Reduced phase space approach to Kasner universe and the problem of time in quantum theory

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Abstract
We apply the reduced phase space quantization to the Kasner universe. We construct the kinematical phase space, find solutions to the Hamilton equations of motion, identify Dirac observables and arrive at physical solutions in terms of Dirac observables and an internal clock. We obtain the physical Hilbert space, which is the carrier space of the self-adjoint representation of the Dirac observables. Then, we discuss the problem of time. We demonstrate that the inclusion of evolution in a gravitational system, at classical level as well as at quantum level, leads respectively to canonically and unitarily inequivalent theories. The example of Hubble operator in two different clock variables and with two distinct spectra is given.

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1. Introduction

The standard model of cosmology is based on the remarkably simple solution to general relativity, the Friedman–Robertson–Walker (FRW) universe. It is expected, however, that a slightly perturbed FRW universe, when evolved back in time, at some moment close enough to the big bang singularity, will lose its space-like symmetries. Therefore, in order to understand the singular conditions from which the universe emerged nearly 14 billion years ago, a study of more general cosmological spacetimes is needed.

A general solution of general relativity in the vicinity of cosmological singularity has been studied by Belinskii, Khalatnikov and Lifshitz (BKL) in [1]. In the BKL scenario, as spacetime approaches singularity, the time derivatives of the gravitational field are shown to dominate over all spatial derivatives for relatively long stretches of time. Surprisingly, the evolution of the general gravitational field turns out to be well approximated, at each point separately, by a sequence of the so-called Kasner epochs. Each epoch is a vacuum solution
to the homogenous spacetime model of Bianchi I type. The transitions between epochs are the effect of non-negligible spatial curvature, which arises quickly and vanishes after a relatively short period of time. In the BKL scenario, the universe undergoes an infinite number of chaotic-like transitions and eventually collapses into a singularity in a finite proper time.

It is commonly believed that the incompleteness of classical theory, which breaks down at the singularity, will be overcome by quantization of the gravitational degrees of freedom. For this purpose, the Dirac method of quantization is usually employed (see e.g. [2–4]). In this paper, we focus on quantum theory of the Kasner universe. We follow, however, an alternative way to quantum theory, namely the reduced phase space quantization (see e.g. [5, 6]). Since the Kasner model plays a central role in the BKL description of a generic cosmological singularity, we believe that the present and future investigations into this model supported by current and forthcoming astrophysical and cosmological data can help obtaining new insights into the universe’s origin.

The fact that in canonical general relativity the evolution of gravitational fields coincides with gauge transformation or equivalently that there is no privileged time standard to measure motion gives rise to the so-called problem of time (see e.g. Kuchar [7]). The problem of time consists of a few related though distinguishable issues. Following Kuchar’s terminology, we will treat in this paper the most fundamental issue, namely the multiple choice problem. In essence, it states that two different choices of time may produce different quantum theories. We will show how severe the problem is and examine its origin. In the view of the results obtained in this paper, the proposals for explaining the multiple choice problem existing in the literature are unsatisfactory. For example, in Isham [8] we can read that two different choices of time lead to canonically equivalent theories, which admit unitarily inequivalent quantum representations due to the Van–Hove phenomenon [9]. We will show that in fact the multiple choice problem can be traced back to the canonical formulation of general relativity and thus studied at classical level.

The application of the reduced phase space approach to the Kasner universe turns out to be manageable and quite straightforward. The system consists of a single constraint on the kinematical phase space, which is six dimensional. We identify the (physical) reduced phase space, that is, the space of Dirac observables, which is four dimensional. We consider two examples of clock variables to introduce the physical evolution and construct the so-called true Hamiltonians. We argue that the evolution is free of the singularity present in the classical theory. We compare the spectra of the Hubble operator in two different clock variables and show that they are very different.

Before we start let us introduce the notation that will be used throughout the text. The canonical variables, which follow from the Legendre mapping applied to the Einstein–Hilbert action, parametrize the kinematical phase space, denoted by $\mathcal{P}$. In this space, the Hamiltonian constraint $H$ is introduced. The constraint surface, defined by $H = 0$, is denoted by $\mathcal{S}$. The Dirac observables, denoted by $\mathcal{D}$, are defined by the relation $\{\mathcal{D}, H\} = 0$ and with the domain restricted to the constraint surface. The space of Dirac observables, called the reduced phase space, or the physical phase space, will be denoted by $\mathcal{P}_R$. In Rovelli [10], it is proposed to call kinematical phase space functions by partial observables in order to emphasize that they can be measured by observers, though the outcome of such a measurement made alone cannot be predicted by theory. There is, however, one kinematical degree of freedom for which the theory makes the immediate prediction, i.e. the Hamiltonian constraint vanishes, $H = 0$. In what follows, by partial observables we mean functions restricted to $\mathcal{S}$ (which seems to be slightly different from Rovelli’s notion), and which will be denoted by $\mathcal{P}_I$. 

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2. Lagrangian formulation

The Hilbert–Einstein action reads

$$S_{HE} = \int_{\Omega \subset M} \sqrt{-g} \, d^3 x \, dt,$$

where $g, R$ are the metric determinant and the Ricci scalar, respectively. The integral is taken over an open subset $\Omega$ of the manifold $M$. We specify action (1) to the case of the vacuum Bianchi I model with $M = R \times \Sigma$, where $\Sigma$ is a compact spacelike leaf and we assume the following metric type:

$$d s^2 = -N^2(t) \, dt^2 + a_1^2(t) \, (dx^1)^2 + a_2^2(t) \, (dx^2)^2 + a_3^2(t) \, (dx^3)^2$$

which leads (1) to the form (see appendix A)

$$S_{HE} = 2 \int_{t_0}^{t_1} \int_{\Sigma} N a_1 a_2 a_3 \left[ \sum_i \frac{1}{N a_i} \left( \dot{a}_i \right)_N \right] + \sum_{i \neq j} \left( \frac{\dot{a}_i}{N a_i} \right) \left( \frac{\dot{a}_j}{N a_j} \right) d^3 x.$$  

Applying the variational principle to (3) gives the Lagrange equations

$$\sum_{i \neq j} \dot{a}_i \dot{a}_j = 0, \quad \dot{a}_i \dot{a}_j = N \left( \frac{\dot{a}_i \dot{a}_j}{N} \right) \forall i \neq j.$$  

The solutions were first found by Kasner in [11]. Later, they were rediscovered by Taub in [12], who gave the solutions in the following form

$$d s^2 = -dt^2 + t^{2p_1} \, dx^2 + t^{2p_2} \, dy^2 + t^{2p_3} \, dz^2,$$

where the constants $p_1, p_2$ and $p_3$ satisfy

$$p_1 + p_2 + p_3 = 1, \quad p_1^2 + p_2^2 + p_3^2 = 1.$$  

All the above solutions, except for $p_1 = 1$, $p_2 = 1$ or $p_3 = 1$, admit a cosmological singularity for $t = 0$.

It is easily seen that action (3), equations of motion (4) and solution (5) are invariant under any time re-parameterization such that $t \mapsto t'(t)$ and $N \mapsto \frac{d t'}{d t} N$. This is the only gauge freedom, which is preserved under the reduction of the Hilbert–Einstein action to the homogenous spacetime. Therefore, by gauge transformation we mean any change of time parameter $t \mapsto t'(t)$.

3. Hamiltonian formulation

Using action (3), we define the momenta

$$\pi^N := \frac{\partial L}{\partial \dot{N}} = 0, \quad \pi^i := \frac{\partial L}{\partial \dot{a}_i} = -\frac{2}{N} (a_i \dot{a}_i).$$

The Legendre mapping (7) is singular, and its range is the submanifold of the phase space given by $\pi^N = 0$. The Hamiltonian reads

$$H_0 = \pi^N \dot{N} + \sum \pi^i \dot{a}_i - L = \frac{1}{2} \sum_i \pi^i \dot{a}_i.$$  

1 For the sake of simplicity, from now on we drop the integration over the compact space-like leaf $\Sigma$ whenever it should appear.
The Dirac analysis [2] leads to the reduction of phase space by the conjugate pair \((N, \pi^N)\) and the introduction of the Hamiltonian constraint

\[
H := \frac{N}{8} \sum_{i \neq j \neq k} \pi^i \pi^j \pi^k (\pi^i a_j - \pi^j a_i - \pi^k a_k) \approx 0, \tag{9}
\]

where now the lapse \(N\) is a Lagrange multiplier. One may verify that the vanishing of Hamiltonian constraint (9) and Hamilton’s equations are equivalent to the first and the second of the Euler–Lagrange equations in (4), respectively.

### 3.1. New variables and motion

We introduce the new canonical variables

\[
X_i := \frac{1}{2} a_i a_k, \quad P_i := -\frac{d_i}{N}, \tag{10}
\]

in which the Hamiltonian constraint (9) reads

\[
H = -\frac{N}{4\sqrt{2}} \sum_{i > j} \sqrt{X_i X_j} P_j. \tag{11}
\]

The symplectic form on the kinematical phase space is defined as

\[
\omega := \sum_i dX_i \wedge dP_i \tag{12}
\]

and its minus inverse is the Poisson bracket, i.e.

\[
\omega^{-1} = \sum_i \left( \frac{\partial}{\partial X_i} \frac{\partial}{\partial P_i} - \frac{\partial}{\partial P_i} \frac{\partial}{\partial X_i} \right). \tag{13}
\]

The Hamilton equations in the gauge \(N = 4\sqrt{2}\sqrt{X_1 X_2 X_3}\) read

\[
\dot{X}_i = \frac{\partial H}{\partial P_i} = -X_i (X_j P_j + X_k P_k) \tag{14}
\]

\[
\dot{P}_i = -\frac{\partial H}{\partial X_i} = P_i (X_j P_j + X_k P_k). \tag{15}
\]

From combining the above equations into one:

\[
\dot{X}_i P_i + X_i \dot{P}_i = (X_i P_i)_j = 0, \tag{16}
\]

we obtain that \(\Gamma_i := X_i P_i\) are constants of motion (as we will see in a moment, they may be identified with some of the Dirac observables). Putting this back to (14), (15), we find that

\[
X_i (t) = X_i (t_0) e^{-(\Gamma_j + \Gamma_k) (t - t_0)}, \quad P_i (t) = P_i (t_0) e^{i(\Gamma_j + \Gamma_k) (t - t_0)}, \tag{17}
\]

where \(P_i (t_0)\) and \(X_i (t_0)\) are the initial conditions for the Hamilton equations and \(t_0\) will be specified later. The physical solutions (17) should satisfy the Hamiltonian constraint (11), which can now be rewritten as

\[
\sum_{i > j} \Gamma_i \Gamma_j \approx 0. \tag{18}
\]

The change of the arrow of time \(t \mapsto -t\) in (17) is equivalent to the sign change \(\Gamma_i \mapsto -\Gamma_i\) for all \(i\)’s, so we can add the condition

\[
\sum_i \Gamma_i > 0 \tag{19}
\]
which ensures that the singularity is approached as the time $t$ grows. Moreover, the following three cases:

$$\Gamma_1 = \Gamma_2 = 0, \quad \Gamma_2 = \Gamma_3 = 0, \quad \Gamma_1 = \Gamma_3 = 0,$$

(20)
can be shown to correspond to the Milne space, which can be isometrically embedded in Minkowski spacetime and thus are non-singular (i.e. the coordinates are singular, not the spacetime itself). We exclude them from the phase space.

### 3.2. Dirac’s observables

It is known that for the Hamiltonian satisfying $dH \neq 0$ in a neighborhood of the constraint surface $H = 0$, one may locally introduce such a canonical parametrization of the kinematical phase space that the canonical coordinates

$$(X_i, P_i), \quad i = 1, \ldots, n,$$

(21)
are replaced with the new canonical pairs

$$(H, T), (\tilde{X}_i, \tilde{P}_i), \quad i = 1, \ldots, n - 1,$$

(22)
such that the variable $T$ is canonically conjugate to $H$ and the symplectic form now reads

$$\omega = dT \wedge dH + d\tilde{X}_i \wedge d\tilde{P}_i.$$

(23)

It is now easily seen that the space of functions which commute with the Hamiltonian $H$ is given by

$$\{H, D_i\} = 0 \Rightarrow D_i = D_i(\tilde{X}_i, \tilde{P}_i, H)$$

(24)
which restricted to the constraint surface $H = 0$ can be identified with the following space of functions:

$$D_i = D_i(\tilde{X}_i, \tilde{P}_i).$$

(25)

An easy way to find all the Dirac observables is by pulling back the symplectic form $\omega$ to the constraint surface

$$\omega|_{H=0} = d\tilde{X}_i \wedge d\tilde{P}_i$$

(26)
and ensuring that the pulled-back two-form is in the canonical form. Obviously, this recipe does not depend on gauge as

$$\omega = (NH) \cdot dT \wedge d\frac{1}{N} + \frac{1}{N} \cdot dT \wedge d(NH) + d\tilde{X}_i \wedge d\tilde{P}_i$$

(27)
so $\omega|_{N=0} = \omega|_{H=0}$ for any $N \neq 0$.

In what follows, we will obtain the complete set of Dirac observables by restricting the symplectic form $\omega$ introduced in (12) to the constraint surface (18). Applying the mapping

$$\Gamma_1 = \frac{1}{2} x - \frac{1}{2} y + z$$

$$\Gamma_2 = \frac{1}{2} x - \frac{1}{2} y - z$$

$$\Gamma_3 = \frac{3}{4} x + \frac{5}{4} y,$$

(28)
one arrives at the following form of the constraint (18):

$$x^2 - y^2 - z^2 = 0.$$
embedding of the constraint surface in the kinematical phase space by

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the lapse function

and leads to \( r > 0 \). The exclusion of the Milne space cases (20), which are equivalent to \( \phi = 0 \) and \( \cos \phi = -\frac{3}{2} \), restricts the parameter \( \phi \) in the following way:

where \( \phi_1 \) and \( \phi_2 \) are the solutions to \( \cos \phi = -\frac{3}{2} \). The starting kinematical phase space was parameterized by the six coordinates \( (X_i, P_i) \). Since \( X_i > 0 \), we could use the coordinates \( (X_i, \Gamma_i) \) as well. Thus, constraint surface (18) may be parameterized by the five coordinates \( (X_i, r, \phi) \).

The complete set of Dirac observables and their commutation relations can be found by restricting the symplectic form \( \omega \) in \( \mathcal{P} \) to the constraint surface \( \mathcal{S} \). Let us denote the embedding of the constraint surface in the kinematical phase space by \( E : \mathcal{S} \hookrightarrow \mathcal{P} \) so that \( E^* : C^\infty(\mathcal{P}) \ni (P_i, X_i) \rightarrow (r, \phi, X_i) \in C^\infty(\mathcal{S}) \) is the restriction of the kinematical phase space functions to the constraint surface functions:

\[
E^* \left( \sum \mathrm{d}X_i \wedge \mathrm{d}P_i \right) = E^* \left( \sum \mathrm{d}X_i \wedge \frac{\mathrm{d}\Gamma_i}{X_i} \right)
\]

\[
= d \left[ \left( \frac{1}{2} - \frac{1}{2} \cos \phi + \sin \phi \right) \ln X_1 + \left( \frac{1}{2} - \frac{1}{2} \cos \phi - \sin \phi \right) \ln X_2 \right] + \frac{3}{4} + \frac{5}{4} \cos \phi \ln X_3 \wedge dr + d \left[ \frac{1}{2} r \sin \phi - r \cos \phi \right] \ln X_1
\]

\[
+ \left( \frac{1}{2} r \sin \phi - r \cos \phi \right) \ln X_2 + \frac{3}{4} \ln r \sin \phi \ln X_3 \right] \wedge d\phi
\]

\[
= \mathrm{d}O_1 \wedge dr + \mathrm{d}O_2 \wedge d\phi,
\]

where we have defined

\[
O_1 = \left( \frac{1}{2} - \frac{1}{2} \cos \phi + \sin \phi \right) \ln X_1 + \left( \frac{1}{2} - \frac{1}{2} \cos \phi - \sin \phi \right) \ln X_2 + \left( \frac{3}{4} + \frac{5}{4} \cos \phi \right) \ln X_3
\]

\[
O_2 = \left( \frac{3}{4} + \frac{5}{4} \cos \phi \right) \ln X_3 + \left( \frac{1}{2} r \sin \phi - r \cos \phi \right) \ln X_2 + \frac{3}{4} r \sin \phi \ln X_3.
\]

The space of Dirac’s observables is called the reduced phase space \( \mathcal{P}_R : (r, \phi, O_1, O_2) \in R_+ \times I \cup I^2 \cup I^3 \times R \times R \). Apparently, the space of Dirac observables in the Kasner universe is not simply connected. The four Dirac observables together with any constraint surface function \( t \) such that

\[
\{ t, H \}_{H=0} \neq 0
\]

form a coordinate system \((r, \phi, O_1, O_2, t)\) on the five-dimensional constraint surface \( \mathcal{S} \) equipped with the two-form:

\[
\omega_S := \sum \mathrm{d}X_i \wedge \mathrm{d}P_i \bigg|_{H=0} = \mathrm{d}O_1 \wedge dr + \mathrm{d}O_2 \wedge d\phi
\]

induced from the symplectic form \( \omega \) on the kinematical phase space \( \mathcal{P} \). It should be added that the freedom in the choice of the fifth coordinate \( t \) on \( \mathcal{S} \) is bigger than the freedom in choosing the lapse function \( N : \mathcal{S} \hookrightarrow R_+ \), which fixes only the first derivative of \( t \) with respect to the Hamiltonian vector field, i.e. \( \{ t, H \}_{H=0} = N^{-1} \), where \( H \) itself is taken with the lapse equal 1.
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3.3. Partial observables

Solutions found in (17) include both the physical and non-physical sector. In the physical sector, however, all the solutions should be expressible in terms of coordinates on $S$. Setting $X_1(t_0) = 1$, we express all the constants occurring in (17), that is, $\Gamma_i, X_i(t_0), P_i(t_0)$, in terms of the Dirac observables $O_1, O_2, \phi$, and arrive at

$$P_1 = \frac{1}{2} r(1 - \cos \phi + 2 \sin \phi) \exp \left(\frac{1}{2} r(5 + 3 \cos \phi - 4 \sin \phi)(t - t_0)\right)$$

$$P_2 = \frac{1}{2} r(1 - \cos \phi + 2 \sin \phi) \exp \left(\frac{1}{2} r(5 + 3 \cos \phi + 4 \sin \phi)(t - t_0)\right)$$

$$P_3 = \frac{1}{2} r(3 + 5 \cos \phi) \exp(r(1 - \cos \phi)(t - t_0))$$

$$X_1 = \exp(-\frac{1}{4} r(5 + 3 \cos \phi - 4 \sin \phi)(t - t_0))$$

$$X_2 = \exp(-\frac{1}{4} r(5 + 3 \cos \phi + 4 \sin \phi)(t - t_0))$$

$$X_3 = \exp(-r(1 - \cos \phi)(t - t_0))$$

The above solutions are solutions (17) restricted to the constraint surface $S$. The variable $t$ parameterizes the gauge orbits in the constraint surface $S$. After the specification of the value of $t_0$ for each gauge orbit, that is, defining $t_0$ as a function of Dirac observables, the variable $t$ becomes the fifth coordinate, which assigns a specific value to each point in $S$.

In analogy to the Friedman cosmology, we will be interested in the Hubble and deceleration parameters, which in the Kasner model are introduced for each of the three directions (see appendix A) and read

$$H_1 = -\frac{r(1 - \cos \phi + 2 \sin \phi)}{32} \exp \left(\frac{r}{4} (7 + \cos \phi)(t - t_0)\right)$$

$$H_2 = -\frac{r(1 - \cos \phi - 2 \sin \phi)}{32} \exp \left(\frac{r}{4} (7 + \cos \phi)(t - t_0)\right)$$

$$H_3 = -\frac{r(3 + 5 \cos \phi)}{64} \exp \left(\frac{r}{4} (7 + \cos \phi)(t - t_0)\right)$$

$$q_1 = \sqrt{2} \frac{7 + \cos \phi}{1 - \cos \phi + 2 \sin \phi} - 1$$

$$q_2 = \sqrt{2} \frac{7 + \cos \phi}{1 - \cos \phi - 2 \sin \phi} - 1$$

$$q_3 = 2\sqrt{2} \frac{7 + \cos \phi}{3 + 5 \cos \phi} - 1.$$

We note that the deceleration parameters $q_i = 2\sqrt{2} \left(\sum \frac{H_i}{H_0}\right) - 1$ are constants of motion, i.e. Dirac’s observables. All the above six quantities determine and are determined by the components of the connection and curvature matrices (see appendix A). Therefore, they represent the local properties of the Kasner universe and do not form the complete space of observables in the compact universe.
For $t$ to be a function on $S$, we need to specify $t_0$ as a function of Dirac observables. We note that the choice

$$t_0 := \frac{O_1(7 \sin \phi - 4 \cos \phi) + \frac{1}{2} O_2(1 + 3 \cos \phi + 4 \sin \phi)}{\frac{7}{2}(7 + \cos \phi)(5 + 3 \cos \phi - 4 \sin \phi)}$$

simplifies nicely the formulas for the Hubble parameters:

$$H_1 = -\frac{r(1 - \cos \phi + 2 \sin \phi)}{32} \exp \left( \frac{r}{4}(7 + \cos \phi)t \right)$$

$$H_2 = -\frac{r(1 - \cos \phi - 2 \sin \phi)}{32} \exp \left( \frac{r}{4}(7 + \cos \phi)t \right)$$

$$H_3 = -\frac{r(3 + 5 \cos \phi)}{64} \exp \left( \frac{r}{4}(7 + \cos \phi)t \right)$$

and leaves the formulas for deceleration parameters unchanged.

We want, however, more than that and apart from simplicity we require that the time coordinate satisfies two extra conditions: (a) has a clear physical meaning and (b) the singularity occurs at its finite value. A distinguished choice is the cosmological time, for which the lapse function $N_{\cos} = 1$ and the singularity is reached at $t_{\cos} = 0$ (for all gauge orbits).

We use the relation $N \, dt = N_{\cos} \, dt_{\cos}$ to obtain the formula

$$t_{\cos} = \int_{t_i}^{t} \frac{dt_{\cos}}{dt} = \int_{\infty}^{t_i} \frac{N}{N_{\cos}} \, dt,$$

where $t = t_i$ defines the four-dimensional boundary of the constraint surface $S$, at which the singularity occurs. Then, we insert $N = 4\sqrt{2} \sqrt{X_1 X_2 X_3}$ and obtain

$$t_{\cos} = -\frac{16\sqrt{2}}{r(7 + \cos \phi)} \exp \left( -\frac{r}{4}(7 + \cos \phi)t \right).$$

This time redefinition simplifies the formulas for the Hubble parameters even further:

$$H_1 = \frac{1 - \cos \phi + 2 \sin \phi}{\sqrt{2}(7 + \cos \phi) t_{\cos}}$$

$$H_2 = \frac{1 - \cos \phi - 2 \sin \phi}{\sqrt{2}(7 + \cos \phi) t_{\cos}}$$

$$H_3 = \frac{3 + 5 \cos \phi}{2\sqrt{2}(7 + \cos \phi) t_{\cos}}.$$
4. Problem of time

All internal clocks are given by the formula
\[ \tau = \int_0^{t_{\text{cos}}} N^{-1} dt_{\text{cos}} + \tau_0, \]  
(62)
where \( N(t_{\text{cos}}, D_i) > 0 \) is a function of the cosmological time and Dirac observables and \( \tau_0(D_i) \) is any function of Dirac observables. Due to the change of the time parameter \( t \mapsto \tau \), any time-dependent function on the constraint surface, i.e. any partial observable, is transformed accordingly:
\[ \mathcal{P}(D_i, t) \mapsto \tilde{\mathcal{P}}(D_i, \tau) = \mathcal{P}(D_i, \tau(D_i)). \]  
(63)
Thus, in general, \( \mathcal{P} \) and \( \tilde{\mathcal{P}} \) will have different dependence on Dirac observables and after quantization they may have different spectra. Therefore, it is meaningless to speak about spectra of partial observables, like energy density, curvature or volume, without reference to the choice of internal clock. To support this statement, it is enough to note that the commutation relation
\[ \{\mathcal{P}_1, \mathcal{P}_2\} \mapsto \{\tilde{\mathcal{P}}_1, \tilde{\mathcal{P}}_2\} = \{\mathcal{P}_1, \mathcal{P}_2\} + \frac{\partial \mathcal{P}_1}{\partial t}\{t(\tau, D_i), \mathcal{P}_2\} + \frac{\partial \mathcal{P}_2}{\partial t}\{\mathcal{P}_1, t(\tau, D_i)\} \]  
(64)
becomes altered after the change of time. Note that the commutation relations between the Dirac observables can be obtained from the form \( \omega_S \) given in (40), where any variable chosen to play a role of time is interpreted as an external parameter. Thus, in the constraint surface the gauge transformation is not canonical and consequently it cannot be unitary in quantum theory. This implicates that the spectral properties of the same operator in different gauges should be, in general, different.

The gauge transformation has another interesting feature. Suppose that we are given any two partial observables, which monotonically increase with time and whose range is identical. For example, let it be the curvature \( C \) and energy density \( \rho \). Then, there is always such a gauge transformation \( \tau \mapsto \tau' \) that energy density in one gauge is functionally identical with the curvature in another gauge, that is, \( \rho_1 \equiv C_{1'}. \) In effect, the spectral properties can be shared by many different partial observables. If we drop the assumption about the identity of ranges, the two different partial observables will still share the identical dependence on Dirac observables for some time during the evolution.

Obviously, one is unable to study the cosmological singularity problem without the notion of evolution, for example, just by the inspection of Dirac observables. Thus, this gives rise to the very interesting question of the possible dependence between the choice of time and the fate of singularity in quantum theory.

4.1. Geometrical formulation of the problem of time

Let us take a closer look at the structure of systems with a Hamiltonian constraint. The constraint equation \( H = 0 \) defines the embedding \( E : S \mapsto \mathcal{P} \) of the constraint surface \( S \) into the kinematical phase space \( \mathcal{P} \) having its dimension increased by 1. The constraint surface \( S \) is therefore odd-dimensional. All the physical motion takes place in the surface and the vectors tangent to the trajectories (gauge orbits) are given by the Hamiltonian vector field \( X_H \) (gauge generator), defined in the standard way:
\[ X_H : \omega(\cdot, X_H) = -dH, \]  
(65)
where \( \omega \) is the symplectic form in \( \mathcal{P} \) and the Hamiltonian vector field \( X_H \big|_{H=0} \) is restricted to the constraint surface, will be denoted by \( X_H \) for brevity.
The constraint surface is equipped with the two-form $\omega_S$ induced from the kinematical phase space, $\omega_S := E^\ast \omega_0$. The form $\omega_S$ is a singular closed two-form of maximal rank. It is represented at each point $p \in S$ by an antisymmetric matrix $\omega_S(p) : T_pS \mapsto T^*_pS$ in the tangent space of the odd-dimensional manifold. Its null vector is $X_H$, satisfying $\omega_S(\cdot, X_H) = 0$. The null vector $X_H$ is a generator of the line bundle with the projection (submersion): $\pi : S \mapsto \mathcal{P}_R$ from the constraint surface to the reduced phase space. The pullback $\pi^\ast$ is understood as an injection from the space of functions $D$ such that $X_H(D) = 0$ to the space of all observables.

The diagram below illustrates the relations between $\mathcal{P}$, $S$ and $\mathcal{P}_R$:

\[ \mathcal{P} \xrightarrow{\text{Embedding, } E} S \xrightarrow{\text{Projection, } \pi} \mathcal{P}_R. \]  

(66)

Since the form $\omega_S$ is singular, it cannot be inverted into the Poisson structure (which should be quantized). Suppose, we introduce a projection on the tangent space at $p \in S$, denoted by $P_p : T_pS \mapsto T_pS$, such that $P_p(X) = 0 \Leftrightarrow X \sim X_H(p)$. Then, the matrix $\omega_S(p)$ can be inverted on the restricted domain $\{X \in T_pS : P_p(X) = X\}$. Though it enables to derive the inverse of $\omega_S$, this construction is ambiguous due to ambiguity in the choice of the projection $P_p$. Now, the (minus) inverse $-\omega^{-1}_{S,p} : T^*_pS \mapsto T_pS$ is the Poisson bracket.

The generalization of the above construction follows straightforwardly. Suppose we attach to each point $q \in S$ a projection $P_q$ of the considered type. In addition, we assume that there exists a slicing of $S$ such that the tangent space to a slice at any $q \in S$ is identical with the range of $P_q$. Let the slicing be given by a function $t : S \mapsto R$. Now the Poisson structure for each $q \in S$ is given by the inverse of the form $\omega_S$ restricted to the hypersurface $t = \text{const}$ containing $q$, and let it be denoted by $-\omega^{-1}_{S,t}$.

The construction of $-\omega^{-1}_{S,t}$ may be achieved by exploiting the simple relation that determines the induced Poisson structure

\[ -\omega^{-1}_{S,t}(t, D_1) := \{t, D_1\}_S = 0 \]  

(67)

with all other commutation relations being fixed uniquely by the independent-of-the-choice-of-time commutation relation between Dirac observables.

### 4.2. Canonical transformations in the constraint surface

Once a slicing is introduced in the constraint surface, we arrive at the triple $(\tilde{S}, \omega_S, t)$. Such a structure is well known in classical mechanics and is called a contact manifold. The restriction of $\omega_S$ to the constant time hypersurfaces forms a symplectic submanifold with the symplectic form $\omega_{S,t}$. The form $\omega_{S,t}$ can be pulled back to the constraint surface, $\tilde{\omega}_{S,t} = t^\ast \omega_{S,t}$. It should be noted that in general $\tilde{\omega}_{S,t} \neq \omega_S$. The relation between $\tilde{\omega}_{S,t}$ and $\omega_S$ is the subject of the theory of canonical transformations and will be discussed below.

One may think of a canonical transformation as a symplectomorphism; however, the contact manifold provides a better avenue to define this notion. Let us cite the definition of the canonical transformation from Abraham and Marsden [13].

**Definition.** Let $(\mathcal{P}_1, \omega_1)$ and $(\mathcal{P}_2, \omega_2)$ be symplectic manifolds and $(R \times \mathcal{P}_1, \tilde{\omega}_1)$ the corresponding contact manifolds. A smooth mapping $F : R \times \mathcal{P}_1 \mapsto R \times \mathcal{P}_2$ is called a canonical transformation if each of the following holds:

1. $F$ is a diffeomorphism;
2. $F$ preserves time; that is, $F^\ast t = t$;
3. there is a function $K_F \in C^\infty(R \times \mathcal{P}_1)$ such that $F^\ast \tilde{\omega}_2 = \omega_K$, where $\omega_K = \tilde{\omega}_1 + dK_F \land dt$.

In what follows, we will use the symbol $H_F$ instead of $K_F$. There are a few observations that can be made in effort to understand the above definition. First, we note that the slicing of the constraint surface

\[ S \mapsto R \]  

(68)
is needed in order to introduce the canonical transformations. However, the lack of this slicing is the essence of gauge invariance and it can only be postulated. Once it is done, any canonical transformation, according to condition D2, preserves chosen time.

This leads us to the next observation that different choices of time must produce canonically inequivalent theories. It confirms our earlier result that the choice of slicing fixes the Poisson structure, which is related to defining an ambiguous procedure by which a non-invertible matrix \((\omega_{S1})\) can be inverted \((\omega_{S1}^{-1})\).

Another observation is as follows. Suppose there is a given slicing \(t\). The constraint surface can be parametrized as \(S = t \times \mathcal{P}_R\), where \(\mathcal{P}_R\) is the reduced phase space. We note that \(\omega_{S1} = \omega_R\) and that \(\omega_S = \tilde{\omega}_R(= t^*\omega_R)\). In this contact manifold, there is no Hamiltonian, since the reduced phase space consists of Dirac observables for which \(\mathcal{D}_i = 0\). Now we may introduce the evolution into the system by considering time-dependent reparametrization of the constant time hypersurfaces. As we will see below this will render a non-vanishing Hamiltonian.

Consider the following canonical transformation \(F : S \mapsto S\), such that \(F^* : \mathcal{D}_i \mapsto \mathcal{D}_i(q, p, t)\), \(F^*t = t\) and:

\[
F^*\omega_S = \tilde{\omega}_{S1} + dH_T \wedge dt, \tag{69}
\]

where \(\tilde{\omega}_{S1} = t^*\omega_{S1}\) is the pullback of the symplectic from \(\omega_{S1}\) living in the leaf \(t = \text{const}\), and parametrized with new coordinates \((q, p)\). The new coordinates are in general time dependent.

In the coordinates \((\mathcal{D}_i, t)\), the null vector of the form \(\omega_S\) is given by \(X_H = \partial_t\). The canonical transformation \(F\) changes the coordinates and the coordinate expression for \(X_H\) accordingly:

\[
F^*X_H = \partial_t + X_T = \partial_t - \omega_{S1}^{-1}(\cdot, H_T) = \partial_t + \{\cdot, H_T\}. \tag{70}
\]

Now it is seen that the evolution of the observables in new coordinates is not only given through the explicit dependence on time \(t\) but also through the true Hamiltonian \(H_T\).

However, not all time-preserving diffeomorphisms are canonical transformations. Therefore, it is useful to introduce an alternative formulation which relies on a generating function \(W\):

\[
p_t, dq^i + H_T dt - F^*\theta_R = dW, \tag{71}
\]

where \(\theta_R\), satisfying \(-d\theta_R = \omega_R\), is the canonical (Poincaré) one-form in the reduced phase space, and \((p_i, q^i)\) are the new canonical pairs. \(W\) is a generating function such that:

\[
W = W(q^i, q, t), \quad p_{D,i} = \frac{\partial W}{\partial q^i}, \quad p_t = \frac{\partial W}{\partial q}, \tag{72}
\]

and the relation between \(W\) and \(H_T\) reads

\[
H_T \left( t, q^i, \frac{\partial W}{\partial q} \right) - \frac{\partial W}{\partial t} = 0. \tag{73}
\]

The final remark is that the true Hamiltonian is quite arbitrary and it does not depend on the particular choice of time but rather on the choice of basic variables on the constant time submanifolds once time is given.

Let us sum up. In the kinematical phase space \(\mathcal{P}\), the symplectic form, \(\omega\), and the Poisson bracket, \(-\omega^{-1}\), can be considered interchangeably. However, in the constraint surface \(S\), the induced two-form, \(\omega_S\), is singular and one cannot define the Poisson bracket in \(S\) unambiguously. The bracket is needed to compute the commutation relations between partial observables prior to quantization. The choice of the clock variable \(t : S \mapsto R\) is equivalent to the choice of the following commutation relation:

\[
\{ t, \mathcal{D}_i \}_S = 0. \tag{74}
\]

We denote by \(q_{D}^i\) and \(p_{D,i}\), the reduced phase space basic variables.
The last relation fixes the Poisson bracket between any pair of partial observables on $S$. In principle, one can choose any function $t : S \mapsto R$ admitting $X_H(t) > 0$ to slice the constraint manifold. The fact that different slicings lead to canonically inequivalent theories is confirmed by formula (74).

It should be emphasized that the Poisson bracket between any pair of Dirac observables is given uniquely in a constrained system. There is the unique two-form in the reduced phase space, $\omega_R$, such that its pullback to the constraint surface gives $\pi^*(\omega_R) = \omega_S$. The form $\omega_R$ is invertible, since the reduced phase space $R$ is even-dimensional, and the Poisson bracket can be computed. This is in agreement with the fact that the Poisson bracket between Dirac observables in the kinematical phase space, $P$, is given uniquely and independently of the choice of time.

4.3. Problem of time in Dirac quantization

In the Dirac quantization, the kinematical phase space is quantized so that the kinematical Hilbert space is obtained and the Hamiltonian constraint is promoted to a self-adjoint operator $H \mapsto H$. Then, the theory is constructed via the solutions to the quantum constraint equation, i.e.

$$\hat{H}\psi = 0.$$  

(75)

The solutions $\psi$ normally do not belong to the kinematical Hilbert space, and the Hilbert space structure needs to be reintroduced. There is the idea, called ‘deparameterization’, which cures the problem and at the same time nicely introduces the concept of evolution of the system. The idea is to reformulate the constraint equation $H = 0$ in such a way that the quantum constraint equation (75) gets a Schrödinger-like form [14, 15]. This procedure is very closely related to another procedure used for the Dirac quantization, namely the group averaging method [16]. Therefore, we will focus here only on the idea of deparameterization while keeping in mind that the problem of time is in fact method-independent and can also be formulated in the context of group averaging.

Suppose that we consider a gravitational system including a scalar field. In this case (see e.g. [15]), $H \approx p^2 - CGR$ and we obtain a Schrödinger-like equation

$$-i\hbar \frac{d}{d\phi} \psi = \sqrt{CGR} \psi$$

(76)

so that the scalar field, $\phi$, plays a role of a time parameter. The non-vanishing true Hamiltonian, $\sqrt{CGR}$, is expressed in terms of the rest of the rest of the kinematical degrees of freedom, here the gravitational ones. They are supposed to parameterize the reduced phase space and play a role of (partial) observables in quantum theory. It must be noted, however, that the commutation relations between these partial observables are postulated. They are parachuted from the kinematical phase space in an ad hoc manner. Since the observables are physical only in the constraint surface, any kinematical degree of freedom, $P$, forms the following equivalence class:

$$P_i \sim P'_i \iff P_i \approx P'_i \iff P_i = P'_i + C_i,$$

(77)

where $C_i$ is a constraint. But then, the Poisson bracket between the equivalence classes on the constraint surface is quite easily shown to be ill-defined (non-unique):

$$\{P_i + C_i, P_j + C_j\} = \{P_i, P_j\} + \{C_i, P_j\} + \{P_i, C_j\} + \{C_i, C_j\},$$

(78)

where only the term $\{C_i, C_j\} \approx 0$ weakly vanishes. The terms $\{C_i, P_j\}$ and $\{P_i, C_j\}$ do not vanish in the constraint surface and make the Poisson structure ill-defined.
The non-existence of the Poisson bracket in the constraint surface $S$ was proved in the previous subsection and is due to the fact that the constraint surface is odd dimensional. Therefore, in order to encode dynamics into quantum theory, one needs to postulate the Poisson bracket between partial observables or between a partial and Dirac one, so that relation (74) is fixed. Having this done, the time parameter is determined as the only partial observable which commutes with all the other, partial and Dirac, observables. Then, the time parameter $t : S \mapsto \mathbb{R}$, together with the Dirac observables, introduces the ‘no-Hamiltonian’ parameterization of the constraint surface $S = \mathbb{R} \times \mathcal{P}_R$. In the scalar field case $t = \phi$, one has

$$\{\phi, D_i\}_S = 0.$$ (79)

Observe once again that in a constrained system, only the Poisson commutation between any pair of Dirac observables whatever its parametrization (see appendix B) is well defined:

$$\{D_i + C_i, D_j + C_j\} = \{D_i, D_j\} + \{D_i, C_j\} + \{C_i, D_j\} + \{C_i, C_j\} \approx \{D_i, D_j\},$$ (80)

since a Dirac observable by definition commutes weakly with a constraint, i.e. $\{D_i, C_j\} \approx 0$ (in opposition to what happens in (78)).

To sum up, in the Dirac quantization, the problem of time persists. As before, this is so due to the fact that time-dependent observables are gauge-variant quantities and their Poisson commutator relations are undefined. In this procedure, an ambiguous Poisson structure can be postulated by parachuting the Poisson structure of $2n - 2$ kinematical degrees of freedom.

5. Choice of time and spectra of partial observables

So far we have shown that the Poisson bracket between partial observables depends on the choice of time. In what follows, we will show how this fact affects spectral properties of time-dependent quantities. Let us study the Hubble observable in a fixed direction (59):

$$H_1 = \frac{1 - \cos \phi + 2 \sin \phi}{\sqrt{2(7 + \cos \phi)} t_{\text{cos}}}.$$ (81)

First we note that the evolution of the Hubble observable, in the cosmological time $t_{\text{cos}}$, is not canonical. For from (81), we have

$$d\phi = \frac{\sqrt{2} t_{\text{cos}} (7 + \cos \phi)^2}{2 + 8 \sin \phi + 14 \cos \phi} \left( dH_1 + \frac{H_1}{t_{\text{cos}}} dt_{\text{cos}} \right),$$ (82)

which after substituting for $d\phi$ in (40) leads to

$$\omega_S = \cdots + \frac{\sqrt{2} H_1 (7 + \cos \phi)^2}{2 + 8 \sin \phi + 14 \cos \phi} d\Omega_2 \wedge dt_{\text{cos}}$$ (83)

which according to the theory of canonical transformations (see the definition in the previous section) should have the form of (69), so that the one-form

$$\frac{\sqrt{2} H_1 (7 + \cos \phi)^2}{2 + 8 \sin \phi + 14 \cos \phi} d\Omega_2$$ (84)

should be equal to the derivative of a true Hamiltonian, $dH_T$, which here would be a generator of the canonical motion of $H_1$. The existence of such a generator would allow us to construct a quantum theory in which the evolution of $H_1$ would be unitary. This apparently does not hold, since the above one-form is not closed. In what follows, we will replace the cosmological time with a different clock variable.
For brevity, let us restrict to \( \phi \in (0, \phi_1) \) and redefine time \( t_{\text{cos}} \) in two ways:

\[
t_{\text{cos}} = \frac{1 - \cos \phi + 2 \sin \phi}{\sqrt{2}(1 + \cos \phi)} (t_1 + O_1) \quad (85)
\]

\[
t_{\text{cos}} = \frac{1 - \cos \phi + 2 \sin \phi \left( \frac{\pi}{\phi_1} \sin \left( \frac{\pi}{\phi_1} \phi \right) \right) t_2 + O_2}{\sqrt{2}(1 + \cos \phi)}. \quad (86)
\]

Both \( t_1 \) and \( t_2 \) are well defined, with \( t_1 \in (-O_1, \infty) \) for a given \( O_1 \) and \( t_2 \in \left( -\frac{O_1}{\frac{\pi}{\phi_1} \sin \left( \frac{\pi}{\phi_1} \phi \right)}, \infty \right) \) for a given \( O_1 \) and \( \phi \). The times are half-lines and the left endpoints signal the singularity.

Now, the Hubble observable (81) takes the form

\[
H_1 = \frac{1}{t_1 + O_1} = \frac{1}{\phi_1} \sin \left( \frac{\pi}{\phi_1} \phi \right) t_2 + O_2. \quad (87)
\]

The difference between the above formulae is due to the different choice of time, i.e. a different parametrization of the constraint surface, though the function \( H_1 : S \mapsto R \) itself remains unchanged, i.e. attaches real numbers to points in the constraint surface uniquely.

Let us see that definitions (85) and (86) lead to canonical motion in \( H_1 \). First let us examine the evolution in \( t_1 \). Introduce

\[
T_1 := t_1 + O_1
\]

so that

\[
H_1 = \frac{1}{T_1} \quad (89)
\]

and

\[
\omega_S = dT_1 \wedge dr + dO_2 \wedge d\phi + dH_T \wedge dr_1, \quad (90)
\]

where \( H_T = r \) is a true Hamiltonian, which generates the canonical motion of \( H_1 \), in \( t_1 \). For each constant time slice, the symplectic form (90) may be inverted to the Poisson structure

\[
\{ \cdot, \cdot \} \bigg|_{t_1=\text{const}} = \frac{\partial}{\partial T_1} \frac{\partial}{\partial r} - \frac{\partial}{\partial r} \frac{\partial}{\partial T_1} + \frac{\partial}{\partial O_2} \frac{\partial}{\partial \phi} - \frac{\partial}{\partial \phi} \frac{\partial}{\partial O_2}. \quad (91)
\]

Now let us examine the evolution in \( t_2 \). Introduce

\[
T_2 := \frac{\pi}{\phi_1} \sin \left( \frac{\pi}{\phi_1} \phi \right) t_2 + O_2
\]

so that

\[
H_1 = \frac{1}{T_2} \quad (93)
\]

and

\[
\omega_S = dO_1 \wedge dr + dT_2 \wedge d\phi + dH_T \wedge dr_2, \quad (94)
\]

where \( H_T = -\cos \left( \frac{\pi}{\phi_1} \phi \right) \) is a true Hamiltonian, which generates the canonical motion of \( H_1 \), in \( t_2 \). For each constant time slice, the symplectic form (94) may be inverted to the Poisson structure

\[
\{ \cdot, \cdot \} \bigg|_{t_2=\text{const}} = \frac{\partial}{\partial O_1} \frac{\partial}{\partial r} - \frac{\partial}{\partial r} \frac{\partial}{\partial O_1} + \frac{\partial}{\partial T_2} \frac{\partial}{\partial \phi} - \frac{\partial}{\partial \phi} \frac{\partial}{\partial T_2}. \quad (95)
\]

3 This phase space sector consists of all the solutions modulo the interchange of the axes in the homogenous leaf.
5.1. Warm-up: quantization of Dirac observables

We have identified the four-dimensional space of Dirac observables, \((r, \phi, O_1, O_2) \in \mathbb{R}_+ \times (0, \phi_1) \times \mathbb{R} \times \mathbb{R}\), equipped with the symplectic form \(\omega_E\) identical with \(\omega_S\) in (40). By inverting the form in the reduced phase space, one can find the Poisson bracket

\[\{O_1, r\} = 1, \quad \{O_2, \phi\} = 1.\]  

We assign the following operators to the corresponding Dirac observables:

\[r \mapsto \hat{r} = r, \quad O_1 \mapsto \hat{O}_1 = i \frac{\partial}{\partial r}, \quad \phi \mapsto \hat{\phi} = \phi, \quad O_2 \mapsto \hat{O}_2 = i \frac{\partial}{\partial \phi}\]  

so that the following algebra homomorphism is obtained:

\[\hat{\{\hat{O}_1, \hat{r}\}} = 1, \quad \hat{\{\hat{O}_2, \hat{\phi}\}} = 1.\]  

and the physical Hilbert space is defined as

\[\mathcal{H}_{\text{phys}} = L^2(\mathbb{R}_+ \times (0, \phi_1), \, dr \, d\phi).\]  

The formally self-adjoint operator \(i \frac{\partial}{\partial r}\), defined on a half-line, can be made into a self-adjoint operator by the following assignment:

\[i \frac{\partial}{\partial r} = \sqrt{-\frac{\partial^2}{\partial r^2}},\]  

where the Laplacian \(-\frac{\partial^2}{\partial r^2}\) acts on the closure (in the ‘operator norm’) of the following space [17]:

\[\{\psi \in \mathcal{H}_{\text{phys}} : \psi(r = 0) = \mu \cdot \partial_r \psi(r = 0)\},\]  

where \(\mu \geq 0\) enumerates unitarily inequivalent self-adjoint realizations of \(-\frac{\partial^2}{\partial r^2}\). The values \(\mu = 0\) and \(\mu = \infty\) correspond to the Dirichlet and Neumann condition, respectively. The spectrum reads

\[sp_{R_+}(i \partial_r) = R_+.\]  

The formally self-adjoint operator \(i \partial_\phi\) is also unbounded and enjoys many unitarily inequivalent essentially self-adjoint realizations in the space [17]

\[\{\psi \in \mathcal{H}_{\text{phys}} : \psi(0) = e^{i2\pi \kappa} \psi(\phi_1)\} ,\]  

where 0 and \(\phi_1\) are the boundary points of the domain. The parameter \(\kappa \in [0, 1)\) enumerates unitarily inequivalent representations of \(i \partial_\phi\). Its spectrum reads

\[sp(i \partial_\phi) = \frac{\kappa}{\phi_1} + \frac{2\pi n}{\phi_1}, \quad n \in \mathbb{Z}.\]  

This completes the quantization of all the gauge-invariant observables in the Kasner universe. Since the notion of evolution is absent in this model, one cannot ask questions about the fate of singularity.

5.2. Quantization of geometrical observables in two different time variables

5.2.1. Case \(t_1\). Let us use the Schrödinger representation to study the Hubble observable defined in (89) with the Poisson structure given in (91):

\[r \mapsto \hat{r} := -i \frac{d}{dr}, \quad \frac{1}{2} \hat{T}_1 := r, \quad \phi \mapsto \hat{\phi} := \phi, \quad \hat{O}_2 := -i \frac{d}{d\phi}\]  

which act on the Hilbert space

\[\mathcal{H}_{\text{phys}} = L^2(\mathbb{R}_+ \times (0, \phi_1), \, dr \, d\phi).\]  

15
so that the following is satisfied:

\[ \{ \hat{T}_1, r \} = \frac{1}{i}[\hat{T}_1, \hat{r}], \quad \{ \hat{O}_2, \phi \} = \frac{1}{i}[\hat{O}_2, \hat{\phi}] . \]  

(107)

The true Hamiltonian reads

\[ \hat{H}_T = -i \frac{d}{dr} . \]  

(108)

The operator \(-i \frac{d}{dr}\) was discussed in the previous subsection, and we showed that it is essentially self-adjoint in the domain (101). Thus, due to the Stone–von Neumann theorem there exists a unitary operator

\[ U = e^{-i \hat{H}_T} \]  

(109)

which proves that the dynamics of the system is well defined for all \( t \in \mathbb{R} \). This means that the singularity which is reached in finite time in classical theory is resolved at quantum level.

Note that the quantum operators associated with physical measurements (like connection or curvature) may be unbounded. These circumstances, however, are common in quantum theory and do not spoil the singularity resolution.

Let us move to the quantization of \( H_1 \):

\[ \hat{H}_1 = \frac{1}{\hat{T}_1} = \frac{1}{r}, \quad r \in \mathbb{R}_+ , \]  

(110)

which is a well-defined self-adjoint (unbounded) operator on a half-line with the continuous spectrum \( s_{\text{p}}(H_1) = \mathbb{R}_+ \).

5.2.2. Case \( t_2 \). Let us use the Schrödinger representation to study the Hubble observable defined in (93) with the Poisson structure given in (95):

\[ r \mapsto \hat{r} := -i \frac{d}{dr}, \quad \mathcal{O}_1 \mapsto \hat{\mathcal{O}}_1 := r, \quad \phi \mapsto \hat{\phi} := \phi, \quad T_2 \mapsto \hat{T}_2 := -i \frac{d}{d\phi} \]  

(111)

which act on the Hilbert space

\[ \mathcal{H}_{\text{phys}} = L^2(\mathbb{R}_+ \times (0, \phi_1), d\rho d\phi) \]  

(112)

so that the following is satisfied:

\[ \{ \hat{\mathcal{O}}_1, \hat{r} \} = \frac{1}{i}[\hat{\mathcal{O}}_1, \hat{r}], \quad \{ \hat{T}_2, \phi \} = \frac{1}{i}[\hat{T}_2, \hat{\phi}] . \]  

(113)

The true Hamiltonian reads

\[ \hat{H}_T = -\cos \left( \frac{\pi \phi}{\phi_1} \right) . \]  

(114)

The operator \( -\cos \left( \frac{\pi \phi}{\phi_1} \right) \) is bounded, symmetric and hence self-adjoint in the Hilbert space. Due to the Stone–von Neumann theorem, there exists a unitary operator

\[ U = e^{-i \hat{H}_T} \]  

(115)

which proves that the dynamics of the system is well defined for all \( t \in \mathbb{R} \). This again means that the singularity which is reached in finite time in classical theory is resolved at the quantum level.

Let us move to the quantization of \( H_1 \):

\[ \hat{H}_1 = \frac{1}{\hat{T}_2} . \]  

(116)
The operator
\[ \hat{T}_2 = -i \frac{d}{d\phi} \]
has been already discussed and is a well-defined self-adjoint (unbounded) operator with the discrete spectrum
\[ \text{sp} \{ i \partial_\phi \} = \kappa \phi_1 + \frac{2\pi i \phi_1}{n}. \]
Using the spectral theorem and requiring positivity of \( \hat{H}_1 \), we find that the spectrum of the Hubble observable is discrete, bounded and reads
\[ \text{spt}_2 (\hat{H}_1) = \left\{ \left| 1 + \frac{2\pi i \phi_1}{n} \right|, \ n \in \mathbb{Z} \right\}. \]

6. Conclusions
Motivated by the BKL scenario, we started this paper aiming at deriving a quantum theory of the Kasner epoch. This task seemed to be feasible with the use of the reduced phase space method: we defined the kinematical phase space, in which we solved Hamilton's equation of motion; then, we identified Dirac observables and their algebra; finally, we arrived at the physical solutions of the classical theory in terms of Dirac observables and a clock variable. At this point, the quantization is usually performed. However, we realized that the choice of clock variable determined the functional dependence of time-dependent quantities on Dirac observables. In the rest of the paper, we studied the consequences of this fact.

We showed that in addition to the usual ambiguities of quantum theory, in a Hamiltonian constraint system like general relativity, there is also another ambiguity related to the choice of the clock. We have managed to clarify the procedure of encoding evolution in quantum gravity. It turned out that the procedure could be identified with inverting a singular matrix. The matrix is the induced two-form on the constraint surface \( \omega_S \) and its inverse, in a sense, still exists but is ambiguous and represents the Poisson bracket. Different choices of the inverse lead to canonically inequivalent classical theories, which are then quantized. Then the dependence of quantum physics on the choice of time variable can be stated as follows: The Poisson bracket associates a canonical transformation with each phase space function. In classical theory, the Poisson bracket is an auxiliary mathematical structure, which does not affect the physical (observable) content of the theory in the sense that it does not matter which canonical transformation corresponds to which phase space function as long as the equations of motion are equivalent. In quantum theory, however, the physical quantities are associated with operators on the Hilbert space, in which they act as generators of unitary transformations. The correspondence between classical and quantum theory is the one between the canonical transformations and the unitary ones. Therefore, the Poisson structure is not auxiliary but essential for this correspondence and thus all ambiguities in canonical formulations of classical theory are expected to lead to quantum theories with different physical content. Thus, for each choice of time, one may find a distinct spectrum for a given partial observable. We have shown that this is the case for a directional Hubble parameter for which we were able to obtain both continuous and discrete spectrum, depending on the choice of the clock variable. Which spectrum, if any, is the correct one? Answering this question is beyond the framework of general relativity and usual quantum mechanics.

In the view of this result, one should construct all the quantum theories treating all the possible time parameters on equal footing. The relation between the resultant canonically inequivalent theories surely deserves further study. This will be the subject of next papers by the present author.

What is the physical interpretation of the obtained result that theories of gravity with different time parameters are canonically inequivalent? Is the evolution of the universe not an
We consider a manifold $\mathcal{M}$ equipped with the metric
\[ ds^2 = -N^2 \, dt^2 + \sum_i a_i^2 \, (dx^i)^2, \]
where $i = 1, 2, 3,$ and on which we introduce the vector fields and the dual 1-forms
\[ e_0 = \frac{1}{N} \partial_t, \quad e_i = \frac{1}{a_i} \partial_i, \quad \sigma^0 = N \, dt, \quad \sigma^i = a_i \, dx^i, \]
so that the following relations hold:
\[ e_\mu \cdot e_\nu = \eta_{\mu \nu}, \quad \sigma_\mu (e_\nu) = \delta_\mu^\nu, \]
where $\mu, \nu = 0, 1, 2, 3.$ We assume that $[18]$
\[ d \left( \sum_\mu \sigma^\mu e_\mu \right) = \sum_\mu \left( d\sigma^\mu - \sum_\nu \sigma^\nu \omega^\mu_{\ \nu} \right) e_\mu = 0 \]
and obtain the connection $\Omega$:  
\[ d\sigma = \sigma \Omega, \quad \Omega = \|\omega^\mu_{\ \nu}\|, \]
which is a matrix of 1-forms. It is uniquely determined from the condition $\omega_{\sigma \mu} + \omega_{\mu \nu} = 0,$ and equals
\[ \Omega = \begin{pmatrix} 0 & \frac{\dot{a}_1}{N a_2} \sigma^1 & \frac{\dot{a}_2}{N a_3} \sigma^2 & \frac{\dot{a}_3}{N a_1} \sigma^3 \\ \frac{\dot{a}_1}{N a_2} \sigma^2 & 0 & 0 & 0 \\ \frac{\dot{a}_2}{N a_3} \sigma^3 & 0 & 0 & 0 \\ \frac{\dot{a}_3}{N a_1} \sigma^1 & 0 & 0 & 0 \end{pmatrix}. \]

From $\Omega$ we compute the curvature matrix $\Theta$:  
\[ \Theta = \|\theta^\mu_{\ \nu}\| = d\Omega - \Omega^2, \]
which is equal to
\[ \Theta = \begin{pmatrix} 0 & \frac{1}{N a_1} \left( \frac{\dot{a}_1}{a_2} \right) \sigma^0 \sigma^1 & \frac{1}{N a_2} \left( \frac{\dot{a}_2}{a_3} \right) \sigma^0 \sigma^2 & \frac{1}{N a_3} \left( \frac{\dot{a}_3}{a_1} \right) \sigma^0 \sigma^3 \\ \frac{1}{N a_1} \left( \frac{\dot{a}_1}{a_2} \right) \sigma^0 \sigma^1 & 0 & \frac{1}{N a_2} \left( \frac{\dot{a}_2}{a_3} \right) \sigma^1 \sigma^2 & \frac{1}{N a_3} \left( \frac{\dot{a}_3}{a_1} \right) \sigma^1 \sigma^3 \\ \frac{1}{N a_2} \left( \frac{\dot{a}_2}{a_3} \right) \sigma^0 \sigma^2 & \frac{1}{N a_3} \left( \frac{\dot{a}_3}{a_1} \right) \sigma^1 \sigma^2 & 0 & \frac{1}{N a_1} \left( \frac{\dot{a}_1}{a_2} \right) \sigma^2 \sigma^3 \\ \frac{1}{N a_3} \left( \frac{\dot{a}_3}{a_1} \right) \sigma^0 \sigma^3 & \frac{1}{N a_1} \left( \frac{\dot{a}_1}{a_2} \right) \sigma^1 \sigma^3 & \frac{1}{N a_2} \left( \frac{\dot{a}_2}{a_3} \right) \sigma^2 \sigma^3 & 0 \end{pmatrix}. \]
The Riemann curvature tensor is now given by
\[
\theta_{\mu\nu} = \frac{1}{2} \sum_{\alpha,\beta} R_{\alpha\mu\beta} \sigma^{\alpha} \sigma^{\beta}
\]  
from which we calculate the Ricci tensor \( R_{\nu\beta} \):
\[
\| R_{\nu\beta} \| = \begin{pmatrix}
R_{00} & 0 & 0 & 0 \\
0 & R_{11} & 0 & 0 \\
0 & 0 & R_{22} & 0 \\
0 & 0 & 0 & R_{33}
\end{pmatrix},
\]  
where
\[
R_{00} = -\sum_i \frac{1}{N\dot{a}_i} \left( \frac{\dot{N}}{N} \right) \dot{a}_i,
\]
\[
R_{ii} = \frac{1}{N\dot{a}_i} \left( \frac{\dot{N}}{N} \right) \dot{a}_i, \quad \sum_{k \neq i} \left( \frac{\dot{N}}{N} \right) \dot{a}_k \dot{a}_i = -\frac{\ddot{H}_i}{H_i^2}.
\]  
In the Friedman cosmology, it is common to use the Hubble parameter \( H \) and the deceleration parameter \( q \), which in the case of the Kasner universe can also be introduced, for each of the three directions separately:
\[
H_i = \frac{\dot{a}_i}{N\dot{a}_i}, \quad q_i = -\frac{1}{N\dot{a}_i} \left( \frac{\dot{N}}{N} \right) \dot{a}_i = -\frac{\ddot{H}_i}{H_i^2}.
\]  
Note that these parameters determine all the components of the curvature matrix \( \Theta \).

**Appendix B. Parametrization of Dirac observables**

It is important to realize the precise notion of the Dirac observable. It is sometimes claimed that the Dirac observable is a kinematical phase space function, which commutes weakly with the Hamiltonian constraint. This is not precise enough. In a constrained system, the physical motion is realized in the constraint surface, let us say \( H = 0 \). This equality implicates the embedding of the constraint surface into the kinematical phase space, \( E : S \mapsto P \). One cannot pull back functions from \( S \) to functions on \( P \), since the range of \( E \) is restricted only to \( H = 0 \). This means that the Dirac observable cannot be defined as a function of the kinematical phase coordinates. The proper definition is as follows: Dirac’s observable \( D_i \) is a constraint surface function, which commutes with the Hamiltonian constraint \( H \), i.e.
\[
\{ O_D, H \} = 0.
\]  
In the Kasner universe, the above equality in the convenient gauge \( N = 4\sqrt{X_1 X_2 X_3} \) takes the following form:
\[
\sum_{i \neq j \neq k} (X_i P_j + X_j P_k) \left( P \frac{\partial O_D}{\partial P_i} - X_i \frac{\partial O_D}{\partial X_i} \right) = 0
\]  
and we obtain
\[
O_D = O_D(\Gamma_i, \Omega_{ij}),
\]  
where
\[
\Omega_{ij} = (\Gamma_i + \Gamma_j)(\Gamma_j + \Gamma_k) \ln |P_i| - (\Gamma_i + \Gamma_j)(\Gamma_j + \Gamma_k) \ln |P_j|
\]  
and satisfy the relation
\[
\Omega_{ij} - \Omega_{kj} = \Omega_{ik}.
\]
These are solutions to (B.1) in a given gauge. Their restriction to the constraint surface (18) is gauge invariant and gives the four-dimensional space of Dirac observables, \( \mathcal{O}_R \). We could alternatively define the Dirac observable as equivalence classes with the equivalence relation

\[
\mathcal{O}_D \sim \mathcal{O}_d \iff \mathcal{O}_D \approx \mathcal{O}_d \iff \mathcal{O}_D = \mathcal{O}_d + C,
\]

where ‘\( \approx \)’ denotes ‘equals on the constraint surface’ and \( C \approx 0 \) is a constraint. This, however, leads to the ambiguity in ‘parameterization’ of Dirac observable as there is no natural projection from the kinematical phase space to the reduced phase space. The important issue here is that the Poisson bracket is well defined between the equivalence classes (see equation (80)).

**Appendix C. The Kasner metric in terms of the cosmological time and Dirac observables**

Let us express the physical solutions in terms of Dirac observables and cosmological time \( t_{\cos} \):

\[
ds^2 = -dt_{\cos}^2 + 2\tilde{a}_1 \left(-\frac{r(7 + \cos \phi)}{16\sqrt{2}}t_{\cos} \right)^{2\frac{2-2\cos \phi + 4\sin \phi}{7 + \cos \phi}} (dx^1)^2
\]
\[
+ 2\tilde{a}_2 \left(-\frac{r(7 + \cos \phi)}{16\sqrt{2}}t_{\cos} \right)^{2\frac{2-2\cos \phi + 4\sin \phi}{7 + \cos \phi}} (dx^2)^2
\]
\[
+ 2\tilde{a}_3 \left(-\frac{r(7 + \cos \phi)}{16\sqrt{2}}t_{\cos} \right)^{2\frac{3+5\cos \phi}{7 + \cos \phi}} (dx^3)^2.
\]

where

\[
\tilde{a}_1 = e^{\frac{1}{2}(\alpha_1(7\cos^2\phi+4\cos\phi)+(\alpha_2(5\cos^2\phi+4\sin\phi)))},
\]
\[
\tilde{a}_2 = e^{\frac{1}{2}(\alpha_2(7\cos^2\phi+4\cos\phi)+(\alpha_3(5\cos^2\phi+4\sin\phi)))},
\]
\[
\tilde{a}_3 = e^{\frac{1}{2}(\alpha_3(7\cos^2\phi+4\cos\phi)+(\alpha_1(5\cos^2\phi+4\sin\phi)))}.
\]

The minus sign in front of the time, \(-t_{\cos}\), comes from our convention that as time grows the universe approaches the singularity, that is, \( t_{\cos} \in (-\infty, 0) \). Now we can relate the parameters \( p_1 \), \( p_2 \) and \( p_3 \) occurring in the metric (5) to the Dirac observables:

\[
p_1 = \frac{\sum_i \Gamma_i}{\sum_i \Gamma_i} = \frac{2 - 2\cos \phi + 4\sin \phi}{7 + \cos \phi},
\]
\[
p_2 = \frac{\sum_i \Gamma_i}{\sum_i \Gamma_i} = \frac{2 - 2\cos \phi - 4\sin \phi}{7 + \cos \phi},
\]
\[
p_3 = \frac{\sum_i \Gamma_i}{\sum_i \Gamma_i} = \frac{3 + 5\cos \phi}{7 + \cos \phi}.
\]

We note that all the Dirac observables play a role provided that the topology of the universe is compact. If, for instance, we set \( \Sigma \) infinite in all directions, then \( \phi \) is the only Dirac observable, since the values of the scale factors \( a_i \) are non-physical, and consequently \( r \), \( \mathcal{O}_1 \) and \( \mathcal{O}_2 \) are not Dirac observables any longer.

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