are (locally) flat and hence non-singular; the issue of “quantum fuzzing” is therefore irrelevant in any case for this set.

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be torn to pieces. The situation in quantum theory is completely analogous. The same mathematical results can have drastically different consequences because of differences in the physical interpretation.

Could the above result on singularities have been anticipated on general grounds? There is, for example, a viewpoint [24] that there should be a rule of “unanimity”: If generic classical solutions of the theory are singular, the singularity would persist in the quantum theory. This is indeed what we have observed in the type I model above. However, it seems difficult to arrive at such a conclusion on general grounds. Consider, for example, a particle moving in an attractive Coulomb potential, subject to the condition that its angular momentum be zero. One then has radial motion and every classical solution is singular in the sense that the potential energy, for example, diverges in a finite time interval along any dynamical trajectory. The quantum theory, on the other hand is well defined: it corresponds to the spherically symmetric sector of the Hydrogen atom problem. In particular, there is a dense subspace of the Hilbert space on which matrix elements of the potential term $1/r$ remain finite for all times. In this sense, the quantum dynamics is very different from classical dynamics.

To conclude, note that using the prescription of (34) one can also construct a 1-parameter family of Dirac observables starting from the original six Dirac observables $\hat{p}_A$ and $\hat{v}_A$. We saw above that for the three $\hat{p}_A$, the dependence on $t$ drops out. The same is true for the three $\hat{v}_A$. Thus, what distinguishes these six from a generic time dependent Dirac observable $\hat{F}(t)$ is that these six are time independent. To obtain the inner product via reality conditions, it suffices to work with a complete set of Dirac observables which may be time independent. If one can find such a set, deparametrization is not needed to find the inner product on the physical states. However, even in this case, to extract the dynamical content of the theory in the usual sense, we need access to generic time dependent Dirac observables.

### 5.3 The type II model

The general line of argument in the type II case is the same as the one given above: One introduces wavefunctions $\Phi(\tilde{\beta}^0, \tilde{p}_\pm)$; writes out the constraint as an evolution equation of the form (29); shows that the reality conditions lead one to the same inner product as in section 4.2; and, introduces the time-dependent Dirac observables analogous to (34). The only technical difference is that $\hat{p}_+$ is now restricted to take on just positive values.

The one parameter family $\hat{\tilde{\beta}}^0(t)$ corresponding to the classical variable $\tilde{\beta}^0$ is again $t$ times the identity operator on physical states. Since $\tilde{\beta}^0$ can be interpreted as time in the classical Hamiltonian description, the parameter $t$ in the expressions of Dirac operators can be again interpreted as (generalized) time in the quantum theory. What is the relation between this time and the spatial volume $V$? Note that $V$ is still given by $\exp 3\beta^0$ where $\beta^0$ is the original Misner variable. Since we performed a non-trivial canonical transformation

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8See also [2] §6.4, where however the reduced space quantum theory is used and the deparametrization is carried out classically. This approach yields the correct result for simple systems such as the type I model now under consideration. In more general situations, however, one must use a genuinely quantum mechanical deparametrization, e.g., using (34).
to arrive at the tilde variables, the phase space time variable \( \tilde{\beta}^0 \) (and hence the quantum time variable \( t \)) is no longer simply related to the spatial volume. Indeed, the volume is a rather complicated function of the tilde canonical variables,

\[
V^2 = \exp 6\tilde{\beta}^0 = \exp(4\sqrt{3}\tilde{\beta}^0 + 2\sqrt{3}\tilde{\beta}^+) = \sqrt{6}(\exp 4\sqrt{3}\tilde{\beta}^0)\cosh(2\sqrt{3}\tilde{\beta}^+) / \tilde{p}_+ ,
\]

and depends in particular on the momentum variable \( \tilde{p}_\pm \) as well. Nonetheless, the qualitative behavior of \( V^2 \) is similar to that in the type I model. To see this, note first that along classical dynamical trajectories, we have: \( \tilde{p}_\pm = \text{const} \), and \( \tilde{\beta}^\pm = b^\pm - \tilde{p}_\pm \tilde{\beta}^0 / \sqrt{\tilde{p}_+^2 + \tilde{p}_-^2} \), where the constants \( b_\pm \) vary from one trajectory to another. It therefore follows that the volume is again a monotonically increasing function of the “time parameter” \( \tilde{\beta}^0 \). Furthermore, as \( \tilde{\beta}^0 \) tends to \( -\infty \), the volume goes to zero. Finally, in quantum theory, it is straightforward to compute the (time-dependent) 1-parameter family of Dirac observables \( V^2(t) \):

\[
\hat{V}^2(t) = \sqrt{6}e^{4\sqrt{3}t} \cdot e^{i\hat{H}(\tilde{\beta}^0 - t)} \circ (1/2) \left( 1/\tilde{p}_+ \right) \left( \cosh(2\sqrt{3}\tilde{\beta}^+) + \cosh(2\sqrt{3}\tilde{\beta}^+) \right),
\]

where we have chosen the symmetric factor ordering and both sides act on states \( \Phi(\tilde{\beta}^0, \tilde{p}_\pm) \), and where, as is the case for Bianchi type I, the Hamiltonian operator is the “free particle” Hamiltonian:

\[
\hat{\tilde{H}} = \frac{1}{\hbar}\sqrt{\tilde{p}_+^2 + \tilde{p}_-^2}.
\]

While the expression of the resulting operators is complicated, they are all well-defined. One finds again that, in the limit as \( t \) goes to \( -\infty \), the volume operator tends to zero.

To discuss the issue of singularities, we can, as before, analyse the behavior of the Weyl scalar \( W = C_{abcd} C^{abcd} \). As with the volume, the explicit expression is rather complicated:

\[
W = \frac{e^{-8\sqrt{3}\tilde{\beta}^0}}{6 \cdot 18 \cdot 24} \left\{ 6\tilde{p}_+^4 (3\tilde{p}_+^2 + 2\tilde{p}_-^2)(\cosh 2\sqrt{3}\tilde{\beta}^+)^{-2} + 18\tilde{p}_0 \tilde{p}_+^3 \cosh 2\sqrt{3}\tilde{\beta}^+)^{-3} \sinh(2\sqrt{3}\tilde{\beta}^+) - 3\tilde{p}_+^4 (53\tilde{p}_+^2 + 12\tilde{p}_-^2)(\cosh 2\sqrt{3}\tilde{\beta}^+)^{-4} + 108\tilde{p}_0 \tilde{p}_+^5 (\cosh 2\sqrt{3}\tilde{\beta}^+)^{-5} \sinh(2\sqrt{3}\tilde{\beta}^+) + 172\tilde{p}_+^6 (\cosh 2\sqrt{3}\tilde{\beta}^+)^{-6} \right\}
\]

\[
= \frac{e^{-8\sqrt{3}\tilde{\beta}^0}}{6 \cdot 18 \cdot 24} \sum_{i=1}^{5} Q_i(\tilde{p}_0, \tilde{p}_+, \tilde{p}_-) T_i(\tilde{\beta}^+),
\]

where \( Q_i \) are (low order) polynomials of their arguments and the \( T_i \) are hyperbolic trigonometric functions. Along classical trajectories, as \( \tilde{\beta}^0 \) goes to \( -\infty \), \( W \) diverges at least as fast as \( \exp(-4\sqrt{3}\tilde{\beta}^0) \). This is the initial singularity in the classical theory. In the quantum theory, one can again construct the 1-parameter family of Dirac observables \( \hat{W}(t) \) by using (34) and choosing the symmetric factor-ordering:

\[
\hat{W}(t) = \frac{e^{-8\sqrt{3}t}}{6 \cdot 18 \cdot 24} e^{i\hat{H}(\tilde{\beta}^0 - t)} \circ (1/2) \sum_{i=1}^{5} \left( Q_i(\tilde{p}_A) \circ T_i(\tilde{\beta}^+) + T_i(\tilde{\beta}^+) \circ Q_i(\tilde{p}_A) \right) \circ e^{-i\hat{H}(\tilde{\beta}^0 - t)}.
\]
The resulting operator $\hat{W}(t)$ again has the property that $\hat{W}(t) \circ \Phi$ diverges for all states in the physical Hilbert space as $t$ tends to $-\infty$. (For explicit computations, it is convenient to use the representation in which the three $\tilde{\beta}^A$ – rather than $(\tilde{p}_+, \tilde{\beta}^0)$ – are diagonal.) This can be seen also by considering, as for Bianchi type I, the behaviour of the operator corresponding to $V^4(t)\hat{W}(t)$. Similar considerations hold for the rest of the DIMT models.

Thus, the curvature singularity persists in quantum theory for all DIMT models.

To conclude this discussion, we point out how this notion of time can be used to construct a meaningful measurement theory. In the quantum mechanics of closed systems, such as the ones we are considering, to discuss issues such as measurements, conditions under which states decohere and behave semi-classically, and to make concrete physical predictions, one generally begins with the notion of exhaustive sets of mutually exclusive alternatives [26]. For the models under consideration, to obtain such sets we can foliate the domain space of physical states by constant $\beta^0$ (in type I and $\tilde{\beta}^0$ in type II) slices. On a slice $\beta^0 = t_0$, a complete set of alternatives can then be constructed, e.g., using any one complete commuting set of (time dependent) Dirac observables corresponding to that instant of time, $t = t_0$. We can construct histories of physical interest – e.g., states which at time $t_1$ have anisotropies (which essentially represent the 3-metric) in a specified range and which at time $t_2$ have momenta (essentially the extrinsic curvatures) in another specified range, etc. Note also that, unlike in the path integral method, we are not tying ourselves down to a specific configuration space: We can easily switch from one representation to another, because we have full recourse to the Dirac transformation theory. Hence, in this approach, we can incorporate a large number of histories which cannot even be considered in the standard path integral approaches.

Note however that we chose, right in the beginning, a preferred deparametrization which is suggested by the form the constraint assumed after the canonical transformation. What if some one makes another choice? Is there a generalized “transformation theory” associated with such changes? As far as we are aware, one does not even know how to phrase this question precisely in full generality. One can make simple changes. For example, after the canonical transformation to the tilde variables, the constraint took on the same form as that encountered in the treatment of a free relativistic particle in Minkowski space (with, in some models, the non-holonomic constraint $\tilde{p}_+ > 0$.) Therefore, we could have made a “Lorentz transformation” in the $\tilde{\beta}^A$ space and used another choice of time with respect to which the constraint would again have been of the form (29). It is easy to see that the resulting description would have been equivalent to the one given here (provided the appropriate non-holonomic constraint is again imposed in the quantum theory). What, however, if one made a completely different choice of time with respect to which the constraint is again of the desired form? This is the question that is wide open and should become a focus of discussion on the issue of time. The main problem is that we have rather limited understanding of all the choices which render the constraint in the desired form, whence it is difficult to make even a precise conjecture relating the many resulting quantum descriptions.

For the Bianchi type II model, however, the Hamiltonian framework of section 3.1 (see (11)) does present us with another deparametrization which is non-trivially related to the one used in this section. Therefore, at least in this one case, we can raise the question of
equivalence. This is the topic of discussion of the next section.

6 Different Quantization Strategies: Comparison

In this section, we will restrict ourselves to the type II model. In this case, already in the original variables \((\bar{\beta}^A, \bar{\rho}_A)\), prior to the canonical transformation, the scalar constraint admits a conditional symmetry \([10]\). That is, the configuration space, spanned by the three \(\bar{\beta}^A\), admits a vector field \(-\partial/\partial \bar{\beta}^0\) which is a time-like Killing field of the supermetric, along the integral curves of which the potential term in the constraint is constant. In the first subsection, we outline the quantum theory \([11]\) that results directly by using this symmetry to decompose solutions to the constraint into positive and negative frequency parts. A priori, it is not clear that this quantum theory is equivalent to that presented in section 4 since the canonical transformation to the tilde variables mixes coordinates and momenta. (In the language of geometric quantization, the two methods use different polarizations already at the kinematic level, before the imposition of the constraint.) Furthermore, the two approaches adopt quite different techniques to single out the inner product on the space of quantum states. In the second subsection, we show that the two descriptions are in fact equivalent in an appropriate sense.

In each case, one can deparametrize the theory. On the classical phase space, the deparametrizations are equivalent since the canonical transformation leaves \((\bar{\beta}^0, \bar{\rho}_0)\) unaffected; \(\bar{\beta}^0 = \bar{\beta}^0\). In the quantum theory, however, the deparametrizations are not obviously equivalent since the domain spaces of physical states are quite different in the two cases due to the non-triviality of the canonical transformation. Nonetheless, we will see that equivalence does hold in an appropriate sense.

The final result holds also for the type I model. However, in this case, the equivalence is hardly surprising: the barred canonical variables are just linear combinations of the unbarred (or the tilde) variables since the canonical transformation is now trivial.

6.1 Conditional symmetries

Recall from section 3 that, in the type II model, the scalar constraint in the barred variables is given by:

\[
\frac{1}{2} \eta^{AB} \bar{p}_A \bar{p}_B + 6 \exp(-4\sqrt{3}\bar{\beta}^+) = 0. \tag{41}
\]

Consequently, the time-like (with respect to \(\eta^{AB}\)) vector field \(\partial/\partial \bar{\beta}^0\) on the configuration space spanned by the three \(\bar{\beta}^A\) defines a momentum variable \(\bar{\rho}_0\) in the phase space, which Poisson-commutes with the scalar constraint. Hence, the canonical transformation generated by \(\bar{\rho}_0\) is a classical symmetry and \(\partial/\partial \bar{\beta}^0\) is a conditional symmetry in the sense of \([10]\). Therefore, we can forego the construction of a complete set of Dirac observables and the rest of the steps in the quantization program \([1, 4]\) which we used in section 4 and carry out quantization by an entirely different route \([12, 24, 28]\). The idea here is as follows. Consider the vector space \(\bar{V}_{\text{sol}}\) of solutions to the quantum constraint

\[
\eta^{AB} \bar{\delta}_A \bar{\delta}_B \Phi(\bar{\beta}) + 12 \exp(-4\sqrt{3}\bar{\beta}^+) \cdot \Phi(\bar{\beta}) = 0. \tag{42}
\]
To equip $\vec{V}_{\text{sol}}$ with an appropriate Hilbert space structure, we can use the conditional symmetry. The 1-parameter group of diffeomorphisms generated by $\partial/\partial \bar{\beta}_0$ has a well-defined action on the space of solutions to (12). We can therefore seek a Hermitian inner product on $\vec{V}_{\text{sol}}$ such that this action is unitary; i.e., such that the classical symmetry is promoted to the quantum theory.

The final result [11] can be summarized as follows. The Hilbert space consists of normalizable solutions to the positive frequency part of the quantum constraint (42), i.e., to the equation:

$$
-i\hbar \bar{\partial}_0 \Phi(\bar{\beta}^\pm, \bar{\beta}^0) = + \left(-\hbar^2 \bar{\partial}_+^2 - \hbar^2 \bar{\partial}_-^2 + 12(\exp(-4\sqrt{3}\bar{\beta}^+))^{\frac{1}{2}} \circ \Phi(\bar{\beta}^\pm, \bar{\beta}^0) \right)
\equiv \Theta^{\frac{1}{2}} \circ \Phi(\bar{\beta}^\pm, \bar{\beta}^0),
$$

(43)

where the choice of plus sign in the square-root ensures the positivity of frequency and where, for notational simplicity, we have omitted bars on the subscripts of the derivative operators. The physical inner product is given by:

$$
\langle \Psi | \Phi \rangle = \int_{\bar{\beta}^0 = k} \, d\bar{\beta}^+ \wedge d\bar{\beta}^- \, \Psi \Phi,
$$

(44)

where $k$ is a constant, the integral on the right side being independent of the choice of $k$. Denote the Hilbert space by $\mathcal{H}$. It is obvious that the operator $-i\hbar \bar{\partial}_0 \equiv \sqrt{3}$ generating the conditional symmetry is self adjoint on $\mathcal{H}$, whence the symmetry is unitarily implemented. The symmetry thus provides us with a Hilbert space structure on the space of physical states. To compare this structure with that obtained in section 4.2, it is convenient to note that the general solution to (13) is of the form

$$
\Phi(\bar{\beta}^\pm, \bar{\beta}^0) = (\exp \left( \frac{i}{\hbar} \Theta^{\frac{1}{2}} \bar{\beta}^0 \right) \circ \phi(\bar{\beta}^\pm)
$$

(45)

where $\phi(\bar{\beta}^\pm)$ is in $L^2(R^2, d\bar{\beta}^+ \wedge d\bar{\beta}^-)$. There is thus a natural isomorphism between the Hilbert space $\mathcal{H}$ of physical states $\Phi(\bar{\beta}^\pm, \bar{\beta}^0)$ and the Hilbert space $\mathcal{H}_0$ of square-integrable (with respect to measure 1) functions $\phi(\bar{\beta}^\pm)$. In section 4.2, we found that the Bianchi II model admits four time-independent Dirac observables: $\tilde{p}_\pm$ and $\tilde{v}_\pm$. Can we express the corresponding operators on the barred Hilbert space? Using the definition of the canonical transformation which took us to the tilde variables, it is straightforward to express the quantum analogs of three of these observables as operators on the Hilbert space $\mathcal{H}_0$. We have:

$$
\begin{align*}
\hat{\tilde{p}}_+ \circ \phi(\bar{\beta}^\pm) &= (\hat{\tilde{p}}_+^2 + 12 \exp(-4\sqrt{3}\hat{\beta}^+))^{\frac{1}{2}} \circ \phi(\bar{\beta}^\pm), \\
\hat{\tilde{p}}_- \circ \phi(\bar{\beta}^\pm) &= -i\hbar \hat{\partial}_- \phi(\bar{\beta}^\pm), \quad \text{and}, \\
\hat{\tilde{v}}_- \circ \phi(\bar{\beta}^\pm) &= \bar{\beta}^- \cdot \phi(\bar{\beta}^\pm).
\end{align*}
$$

(46)

We will use the Hilbert space $\mathcal{H}_0$ and these three operators thereon in the next subsection. The fourth Dirac observable, $\hat{\tilde{v}}_+$, on the other hand, seems difficult to express as an operator on the barred Hilbert spaces. Its classical analog is $(\tilde{p}_+^2, \tilde{p}_0) / \tilde{p}_0$ and, because of the non-triviality of the canonical transformation from $(\bar{\beta}^+, \bar{p}_+)$ to $(\bar{\beta}^+, \tilde{p}_+)$,
its expression in the barred variables is quite complicated, involving not only square-roots but also logarithms of polynomials in $\tilde{\beta}^+$ and $\tilde{p}_+$. Consequently one encounters severe factor ordering ambiguities in the passage to quantum theory. In this sense then we do not have access to a full set of time independent Dirac observables on the barred Hilbert spaces. In this sense, the quantum theory based on conditional symmetries is not as complete as that constructed in section 4.

6.2 Comparison: Time independent Dirac observables

We now wish to compare the quantum theory obtained in the previous subsection with that obtained in section 4.2. In the quantum description just constructed, the Hilbert space $\mathcal{H}$ is the space of normalizable positive frequency solutions to a Klein-Gordon equation with a static potential, while the Hilbert space $\mathcal{H}$ of section 4 is the space of functions on the right half $L^R_+$ of the null cone in momentum space. One's first impulse may be to conclude that $\mathcal{H}$ is twice as large as $\mathcal{H}$ since there is now no trace of the (non-holonomic) constraint that led us to the half cone. We will show that this conclusion is incorrect.

It is convenient for this purpose to recast the mathematical framework of section 4.2 by emphasizing the role of wave functions $\phi(\tilde{p}_\pm)$ over those of solutions $\Phi(\tilde{p}_\pm, \tilde{p}_0)$ to the quantum constraint. (See Eq. (20).) The Hilbert space $\mathcal{H}_0$ of physical states is then $L^2(R^2, \frac{dp_x dp_y}{\tilde{p}_+})$. The four time independent Dirac operators have the following action on $\mathcal{H}_0$:

$$
\begin{align*}
\hat{p}_+ \circ \psi(\tilde{p}_\pm) &= \tilde{p}_+ \cdot \psi(\tilde{p}_\pm), & \hat{p}_- \circ \psi(\tilde{p}_\pm) &= \tilde{p}_- \cdot \psi(\tilde{p}_\pm) \\
\hat{v}_+ \circ \psi(\tilde{p}_\pm) &= i\hbar \tilde{p}_+ \partial_+ \psi(\tilde{p}_\pm), & \hat{v}_- \circ \psi(\tilde{p}_\pm) &= i\hbar \partial_- \psi(\tilde{p}_\pm),
\end{align*}
$$

and they provide us with a complete set of quantum observables. To relate the two quantum theories, we wish to ask if there is a unitary map from the Hilbert space $\mathcal{H}_0$ to the Hilbert space $\mathcal{H}_0$ introduced in section 6.1, which interacts in the correct way with these observables.

To set up such a map, it is easiest to first find in each space a set of basis vectors corresponding to the same set of commuting Dirac observables. One commuting set is given by $(\tilde{p}_+, \tilde{p}_-)$. Since the corresponding operators act simply by multiplication on $\mathcal{H}_0$, the spectra are trivial to compute on this Hilbert space: both operators have a purely continuum spectrum, that of $\tilde{p}_+$ is given by $(0, \infty)$ while that of $\tilde{p}_-$ is given by $(-\infty, \infty)$. Thus, a simultaneous eigenstate $|\tilde{p}_+, \tilde{p}_-\rangle$ of the two operators is labelled only by the two real numbers, $\tilde{p}_+$ being restricted to be positive; there is no further degeneracy. The form of the inner product on $\mathcal{H}_0$ suggests that we normalize these eigenvectors such that:

$$
\langle \tilde{p}_+, \tilde{p}_- \mid \tilde{p}_+', \tilde{p}_-' \rangle = \tilde{p}_+ \delta(\tilde{p}_+, \tilde{p}_+) \delta(\tilde{p}_-, \tilde{p}_-).
$$

What is the situation with $\mathcal{H}_0$? Since $\tilde{p}_- \equiv \tilde{p}_-$, the operator $\hat{\tilde{p}}_-$ corresponding to $\tilde{p}_-$ is simply $-i\hbar \partial_-$, whose spectrum is continuous with values in the full range $(-\infty, \infty)$. The operator $\hat{\tilde{p}}_+$ is more complicated. The canonical transformation defining the tilde variables yields:

$$
\tilde{p}_+^2 = \tilde{p}_+^2 + 12 \exp(-4\sqrt{3}\tilde{\beta}^+).
$$

Since the “potential” is positive and goes to zero as $\tilde{\beta}^+$ goes to infinity, the spectrum of the operator $\tilde{p}_+^2$ is continuous and takes all values between $(0, \infty)$. The key question is whether
the spectrum is degenerate. If so, the spectrum of its positive square root, \( \hat{p}_+ \), would also be degenerate, and the two quantum descriptions would be inequivalent. There is a standard textbook argument (see, e.g., [29]) which establishes the non-degeneracy of the spectra of Hamiltonians in 1-dimensional potential problems of non-relativistic quantum mechanics. With a small extension to accommodate the fact that the “potential” does not go to zero (in fact diverges) as \( \beta^+ \) tends to \(-\infty\), this argument ensures that the spectrum of \( \hat{p}_+^2 \), and hence also that of \( \hat{p}_+ \), is non-degenerate. (This is in sharp contrast to the spectrum of \( \hat{p}_-^2 = -\hbar^2 \hat{p}_-^2 \) which is obviously 2-fold degenerate; the key difference in the two cases is the presence of the potential term in (48)). Thus, on the Hilbert space \( \mathcal{H}_0 \) as well, the kets \(| \tilde{p}_+ \rangle, | \tilde{p}_- \rangle \) provide us with a complete basis, which we choose to be normalized such that \(| \tilde{p}_+ \rangle, | \tilde{p}_- \rangle \rangle = \hat{p}_+ \delta(\tilde{p}_+, \tilde{p}_+) \delta(\tilde{p}_-, \tilde{p}_-) \). Since the operator \( \hat{p}_- \) has the action \( \hat{p}_- \phi = -i\hbar \partial_- \phi \), the simultaneous eigenfunctions of \( \hat{p}_\pm \) have the functional form: \(| \tilde{\beta}^+, \tilde{\beta}^- | \rangle = (1/\sqrt{2\pi}) \langle \exp \frac{i}{\hbar} \tilde{\beta}^- \hat{p}_- \rangle f_{\tilde{p}_+}(\tilde{\beta}^+) \), where \( f_{\tilde{p}_+}(\tilde{\beta}^+) \) are the suitably normalized eigenfunctions of the operator \( \hat{p}_+ \).

We can now set up the required isomorphism \( U : \mathcal{H}_0 \mapsto \tilde{\mathcal{H}}_0 \):

\[
(U \circ \phi)(\tilde{p}_\pm) := \frac{1}{\sqrt{2\pi}} \int d\tilde{\beta}^+ d\tilde{\beta}^- \langle \exp \frac{i}{\hbar} \tilde{\beta}^- \hat{p}_- \rangle f_{\tilde{p}_+}(\tilde{\beta}^+) \phi(\tilde{\beta}^+) .
\]

It is straightforward to check that \( U \) commutes with the action of the three time independent Dirac operators, \( \hat{p}_+, \hat{p}_-, \hat{v}_- \) which are independently defined on the two Hilbert spaces \( \mathcal{H}_0 \) and \( \tilde{\mathcal{H}}_0 \). So far, the fourth time independent Dirac operator \( \hat{v}_+ \) is defined only on \( \mathcal{H}_0 \): We saw in section 6.1 that, if one tries to define it on \( \mathcal{H}_0 \) directly by using the barred operators, one faces severe factor ordering problems. However, now that we have the map \( U \), we can use it to pull \( \hat{v}_+ \) back to \( \mathcal{H}_0 \) from \( \tilde{\mathcal{H}}_0 \) and simply use the resulting operator \( U \circ \hat{v}_+ \circ U^{-1} \) as the fourth Dirac observable in the barred quantum theory. (This procedure may be regarded as a solution to the factor ordering problem.) By construction, then, all four Dirac operators on \( \mathcal{H}_0 \) have the “correct” commutation relations among themselves. When this is done, both the tilde and the barred descriptions are equipped with a complete set of observables and \( U \) provides the isomorphism between them. In this sense, the two quantum theories are equivalent[9].

### 6.3 Deparametrization

We saw in the previous two subsections that the barred description, by itself, is not as complete as the tilde description since we have direct access only to three of the four time independent Dirac observables. Nonetheless, because the scalar constraint could be recast as a Schrödinger evolution equation (43), we can still deparametrize the theory

---

[9] Note that even though we have fixed the normalization of the basis vectors, there is still the freedom to rescale each basis vector by a phase factor. The condition that the map should commute with the action of the third Dirac observable \( \hat{v}_- \) restricts the phase factor to depend on \( \hat{p}_+ \) only. Thus, the map \( U \) is unique only up to \( U \mapsto \exp iF(\hat{p}_+) \cdot U \), for some real-valued function \( F(\hat{p}_+) \). If we change the map, the image of \( \hat{v}_+ \) on \( \mathcal{H}_0 \) will change. However, the equivalence result holds for any of these \( U \).
satisfactorily and discuss quantum dynamics. We will first expand on this observation and then relate the resulting dynamical description to the one obtained in section 5.

Let us begin with the Hilbert space $\bar{\mathcal{H}}$. The operators $\hat{\beta}_A$ and $\hat{p}_\pm$ are clearly not Dirac operators. Nonetheless, we can follow the procedure of section 5.2 to introduce time dependent Dirac operators $\hat{\beta}_A(t)$ and $\hat{p}_A(t)$. Again, $\hat{\beta}_0(t)$ is a multiple of identity and the true degrees reside in $\hat{\beta}_\pm$ and $\hat{p}_\pm$. As before, a general time dependent Dirac operator has the form:

$$\left(\hat{F}(\hat{\beta}, \hat{p}_A)(t) \circ \Phi\right)(\hat{\beta}^A) := e^{\frac{i}{\bar{\hbar}}\sqrt{\Theta}(\hat{\beta}_0 - t)} \circ F(\hat{\beta}_A, \hat{p}_A) \circ \Phi(\beta_\pm, \beta_0 = t).$$  \hspace{1cm} (50)

Thus, the situation is completely analogous to the one we encountered in section 4; this discussion of quantum dynamics is quite insensitive to whether or not one has access to a complete set of time independent Dirac operators. However, since the analog of the Hamiltonian $H$ in (34) is now $\sqrt{\Theta}/\bar{\hbar}$ and since $\Theta$ involves the complicated potential term (Eq. (43)), the explicit expressions of the resulting time dependent Dirac operators are now quite involved and explicit calculations, correspondingly harder. Nonetheless, in principle, the conditional symmetry approach provides us with the machinery needed for the construction of histories of physical interest, to phrase a variety of dynamical questions and to make physical predictions. Note also that the inner product makes each of the operators $\hat{\beta}_\pm$ and $\hat{p}_\pm$ self adjoint; classical reality conditions are incorporated properly.

Is there a sense in which this analysis of dynamics on $\bar{\mathcal{H}}$ is equivalent to that on $\tilde{\mathcal{H}}$ performed in section 5.3? Thanks to the map $U$ constructed in the previous subsection, the answer is in the affirmative. For a general operator, one must make factor ordering choices on both Hilbert spaces. If the operators are so ordered that, on the $\beta_0 = 0$ and $\tilde{\beta}_0 = 0$ slices, the two operators are related by the map $U$, i.e., $U \circ \hat{F}(t = 0) \circ U^{-1} = \hat{F}(t = 0)$, then the two sets of dynamical predictions, calculated independently on the two Hilbert spaces $\bar{\mathcal{H}}$ and $\tilde{\mathcal{H}}$ will coincide. This happens because the map $U$ sends the Hamiltonian $\hat{\tilde{H}}$ on $\tilde{\mathcal{H}}$ to the operator $\sqrt{\Theta}/\bar{\hbar}$ on $\bar{\mathcal{H}}$. In this sense, the two deparametrizations are quantum mechanically equivalent. This is interesting because the deparametrizations are not related to each other trivially. They do not correspond just to different slicings of a given domain space of wave functions. Indeed, the domain spaces are themselves different in the two cases—one is spanned by the three $\hat{\beta}_A$ and the other by the three $\tilde{\beta}_A$. Because $\hat{\beta}_A$ are mixtures of the $\tilde{\beta}_A$ and their momenta (and vice versa), there is no simple geometrical relation between the two domain spaces and hence between the two sets of slicings.

However, it is important to bear in mind that the difference in the two parametrizations is of a quite special nature. On the full phase space, $\bar{\beta}_0 = \tilde{\beta}_0$, whence the two deparametrizations (i.e., foliations of the constraint surface) agree classically. A difference arises in the quantum theory only because the two descriptions result from choosing different polarizations on the phase space. In a more general situation, one would encounter a difference in the deparametrization already at the classical level: there may exist two distinct foliations of the classical phase space and two related polarizations such that the quantum constraint reduces to the Schrödinger form with respect to each of them. It would be extremely valuable to construct and analyse such an example.
7 Discussion

The four main results of this paper are contained in the four sections, 3-6: existence of canonical transformations which removes the potential term in the dynamical constraint; completion of the quantization program of [1,4]; extraction of dynamics from a frozen formalism; and, comparison between two distinct quantization procedures. Their content and ramifications can be summarized as follows.

First, for a fairly large class of spatially homogeneous models –diagonal, intrinsically multiply transitive ones– we exhibited in section 3 a canonical transformation which removes the “potential” term in the scalar or the Hamiltonian constraint of geometrodynamics. In terms of the new canonical variables, then, the scalar constraint is purely quadratic in momenta. Furthermore, the supermetric turns out to be flat! What distinguishes one model from another is the global topology of the constraint surface, or, of the effective configuration space. Finally, note that in all but type I models, the scalar constraint in the ADM variables –and hence the dynamics of, say, anisotropies– is quite complicated. It is striking that by using the new canonical variables, these complications can be bypassed both classically and quantum mechanically. We effectively map an interacting problem to a free problem. The solution of the free problem is trivial and all the physics of the original problem is coded essentially in the transformation relating the two.

Indeed, we found in section 4 that using the new canonical variables, one can carry out the general quantization program of [1,4] to completion in a straightforward fashion. This exercise did, however, teach us something about the program itself. First, we could isolate a complete set of Dirac observables and, using the reality conditions, equip the space of quantum states with a unique Hermitian structure [21]. This result provides an independent check on the strategy of [1,4] for obtaining the inner product using reality conditions rather than attempting to implement symmetries unitarily. In particular, we saw that it is not necessary to “deparametrize” [12] the theory to obtain the inner product; the issue of constructing a consistent mathematical framework is thus divorced from the conceptual difficulties associated with the problem of time [13]. Second, we gained technical insight on the kind of problems that can arise if the set of observables under consideration fails to be complete even on a set of measure zero on the classical phase space. However, many interesting questions cannot be even phrased purely in terms of the Dirac observables introduced in section 4. Indeed, since there is no notion of time, we cannot address the issue of dynamics. In section 5, we therefore recast the scalar constraint in another form, that of the Schrödinger equation. Thus, one of the arguments of the physical quantum states is now interpreted as time, with respect to which other arguments –representing the “true, dynamical” degrees of freedom– evolve. We could

\footnote{This point is important because there exist interesting constrained systems –including 2+1 dimensional general relativity on a 2-surface with genus \( \geq 2 \)– where a global deparametrization is either difficult or impossible but where the reality conditions suffice to select the inner product [1,4]. Note, however, that the general strategy does not require that the Dirac observables be time independent. If one can isolate a time and find a complete set of time dependent Dirac observables (such as anisotropies in the DIMT models), one can use them to impose the reality conditions with equal ease. This point has been misunderstood in some recent reviews of the quantization program.}
then introduce a 1-parameter family of operators, whose dependence on the parameter provided us with information about their “evolution.” For each value of the parameter, the operator weakly commutes with the constraints; it maps the physical states to other physical states and is therefore a genuine Dirac observable. In this sense, the “de-parametrization” considered here is “covariant.” In particular, a physical state is simply a solution to the quantum constraint equation rather than a restriction of the solution to a suitable “slice” in the effective configuration space. We used the newly introduced, “time-dependent Dirac observables” to analyse how anisotropies evolve and what happens to the classical singularities in the quantum theory. We found that the singularities persist; minisuperspace quantization does not remove them. Finally, one can also use this framework to construct various physically interesting histories and examine, e.g., whether they decohere. In this sense then, we have all the machinery needed in the measurement theory of closed systems [26].

The result on persistence of singularities is at first surprising. After all, dynamics is unitarily implemented by a self-adjoint Hamiltonian and there is a general belief that unitary evolution can not lead to any singularities. We would like to emphasize that this belief is simply unfounded. To see this point, let us return momentarily to the classical Hamiltonian description of, say, the Bianchi I model. In this case, one can find a globally defined, complete set of constants of motion even though almost every dynamical trajectory runs into a singularity. If we choose 4 constants of motion $K_i(β^A, p_A)$ and $β^0$ as coordinates on the constraint surface in phase space, each dynamical trajectory is given simply by $K_i = \text{(const)}_i$; there is no trace of a singularity in this form of the solution. The singularity appears when we examine how quantities like the anisotropies $β^\pm$ or curvature scalars change along the trajectories. Indeed, even as the trajectory plunges into the singularity, the values of $K_i$ remain well-defined, equal to the constants that specify the trajectory. The situation in the quantum theory is similar. Since $p_\pm$ constitute a complete set of commuting observables which commute with the Hamiltonian, dynamics is trivialized: as the wave function evolves, the absolute value of the wave function $|ψ(p_\pm, β^0)|$ remains constant and only the phase oscillates as $\exp β^0 (i\sqrt{p_\pm^2 + p_\mp^2})$. We see no trace of the singularity: The expectation values of any observables made out of $ψ(p_\pm) \text{ and } ˆv_\pm$—which together generate the entire algebra of Dirac observables—remain finite. We see the singularity only when we examine other observables, e.g., the expectation values of anisotropies or curvature scalars. We see no reason to rule out a similar circumstance in more general cases; even in the general context, singularities may persist inspite of unitarity of quantum evolution. In the DIMT models, however, the situation is more striking than what may be expected in the general context: in these cases, we could find complete sets of observables which are constants of motion and therefore remain perfectly well behaved through out the evolution, even when other, (time dependent) observables diverge —signaling a physical singularity. This is a striking illustration of the procedure of mapping a non-trivial model to a trivial one. The non-trivial physics is simply hidden; it does not go away. It can be uncovered by examining the physically interesting observables of the original model in the solution of the trivial one.

Finally, we saw in section 6 that in the type II model, a quantum theory could be
constructed following two different avenues: the quantization program of [1,4]; and the use of conditional symmetries [12,11]. The second approach is closer to traditional quantum field theories where the Hilbert space structure in the quantum theory is dictated by the presence and structure of suitable symmetries. We compared the two approaches in section 6. The framework resulting from the first approach is more complete in that we have direct access to a complete set of (time independent) Dirac observables. In the conditional symmetries approach, it appears very difficult to introduce one of these Dirac observables directly. However, if we “pull back” this last Dirac observable from the Hilbert space constructed in the first approach, the two descriptions are equivalent.

Although the models considered here are dynamically non-trivial, the existence of a multiply transitive isometry group intrinsic to each spatially homogeneous slice makes them exactly soluble. It is this solubility that lies at the heart of the canonical transformations. Therefore, the technical considerations of this paper are not likely to be useful to the discussion of full quantum gravity in 3+1 dimensions. Nonetheless, the qualitative lessons learnt here are likely to be valuable: they provide us with further confidence in the general quantization program of [1,4]; illustrate the simplifications that can be caused by judicious canonical transformations; and suggest how one can use the time dependent Dirac observables to probe dynamics in the setting of a “covariant deparametrization”, and to analyse physical issues such as the fate of singularities within the framework of canonical quantization.

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