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REVIEW ARTICLE

THE PROBLEM OF TIME AND GAUGE INVARIANCE IN THE QUANTIZATION OF COSMOLOGICAL MODELS I. CANONICAL QUANTIZATION METHODS

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This paper is the first of two parts of a work reviewing some approaches to the problem of time in quantum cosmology which were put forward last decade and related to the problems of reparametrization and gauge invariance of quantum gravity. In the present part we recall the basic features of quantum geometrodynamics and minisuperspace cosmological models, and discuss fundamental problems of the Wheeler –DeWitt theory. Various attempts to find a solution to the problem of time are considered in the framework of the canonical approach. Possible solutions are investigated making use of minisuperspace models, that is, using systems with a finite number of degrees of freedom. At the same time, in the last section of the paper we extend our consideration beyond the minisuperspace approximation and briefly review the promising ideas by Brown and Kuchař, who propose that dust interacting only gravitationally can be used for time measuring, and the unitary approach by Barvinsky and collaborators. The latter approach admits both canonical and path integral formulations and anticipates the consideration of recent developments in the path integral approach in the second part of our work.

Проблема времени и калибровочная инвариантность в квантовании космологических моделей. I. Методы канонического квантования
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Статья является первой частью работы, содержащей обзор некоторых подходов к проблеме времени в квантовой космологии, выдвинутых в прошедшее десятилетие и связанных с проблемами репараметризационной и калибровочной инвариантности квантовой теории гравитации. В первой части мы напоминаем основные особенности квантовой геометродинамики и космологических моделей в минисуперпространстве и обсуждаем фундаментальные проблемы теории Уилера–ДеВитта. Различные попытки найти решение проблемы времени рассматриваются в рамках канонического подхода. Возможные решения проблемы исследуются с помощью моделей в минисуперпространстве, т.е. для систем с конечным числом степеней свободы. В то же время в последнем разделе статьи мы расширяем наше рассмотрение за пределы приближения минисуперпространства и даем краткий обзор идей Брауна и Кухаржа, которые высказали предположение, что пыль, взаимодействующая только с гравитацией, может быть использована для измерения времени, а также унитарного подхода Барвинского и его коллег. Последний подход допускает формулировку как в рамках канонических методов, так и в рамках фейнмановского интегрирования по траекториям, что предваряет рассмотрение во второй части нашей работы недавних результатов, полученных с помощью интегрирования по траекториям.

1. Introduction

It is generally accepted now that the initial stages of cosmological evolution must be described by quantum cosmology. The need for a quantum theory of the early Universe is a logical consequence of the fact that classical general relativity is not applicable in the vicinity of a cosmological singularity. As was pointed out by Grishchuk and Zeldovich [36], a full cosmological theory must include a notion about the origin of spacetime itself, which is essentially a quantum gravitational phenomenon. In the framework of such a full theory one

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should consider both the gravitational field and matter quantized.

The standard approach to quantum cosmology includes three basic steps: a classical theory for the dynamics, a quantization prescription in terms of a wave function or a propagator, and interpretation. The second and third steps are highly non-trivial because general relativity includes general covariance as a central feature. Accordingly, the Hamiltonian formulation for the gravitational field is that of a constrained system. Any attempt to save gauge invariance in quantum theory of gravity creates a number of problems.

The problem of time is the most well-known difficulty of the Wheeler–DeWitt quantum geometrodynamics which is a theoretical basis for modern quantum cosmology. This problem is inseparably linked with others among which are the problems of Hilbert space (positive-definite inner product), reparametrization non-invariance and operator ordering. The problem of time has been discussed in a plenty of papers (see, e.g., [12, 14–17, 32, 43, 50, 68–71]. The paper by Vilenkin [71] was one of the first works where the problem of time was considered in the context of quantum cosmology. In the paper by Unruh [68] it was shown that a solution of this problem may require some modification of the theory of gravity (including the Hamiltonian constraint). Isham [43] gave a very informative and profound review of the problem, a classification of existing approaches to the problem of time and many references can be found therein. Philosophical aspects of the problem were discussed in [70, 12].

It is not the purpose of the present paper to give an exhaustive consideration to all approaches to the problem of time which are widespread in modern literature. We also do not intend to repeat earlier papers on this subject. Our aim is to review some ideas put forward in the last decade and to show that the problem of time is closely related to that of reparametrization and gauge invariance of quantum gravity. Understanding the latter circumstance may shed some new light on a possible solution of this problem.

Our work consists of two parts. In the present part we shall recall the basic features of quantum geometrodynamics and minisuperspace cosmological models, discuss the fundamental problems of the Wheeler–DeWitt theory and give a layout of the paper (Sec. 2). Further, in Sec. 3 we shall consider various attempts to find a solution to the problem of time in the framework of the canonical approach. We shall investigate possible solutions making use of minisuperspace models with a finite number of degrees of freedom, which will help us to clarify some points. However, in Sec. 4 we shall expand our consideration beyond the minisuperspace approximation and briefly review the promising ideas by Brown and Kuchař [11] and also by Barvinsky and collaborators [4–6, 8].Barvinsky's programme, which can be presented both in the canonical and in the path integral formalisms, is of great importance for understanding the relationship between imposing a gauge condition and introducing time in quantum gravity.

In the second part of our work we shall consider in more detail two approaches within the scope of Feynman's path integration scheme. The first approach by Simeone and collaborators [24, 30, 33–35, 62–66] is essentially based on Barvinsky's ideas, in particular, on the idea of deparametrization (reduction to physical degrees of freedom). This proposal is gauge-invariant and lies in the course of the unitary approach to quantization of gravity. Another approach by Savchenko, Shestakova and Vereshkov [57–61] is rather radical. It is an attempt to take into account the peculiarities of the Universe as a system without asymptotic states, which leads to the conclusion that quantum geometrodynamics constructed for such a system is, in general, gauge-non-invariant theory. However, this theory is shown to be mathematically consistent, and the problem of time is solved in this theory in a natural way.

2. Quantum cosmology: basic issues

2.1. The gravitational field as a constrained system

The Wheeler–DeWitt (WDW) quantum geometrodynamics is based upon canonical quantization of constrained systems. The first step in this procedure is rewriting of the Einstein–Hilbert action S, which is a functional of the spacetime metric $g_{\mu\nu}(X)$, in a Hamiltonian form. Then the dynamics is given by a succession of spacelike three-dimensional hypersurfaces in four-dimensional spacetime. By introducing the timelike parameter τ and the internal coordinates x^a ($a = 1, 2, 3$), the theory can be written in terms of a new set of variables: the spatial three-metric g_{ab} on a hypersurface and the velocity U^μ with which this surface evolves in spacetime. The normal and tangential components of the velocity U^μ are the lapse and shift functions defined by Kuchař [45] as a generalization of those introduced by Arnowitt, Deser and Misner [2] $N = (-g^{00})^{-1/2}$, $N^a = g^{ab} g_{b0}$. After the extrinsic curvature

$$K_{ab} = \frac{1}{2N}\left(\nabla_a N_b + \nabla_b N_a - \frac{dg_{ab}}{d\tau}\right),$$

describing the evolution of the spacelike hypersurface embedded in spacetime is defined, the Lagrangian form of the Einstein action will be

$$S[g_{ab}, N, N^a] = \int_{\tau_1}^{\tau_2} d\tau \int d^3x\, N ({}^3g)^{1/2} (K_{ab}K^{ab} - K^2 + {}^3R - 2\Lambda), \quad (1)$$

where ${}^3R$ is the scalar curvature of space, $K = g^{ab}K_{ab}$ and Λ is the cosmological constant.

The Hamiltonian form of the action is obtained by defining the canonical momenta

$$p^{ab} = -2G^{abcd}K_{cd},$$
$$G^{abcd} = \frac{1}{4}({}^3g)^{1/2}(g^{ac}g^{bd} + g^{ad}g^{bc} - 2g^{ab}g^{cd}), \quad (2)$$

G^{abcd} being the DeWitt supermetric. Then we have

$$S[g_{ab}, p^{ab}, N, N^a] = \int d\tau \int d^3x \left(p^{ab}\frac{dg_{ab}}{d\tau} - N\mathcal{H} - N^a\mathcal{H}_a\right), \quad (3)$$

where

$$\begin{aligned}\mathcal{H} &= \frac{1}{2}G_{abcd}p^{ab}p^{cd} - ({}^3g)^{1/2}({}^3R - 2\Lambda),\\ \mathcal{H}_a &= -2g_{ac}\nabla_d p^{cd},\\ G_{abcd} &= ({}^3g)^{-1/2}(g_{ac}g_{bd} + g_{ad}g_{bc} - 2g_{ab}g_{cd}).\end{aligned} \quad (4)$$

The lapse and shift functions are not determined; when we require the action to be stationary under an arbitrary variation of N and N^a, the *Hamiltonian and momentum constraints* are obtained:

$$\mathcal{H} = 0, \quad (5)$$

$$\mathcal{H}_a = 0. \quad (6)$$

The presence of these constraints reflects the general covariance of the theory. However, the status of the two constraints is different: a basic role is given to the Hamiltonian constraint (5) which generates the dynamics of 3-geometry (the change of canonical data under transition from one spacelike hypersurface to another). A dynamical character of the Hamiltonian constraint results from the non-standard quadratic dependence of $\mathcal{H}$ on the momenta p^{ab}. It is the reason why the Hamiltonian constraint has no analogy in other gauge theories. The arbitrariness of N leads to the so-called many-fingered nature of time: since the lapse corresponds to the velocity of motion of the three-hypersurface in the normal direction, as N depends on x^a and τ, the separation between two successive hypersurfaces is different at different points of spacetime, and time thus has a local character.

The momentum constraints (6) generate diffeomorphisms of the 3-metric g_{ab} and are similar to constraints in the Yang–Mills theory. In their operator form after quantization, they are considered as the conditions that a wave function is invariant under coordinate transformations of the 3-metric. Since the wave function is also independent of the lapse and shift functions, it leads to the conclusion that the wave function must depend only on 3-geometry. But the latter statement remains to be declarative: it has no mathematical realization. The wave function always depends on a specific form of the metric, which gives rise to reparametrization non-invariance of the WDW quantum geometrodynamics.

2.2. Quantization and fundamental problems of Wheeler–DeWitt theory

In the Dirac canonical quantization, the classical constraints are turned into operators and are imposed on the wave function, which must be annihilated by them. Hence the constraint $\mathcal{H} = 0$ leads to the WDW equation

$$\mathcal{H}\Psi = 0, \quad (7)$$

A solution to this equation corresponding to the observable physical Universe is singled out by boundary conditions which acquire the status of a fundamental law. However, this formulation of the WDW theory is not complete: such questions as the structure of Hilbert space or which quantities should be considered as observables, remain open. At the same time, these questions are of great importance from the viewpoint of the construction of any quantum theory.

The problem of time is a consequence of the fact that the gravitational Hamiltonian is a linear combination of constraints (see (3)), which leads to a static picture of the world. DeWitt [25] commented it as follows: Physical significance can be ascribed only to intrinsic dynamics of the Universe while its four-dimensional description, in particular, its evolution in time, are irrelevant.

At the same time, any possible solution of *the problem of Hilbert space* implies some solution of the problem of time. One cannot determine the structure of Hilbert space if the inner product of state vectors is not defined. The inner product is to be conserved in time, so some definition of time is required. As a rule, time is identified with a function of variables of configurational or phase space. But in this case the status of time variable differs from what it is in ordinary quantum mechanics, namely, an extrinsic parameter related to an observer and marking changes in a physical system.

Another problem, which is closely connected with the problem of time, is *the problem of observables*. According to the Dirac scheme, observables are quantities which have vanishing Poisson brackets with constraints. It is indeed true for electrodynamics where all observables are gauge-invariant. But in the case of gravity this criterion leads to the conclusion that all observables should not depend on time. Then one loses a possibility of describing the time evolution of a gravitational system in terms of observables.

The next problem is that of *reparametrization non-invariance*: at the classical level, the gravitational constraints can be written in various equivalent forms, while at the quantum level, after replacing the momenta by operators, these different forms of the constraints become non-equivalent. It is a consequence of the fact that the DeWitt supermetric G^{abcd} depends, in general, on the lapse function N [41] (in (2) the choice $N = 1$ has been made). In principle, one could replace N with another function of some new variable $\tilde{N}$ and the 3-metric g_{ab}: $N = v(\tilde{N}, g_{ab})$. This leads to changing the supermetric G^{abcd}, so that the corresponding WDW equations would have different solutions. A relation between these solutions can be found in a very restricted class of parametrizations [38]. We shall return to this point in Part II, where it will be argued that reparametrization non-invariance of the WDW equation can be understood as a hidden gauge non-invariance.

Let us also point to *the problem of a global structure of spacetime*. One can apply the canonical quantization procedure only if spacetime has the topology $R \times \Sigma$, where Σ is some 3-manifold. In any other case it is impossible to introduce globally (in the whole spacetime) a set of spacelike hypersurfaces without intersections and other singularities, and it is impossible to introduce a global time. In most papers, simple enough cosmological models are considered, and this problem seems to be not so important. But the existence of this problem, as well as the previous ones, shows that WDW quantum geometrodynamics needs to be modified.

2.3. Interpretation

Apart from mathematical problems, WDW quantum geometrodynamics has no generally accepted interpretation. Of course, the absence of a clear interpretation cannot be a reason to revise a theory if the theory is mathematically consistent. In the case of quantum geometrodynamics, however, the problem of its interpretation results from its mathematical difficulties.

Thus, there does not exist *a precise probability interpretation* of the wave function. It is related to the mathematical problem of Hilbert space discussed above. Some authors have proposed to start from a definition of time allowing one to obtain a Schrödinger equation [37, 20, 28, 18]; in this case, the physical inner product can be defined as

$$(\Psi_2|\Psi_1) = \int dq\, \Psi_2^* \,\hat{\mu}\, \Psi_1,$$

with $\hat{\mu}_{t'} = \delta(t-t')$, so that the integral is evaluated at fixed time t'. The central objection to such a procedure is that the resulting wave functions are solutions of the Wheeler–DeWitt equation (or can be related to them) only in the case of a restricted class of minisuperspace models.

Another possibility is to straightforwardly solve the WDW equation in terms of a set of coordinates including global time [71, 37, 35, 65, 66]: $\{q^i\} = \{t, q^\gamma\}$; in this case the physical inner product can be written as

$$(\Psi_2|\Psi_1) = \frac{i}{2}\int dq \left[\Psi_1^* \frac{\partial \Psi_2}{\partial t} - \Psi_2 \frac{\partial \Psi_1^*}{\partial t}\right], \qquad (8)$$

where the integration is done at fixed t and is restricted to the coordinates q^γ. This does not solve the problem of defining a conserved positive probability because a Klein–Gordon inner product is obtained, which is in general not positive-definite. Since the difficulties arise from the fact that the WDW equation is of second order in all its derivatives, in the recent years there have also been proposals based on Dirac's solution to the problem, and some authors have introduced a spinor wave function for cosmological models [51, 52, 53].

Once adopting the WDW theory, one should admit that a wave function satisfying Eq. (7) describes the past of the Universe as well as its future with all observers being inside the Universe in different stages of its evolution, and all observations to be made by these observers. This picture might be considered within the framework of the many-worlds interpretation of the wave function proposed by Everett [27] and applied to geometrodynamics by Wheeler [73]. However, it does not seem that the WDW quantum geometrodynamics is a mathematical realization of the Everett conception. Indeed, the wave function satisfying Eq. (7) and certain boundary conditions are thought to be a branch of a many-worlds wave function that corresponds to a certain universe, other branches being selected by other boundary conditions. The information about all possible actions of an observer through the whole history of the Universe can be contained *only* in boundary conditions. At the same time, any mathematical realization of the Everett conception implies that a state of a closed system is a superposition, each element of which is a product of some state of the first subsystem and a relative state of the second one, one of the subsystems being a measuring apparatus. To find such a superposition for the Universe we need to define full sets of orthonormal states of the subsystems, which returns us to the problem of Hilbert space.

Barvinsky and Ponomariov [3] discussed a mathematical realization of the Everett conception. Though the full set of orthonormal states was not defined, they showed that, to define an inner product in Hilbert space, one should impose some gauge condition, which makes the wave function depend to a certain extent on this gauge condition. The state described by the wave function was interpreted as a relative state of the Universe for the chosen gauge condition. In Sec. 4.2 we shall comment the central points of the unitary approach to quantum theory of gravity proposed by Barvinsky. It is important that the work of Barvinsky and Ponomariov has demonstrated that in any mathematical realization of the Everett conception a wave function must contain information on both the geometry of the Universe and the reference frame, fixed by a gauge condition with which this geometry could be studied.

Further, the question arises if a theory, in which the wave function depends on a gauge condition, could be gauge-invariant. Barvinsky and his collaborators gave a positive answer to this question. The quantization procedure proposed by them is thought to be a "projection" of the gauge-independent Dirac–WDW formalism [1]. Equivalence with the Dirac–WDW scheme can be proved in the one-loop approximation and for some special quasiclassical states. In [7], Barvinsky wrote that the validity of extrapolating the unitary approach to quantum cosmology is based on the success of quantizing gauge theories in asymptotically flat spacetime in unitary gauges. We would note in this connection that the success of quantization in asymptotically flat spacetime is crucially based on the presence of asymptotic states; the latter makes possible to solve the full set of constraints and gauge conditions within the limits of perturbation theory and to split off the threedimensionally transversal gravitational degrees of freedom from the so-called "nonphysical" ones. In a general situation without asymptotic states it may happen that gauge invariance should be abandoned in a formally consistent formulation. It is worth emphasizing that in both cases fixing a gauge enables one to introduce time in quantum theory of gravity.

2.4. Canonical approach and an outline of this paper

The canonical approach, in a broad sense, unifies such methods as the Dirac quantization [26] and the quantization in unitary gauges which means a transition to a reduced phase space of true physical degrees of freedom (see, e.g., [7]). These methods are close to ordinary quantum theory in the sense that the quantization procedure includes constructing a Hamiltonian formalism.

This part of our work is entirely devoted to canonical methods. The aim of Sec. 3 is to illustrate that without introducing a physical time it is difficult to give a clear interpretation to solutions to the WDW equation for different models. On the other hand, the minisuperspace approach, where one deals with cosmological models with a finite number of degrees of freedom, makes treatable a search for a wave function with all desired properties of a consistent theory, a precise notion of evolution and a well-defined probability. We shall review the most representative developments within this line of work, namely, those which start from different programmes of deparametrization or reduction to physical degrees of freedom as a preliminary step before quantization [4–6, 8, 9, 20–22, 28, 29, 37, 42, 46, 48, 72]. In Sec. 2.5 we shall recall the main features of minisuperspace models used in our further consideration.

A possible solution to the problem of time consists in the identification of time with some function of variables of configurational or phase space. To anticipate our consideration, in Sec. 2.6 we shall formulate a condition to be satisfied by admissible functions. The notion of intrinsic and extrinsic time will also be explained in this section.

The definition of time enables one to come to a Schrödinger equation with a square-root true Hamiltonian. In Sec. 3.1 we shall discuss a relation between the Schrödinger equation and the WDW equation and show that solutions to the Schrödinger equation also satisfy the WDW equation if the Hamiltonian does not depend on the variable defined as time.

In Sec. 3.2 we shall demonstrate, following to Hájícek, that the requirement of unitarity of a resulting theory may be related to a correct choice of the time variable. We shall touch upon the WKB solutions to the WDW equation in Sec. 3.3, and it will be pointed out there that the definition of classically forbidden and allowed regions is difficult for models where a clear notion of time is absent.

The role of identification of time will be illustrated in Sec. 3.4–3.6 for the Taub Universe. The behaviour of the wave function in minisuperspace leads to a certain choice of solutions to the WDW equation considered in Sec. 3.4, while other solutions are discarded. On the other hand, the time identification procedure based on the analogy with the ideal clock results in the opposite choice for discarding the solutions. Namely, as will be shown in Sec. 3.5, solutions to the Schrödinger equation can be used to select a set of solutions to the WDW equation. In some cases it is possible to define a phase time in such a way that the corresponding solution to the WDW equation will have an evolutionary form. An example will be given in Sec. 3.6. In this situation we do not need the Schrödinger equation to select solutions, though there is a correspondence between the solutions to the WDW equation with the time variable and those of the Schrödinger equation considered in the preceding section. Interpretation of these solutions is straightforward if the Hamiltonian is time-independent.

As was mentioned above, a possible way of introducing time into the theory consists in imposing some gauge condition. In the canonical formalism, it may be done by means of a time-dependent gauge condition. This line of work will be discussed in Sec. 3.7. A weak point of this approach is that different gauge choices lead to nonequivalent quantizations.

In Sec. 3.8 we shall consider a coordinate choice which gives rise to the WDW equation with a time-inedpendent Hamiltonian. In this case there exists a direct correspondence between the WDW and Schrödinger equations and their solutions. Unfortunately, this correspondence exists only for a limited class of models.

Sec. 3.9 will be devoted to rather an exotic two-component approach, in which the WDW equation is reduced to a set of first-order equations with respect to time. It resembles the transition from the Klein–Gordon equation to the Dirac equation and requires introducing a spinor wave function. This procedure also leads to a Schrödinger equation and an appropriate interpretation.

A disadvantage of the methods presented in Sec. 3 is that they can be applied to restricted classes of models. Their application depends to a large txtent on the choice of suitable coordinates and the resulting form of the Hamiltonian constraint. In Sec. 4 we shall briefly review general approaches formulated for the full gravitational theory. In Sec. 4.1 we shall consider an interesting idea by Brown and Kuchař [11] that dust interacting only gravitationally can serve as a time variable. This proposal leads to a special form of the constraints and, eventually, to a Schrödinger equation. It lies entirely within the scope of the canonical formalism. On the other hand, the Barvinsky's approach [4–6, 8], which we have already mentioned in Sec. 2.3 and whose main points we shall recall in Sec. 4.2, admits both the canonical and path integral formulations. It anticipates a consideration of recent developments in the path-integral approach in the second part of our work.

2.5. Minisuperspace models

If all but a finite number of degrees of freedom of the classical theory are set to zero, we obtain the *minisuperspace approximation*; the choice of an homogeneous lapse and zero shift lead to an action whose Hamiltonian form is

$$S[q^i, p_i, N] = \int_{\tau_1}^{\tau_2} \left(p_i \frac{dq^i}{d\tau} - N\mathcal{H} \right) d\tau, \tag{9}$$

where

$$\mathcal{H} = G^{ij}\, p_i p_j + V(q). \tag{10}$$

Here G^{ij} is a reduced version of the DeWitt supermetric and V is the potential, which depends on the curvature and includes terms corresponding to coupling between the gravitational field and matter fields; it is understood that spatial integration has already been performed, so that only integration on τ remains. As the shift is null, the momenta read $p_i = \frac{1}{N} G_{ij} \frac{dq^j}{d\tau}$. On the classical path we have the Hamilton canonical equations

$$\frac{dq^i}{d\tau} = N[q^i, \mathcal{H}], \qquad \frac{dp_i}{d\tau} = N[p_i, \mathcal{H}] \tag{11}$$

and the minisuperspace version of the Hamiltonian constraint

$$\mathcal{H} = 0.$$

The evolution of the lapse N is arbitrary, as it is not determined by the canonical equations. Hence, the separation between two successive spatial three-surfaces, although globally the same, is still undetermined: this is the minisuperspace version of the many-fingered nature of time of the full theory.

The spatial line element of an isotropic and homogeneous cosmological model has the form

$$dl^2 = g_{ab} dx^a dx^b$$

where g_{ab} is the space metric, whose components are functions of time. The isotropy and homogeneity hypothesis leads to the fact that the curvature depends on only one parameter: for $k = 0$ we have a flat universe, for $k = -1$ the universe is open, and for $k = 1$ the universe is closed. The spacetime metric has then the Friedmann–Robertson–Walker form [49]

$$\begin{aligned} ds^2 &= N^2 d\tau^2 \\ &- a^2(\tau) \left(\frac{dr^2}{1 - kr^2} + r^2 d\theta^2 + r^2 \sin^2\theta d\varphi^2 \right), \end{aligned} \tag{12}$$

where $a(\tau)$ is the spatial scale factor.

The hypothesis of homogeneity and isotropy completely determines the form of the space metric leaving free only the curvature; restricting the hypothesis to homogeneity without any other symmetry assumption allows for much more freedom. Homogeneity implies that the metric properties are the same at any point of space. A mathematical formulation of this is given by a set of transformations which leave the metric unchanged. For a homogeneous non-Euclidean space, the transformations of the symmetry group leave invariant three linear differential forms; these forms are not total differentials of functions of the coordinates, but they read

$$\sigma^i = e^i_a dx^a$$

where $a = 1, 2, 3$ and e^i are three independent vectors. The differential forms fulfil $d\sigma^i = \epsilon_{ijk} \sigma^j \times \sigma^k$. The invariant space metric can then be written as [49]

$$dl^2 = g_{ij} \sigma^i \sigma^j = g_{ij} (e^i_a dx^a)(e^j_b dx^b),$$

so that the spatial metric tensor has the components

$$g_{ab} = g_{ij} e^i_a e^j_b.$$

Possible anisotropic cosmologies are comprised by the Bianchi models and the Kantowski–Sachs model [55]. By introducing the diagonal 3×3 matrix β_{ij} their spacetime metrics can be written as

$$ds^2 = N^2 d\tau^2 - \mathrm{e}^{2\Omega(\tau)} (\mathrm{e}^{2\beta(\tau)})_{ij} \sigma^i \sigma^j. \tag{13}$$

However, the spatial geometry of Bianchi models is essentially different from that of the Kantowski–Sachs model, because a continuous transformation carrying from the latter to the Bianchi form does not exist.

2.6. Global phase time

A globally good time is a function $t(q^i, p_i)$ which monotonically increases along a dynamical trajectory, that is, each surface $t = \mathrm{const}$ in phase space is crossed by a dynamical trajectory only once; hence the successive states of the system can be parametrized by this function. This means that $t(q^i, p_i)$ must fulfil the condition

$$\mathrm{H}^A \frac{\partial t}{\partial x^A} > 0 \tag{14}$$

where H^A are components of the Hamiltonian vector

$$\mathbf{H} \equiv (\mathrm{H}^q, \mathrm{H}^p) = \left(\frac{\partial \mathcal{H}}{\partial p}, -\frac{\partial \mathcal{H}}{\partial q} \right). \tag{15}$$

The definition of Poisson brackets clearly leads to the equivalent condition [37]

$$[t, \mathcal{H}] > 0. \tag{16}$$

(If we define a scaled constraint

$$H = \mathcal{F}^{-1} \mathcal{H}, \quad \mathcal{F} > 0,$$

it can easily be shown that H and $\mathcal{H}$ are equivalent, in the sense that they describe the same parameterized system: their field lines, which coincide with the classical trajectories, are proportional on the constraint surface. Thus if we can find a function $\bar{t}(q^i, p_i)$ with the property

$$[\bar{t}, H] > 0,$$

we know that $\bar{t}(q^i, p_i)$ monotonically increases along the dynamical trajectories associated to both H and $\mathcal{H}$, and it is also a global phase time.)

Since the supermetric G^{ik} does not depend on the momenta, a function $t(q^i)$ is a global time if the bracket

$$[t(q^i), \mathcal{H}] = [t(q^i), G^{ik} p_i p_k] = 2\frac{\partial t}{\partial q^i} G^{ik} p_k \tag{17}$$

is positive-definite. Hence if the supermetric has a diagonal form and one of the momenta vanishes at a given point of phase space, then no function of only its conjugated coordinate can be a global time. For a constraint whose potential can be zero for finite values of the coordinates, the momenta p_k can be all equal to zero at a given point, and $[t(q^i), \mathcal{H}]$ can vanish. Hence an *intrinsic time* $t(q^i)$ [47] exists only if the potential in the constraint has a definite sign. In the most general case, a global phase time should be a function including the canonical momenta; this is called an *extrinsic time* $t(q^i, p_i)$ [44, 74], because the momenta are related to the extrinsic curvature K_{ab} which describes the evolution of spacelike three-dimensional hypersurfaces in four-dimensional spacetime: in the case of no matter fields, we have

$$p_i \equiv p^{ab} = -2G^{abcd} K_{cd}.$$

The existence of time in terms of only the coordinates is related to the fact that, in some special cases which do not represent the general features of gravitation, the coordinates can be obtained in terms of the momenta with no ambiguities; however, this is not always possible, and a consistent quantization can require working with an extrinsic time.

3. Canonical quantization

Imposing the operator form of the original Hamiltonian constraint on a wave function yields the usual WDW equation, which is second-order in all its derivatives. A Schrödinger equation, instead, requires a preliminary definition of time, and then it includes the notion of a true (non-vanishing) Hamiltonian. Though the WDW equation is the most common choice for the canonical quantization of minisuperspaces, it is difficult to interpret the resulting wave function in terms of a conserved positive-definite inner product. The Schrödinger quantization, instead, allows one to define a conserved inner product, and then a clear probability interpretation can be given to the wave function.

In some cases, a Schrödinger equation has been obtained by splitting the constraint into two disjoint sheets given by the two signs of the momentum p_0 conjugated to a coordinate q^0 identified as time; this yields a canonical quantization consisting in two equations of first order in $\partial/\partial q^0$. Thus we have a pair of Hilbert spaces, each with its corresponding Schrödinger equation. In this case we can say that the Schrödinger quantization preserves the topology of the constraint surface, that is, splitting of the classical solutions into two disjoint subsets has its quantum version in splitting of the theory into two Hilbert spaces [67].

The subtleties involved in splitting of the original constraint into two constraints, namely $K^+ = 0$ and $K^- = 0$, were first carefully considered by Blyth and Isham [10]. These two constraints together are classically equivalent to the original Hamiltonian constraint $H = 0$, which is quadratic in all momenta; that is, classical dynamics takes place in one of the two sheets of the constraint surface determined by the sign of a non-vanishing momentum. But at the quantum level this equivalence is no more fulfilled if time appears in the potential: a function in the kernel of the operator $\hat{K}^+$ or $\hat{K}^-$ is not annihilated by the operator $\hat{H}$, but by $\hat{H}$ plus terms corresponding to a commutator between $\hat{p}_0$ and the square-root true Hamiltonian resulting from its time-depending potential. It must be emphasized that these terms cannot be eliminated by operator ordering.

We shall then begin with a discussion of the mentioned work by Blyth and Isham; also, Hájícek's thorough discussion of the relation between unitarity and the identification of time [37] is reproduced and commented in detail. Then a review of two standard procedures will follow, one by Halliwell and the other by Moncrief and Ryan, in the framework of a WDW equation straightforwardly obtained from the constraints of different homogeneous models *without* a previous analysis of the problem of time. We shall emphasize unsatisfactory points of such a procedure, and then show some improvements based on the identification of global time as a step before quantization. Within this context, we shall also discuss the role of the Schrödinger equation, both as an auxiliary tool for selecting solutions of the WDW equation and as the central equation for quantization; in particular, we analyse an interesting approach starting with identification of time by means of gauge fixing and also a two-component formulation inspired in Dirac's solution to the problems of the Klein–Gordon equation.

3.1. WDW equation and Schrödinger equation

A good introduction to the problem of choosing between these two formulations can be found in an early work by Blyth and Isham, Ref. [10]. Within the context of canonical quantization of a Friedmann–Robertson–Walker universe with matter in the form of a scalar field, the authors carefully study the reduction procedure leading to a Schrödinger equation and establish its inequivalence with the standard WDW approach. The analysis starts with identification of one of the canonical coordinates of the model as a time variable (in practice, the scale factor; see below), thus reducing the system and treating it in the usual canonical form with a true time and a true non-vanishing Hamiltonian. The result is the time-dependent Schrödinger equation

$$i\frac{\partial \Psi}{\partial t} = h\Psi, \tag{18}$$

where h is a square-root true Hamiltonian. This requires a definition by means of the spectral theorem, assuming that the square root is taken on a positive-definite self-adjoint operator. This point relies on the correct identification of time (see the next section); for example, the scale factor is a bad time variable for any model allowing for $p_\Omega = 0$.

The usual WDW approach would lead, instead of (18), to the second-order equation

$$-\frac{\partial^2\Psi}{\partial t^2} = h^2\Psi, \tag{19}$$

which in the most general case is not equivalent to (18). In fact, by acting with h on both sides of the Schrödinger equation, the result obtained is

$$-\frac{\partial^2\Psi}{\partial t^2} - i\frac{\partial h}{\partial t}\Psi = h^2\Psi. \tag{20}$$

Clearly the solutions of (18) and (19) will then be different, unless the potential in the square-root Hamiltonian h does not depend on the variable defined as time. In the case that h commutes at different times, integration of (18) yields

$$\Psi(x,t) = \exp\left(-i\int_{t_0}^{t} h(s)ds\right)\Psi(x,t_0), \tag{21}$$

where x stands for the true degrees of freedom of the system. A decomposition in terms of eigenstates $\Psi_E(x,t)$ can be given, with

$$\Psi_E(x,t) = \exp\left(-i\int_{t_0}^{t} E(s)ds\right)\Psi_E(x,t_0),$$

and $\Psi_E(x,t_0)$ a solution of the equation

$$h^2(x,t_0)\Psi_E(x,t_0) = E^2\Psi_E(x,t_0).$$

Here there is no problem with the square of the true Hamiltonian h^2 because this is an eigenvalue equation for a fixed time t_0. Once a definite solution is obtained, it can be provided with physical meaning because the corresponding inner product is well defined, which is not the case for the Klein–Gordon type equation (19). Though the first choice of time by the authors is the scale factor, other choices are also explored, including extrinsic times. This is unavoidable for any Friedmann–Robertson–Walker model with a constraint including a potential which can be zero for finite values of the coordinates.

3.2. Unitarity and time

Here we shall reproduce and analyse the early work by Hájícek where the relation existing between a correct choice of time and the obtention of a unitary theory [37] is clearly established, and the analogy between the existence of a global phase time for a parametrized system and the possibility of a globally good gauge choice for a gauge system is discussed.

Instead of the models studied by Hájícek, we shall consider a generic (scaled) constraint of the form

$$-\tilde{p}_1^2 + \tilde{p}_2^2 + A\mathrm{e}^{(a\tilde{q}^1 + b\tilde{q}^2)} = 0 \tag{22}$$

with $a \neq b$, where we have used tildes to denote that the variables are not necessarily the original ones, but a set $\{\tilde{q}^i, \tilde{p}_i\}$ including the coordinate $\tilde{q}^0$ which is a global time. This Hamiltonian corresponds to some models of interest, like dilaton cosmologies, the Kantowski–Sachs universe and even the Taub universe after a canonical transformation. It is easy to show that a coordinate change exists, leading to

$$H = -p_x^2 + p_y^2 + \zeta\mathrm{e}^{2x} = 0 \tag{23}$$

with $\mathrm{sign}(\zeta) = \mathrm{sign}(A/(a^2 - b^2))$. Depending on the sign of the constant A in the constraint (22), these models admit as global phase time the coordinates x or y. In case $\zeta > 0$, the time is $t = \pm x$, so that, following Ref. [37], we can define the reduced Hamiltonians as $h_\pm = \pm\sqrt{p_y^2 + \zeta\mathrm{e}^{2x}}$, and we can write the Schrödinger equations

$$i\frac{\partial}{\partial x}\Psi(x,y) = \mp\left(-\frac{\partial^2}{\partial y^2} + \zeta\mathrm{e}^{2x}\right)^{1/2}\Psi(x,y) \tag{24}$$

(note that in this case we obtain a time-dependent potential). If, instead, we have $\zeta < 0$, the time is $t = \pm y$ and the reduced Hamiltonians corresponding to each sheet of the constraint surface are $h_\pm = \pm\sqrt{p_x^2 - \zeta\mathrm{e}^{2x}}$; the associated Schrödinger equations are

$$i\frac{\partial}{\partial y}\Psi(x,y) = \mp\left(-\frac{\partial^2}{\partial x^2} - \zeta\mathrm{e}^{2x}\right)^{1/2}\Psi(x,y). \tag{25}$$

For both $\zeta > 0$ and $\zeta < 0$ we have a pair of Hilbert spaces, each one with its corresponding Schrödinger equation, and a conserved positive-definite inner product allowing for the usual probability interpretation of the wave function. This is analogous to the obtention of two quantum propagators, one for each disjoint theory, mentioned in the context of path integral quantization [67, 8].

A point to be remarked is that, as a result of a correct time definition, in both cases the reduced Hamiltonians are real, so that the evolution operator is self-adjoint, and the resulting quantization is unitary. Instead, a wrong choice of time, like for example $t = \pm x$ in the case $\zeta < 0$, leads to a Hamiltonian for a reduced system which is not real for all allowed values of the variables, and we obtain a non-unitary theory.

There is an aspect, however, which should be marked, though it was not emphasized in Ref. [37]. In the case $\zeta > 0$ the Schrödinger equations can be obtained starting from the constraint written as a product of two linear constraints:

$$\left(-p_x + \sqrt{p_y^2 + \zeta\mathrm{e}^{2x}}\right)\left(p_x + \sqrt{p_y^2 + \zeta\mathrm{e}^{2x}}\right) = 0, \tag{26}$$

and it is then clear that the potential depends on time. Therefore, though at the classical level this product is equivalent to the constraint (22), in its operator version the two constraints differ in terms associated to the commutators between p_x and the potential ζe^{2x}. Hence, depending on which of the two classically equivalent constraints we start from, we obtain different quantum theories. Observe that this problem appears in the case for which the WDW equation leads to a result in which the identification of positive and negative-energy solutions is not apparent, at least in the standard form: for the case $\zeta > 0$, $t = \pm x$ we obtain the WDW solutions

$$\Psi_\omega(x,y) = \left[a_+(\omega)e^{i\omega y} + a_-(\omega)e^{-i\omega y}\right] \times \left[b_+(\omega)J_{i\omega}(\sqrt{|\zeta|}e^x) + b_-(\omega)N_{i\omega}(\sqrt{|\zeta|}e^x)\right], \quad (27)$$

with $J_{i\omega}$ and $N_{i\omega}$ the Bessel and Neumann functions of imaginary order, respectively; note that the time dependence appears in the argument of Bessel functions. Instead, for $\zeta < 0$, $t = \pm y$, the solutions are of the form

$$\Psi_\omega(x,y) = \left[a_+(\omega)e^{i\omega y} + a_-(\omega)e^{-i\omega y}\right] \times \left[b_+(\omega)I_{i\omega}(\sqrt{|\zeta|}e^x) + b_-(\omega)K_{i\omega}(\sqrt{|\zeta|}e^x)\right], \quad (28)$$

where $I_{i\omega}$ and $K_{i\omega}$ are modified Bessel functions. In this case the usual factors $\sim e^{i\omega t}$ associated with definite energy states are obtained; moreover, now the WDW solutions are the same, corresponding to the Schrödinger equation, so that the inner product is well defined.

We insist on a point regarding the topology of the constraint: the choice of a Schrödinger formulation always preserves the classical geometry of the constraint surface [13, 67]; in the case of a time-dependent potential this is achieved by introducing the commutator mentioned above, whose form is $\left[\sqrt{\sum(\hat{\tilde{p}}_r)^2 + V(\hat{\tilde{q}}^i)}, \hat{\tilde{p}}_0\right]$ (where $r \neq 0$, and V stands for the potential in the scaled Hamiltonian constraint H). It is clear that this cannot be avoided by any operator ordering.

3.3. Approximate solutions of the WDW equation

The impossibility of explicitly integrating the WDW equation except for a limited class of models has led to several attempts of quantization based on approximations valid for different regions of phase space. Consider the Hamiltonian constraint of a closed ($k = 1$) homogeneous and isotropic universe with a scalar field ϕ and zero cosmological constant; assume a generic dependence of the potential with ϕ, namely $V(\phi)$. The associated WDW equation obtained by replacing $p \to -i\partial/\partial q$ (and considering a trivial factor ordering) reads

$$\left(\frac{\partial^2}{\partial\Omega^2} - \frac{\partial^2}{\partial\phi^2} + V(\phi)e^{6\Omega} - e^{4\Omega}\right)\Psi(\Omega,\phi) = 0. \quad (29)$$

Halliwell analysed the region of phase space such that $|V'/V| \ll 1$ and found solutions whose variation with the matter field was small, so that the ϕ derivative can be neglected. In the region where the scale factor is small, the resulting WKB solutions have the exponential form [39]

$$\Psi(\Omega,\phi) \sim \exp\left(\pm\frac{1}{3V(\phi)}(1 - e^{2\Omega}V(\phi))^{3/2}\right) \quad (30)$$

and are associated with a classically forbidden region. For large values of the scale factor, the WKB solutions have the oscillatory form

$$\Psi(\Omega,\phi) \sim \exp\left(\pm\frac{i}{3V(\phi)}(e^{2\Omega}V(\phi) - 1)^{3/2}\right). \quad (31)$$

These solutions correspond to what is considered the classically allowed region. Both kinds of solution can be matched by means of the usual WKB matching procedure. In case $e^{2\Omega}V(\phi) \ll 1$, it can be shown that the oscillatory wave function is peaked about a solution of the form

$$e^{\Omega} \sim e^{\sqrt{V}\tau}, \qquad \phi \sim \phi_0,$$

which corresponds to an inflationary behaviour. (For the case $V(\phi)=0$ an exact solution can be easily obtained in terms of modified Bessel functions. This is also the case if $V(\phi)=0$ in a flat ($k = 0$) model with a nonzero cosmological constant). Depending on the form of $V(\phi)$, the regions considered by Halliwell may be related to those to which the analysis should be restricted if one were to define an intrinsic time in the case of models for which this cannot be done globally. We should signal that the absence of a notion of time within this formulation, besides making unclear the interpretation of the formalism, makes not completely justified the identification of classically forbidden or allowed regions, since this would require a separation between true degrees of freedom and time; we will return to this point, with more detail, in the following paragraph.

3.4. Exact solutions without time

In the literature we can find different exact solutions to the WDW equation for minisuperspace models. An example among those which do not start from an explicit deparametrization is the solution found for the Taub universe (see the next section) by Moncrief and Ryan [54] in the context of an analysis of a Bianchi type-IX universe with rather a general operator ordering of the Hamiltonian constraint [40]. In the case of the most trivial ordering they found the following general solution to the WDW equation:

$$\Psi(\Omega,\beta_+) = \int_0^\infty d\omega\, F(\omega) \times K_{i\omega}\left(\frac{1}{6}e^{2\Omega-4\beta_+}\right)K_{2i\omega}\left(\frac{2}{3}e^{2\Omega-\beta_+}\right), \quad (32)$$

where $K_{i\omega}$ are modified Bessel functions of imaginary argument; modified functions I would also appear, but they are discarded because they are not well-behaved for $\beta_+ \to \pm\infty$ (see below). In the particular case that $F(\omega) = \omega \sinh(\pi\omega)$, Moncrief and Ryan showed that the wave function can be written in the form

$$\Psi(\Omega, \beta_+) = R(\Omega, \beta_+) \mathrm{e}^{-S} \tag{33}$$

with

$$S = \frac{1}{6} \mathrm{e}^{2\Omega} \left(\mathrm{e}^{-4\beta_+} + 2\mathrm{e}^{2\beta_+} \right).$$

This wave function has a nice feature that for values of Ω near the singularity (that is, the scale factor near to zero), the probability is spread over all possible degrees of anisotropy given by β_+, while for large values of the scale factor the probability is peaked around the isotropic Friedmann–Robertson–Walker closed universe; the authors, however, abstain from a naive interpretation of the wave function, and they note that there are different probability interpretations that would not agree with this one.

There are two central objections to this straightforward procedure, and both arise from the absence of a notion of time in the formalism: first, since time has not been identified, it is not possible to speak about a conserved probability, hence the meaning of the wave function is not clear at all. Second, the choice of a set of solutions made by discarding the modified Bessel functions I would only be justified by a bad behaviour of the wave function in a region of the configuration space determined by the form of the potential of *a true Hamiltonian*. This is not the case, because a true Hamiltonian is necessarily related to a physical time, which is lacking in this formulation; in fact, we shall immediately see that a careful analysis of this point leads to the exactly opposite choice for discarding Bessel functions. The procedure (see the next section) will be based in an intermediate line of work consisting in combining the WDW equation with a Schrödinger equation.

3.5. Boundary conditions for WDW solutions from a Schrödinger equation

The problem mentioned in the two above examples could be solved by an approach beginning with the identification of a global phase time like that in Ref. [18], whose authors obtain a Schrödinger equation and use its solutions to select a set of solutions of the WDW equation. The underlying idea is that a typical constraint of a parametrized system, which is linear in the momentum conjugated to the true time, is hidden in the formalism of gravitation. This is an extension of the analogy between an ideal clock and empty isotropic models [9, 28, 23]: The constraint of the ideal clock

$$\mathcal{H} = p_t - t^2 = 0$$

yields the Schrödinger equation

$$i \frac{\partial \Psi}{\partial t} = -t^2 \Psi, \tag{34}$$

which is of parabolic form and has the only solution $\Psi = \mathrm{e}^{it^3/3}$. As a first step to obtain the constraint of a minisuperspace, a canonical transformation leading to a constraint quadratic in the momenta is performed: defining $Q = p_t$, $P = -t$, we obtain

$$\mathcal{H} = -P^2 + Q = 0.$$

(The Hamiltonian of empty isotropic models results from the second transformation $Q = \tilde{V}(\Omega)$, $P = p_\Omega (d\tilde{V}/d\Omega)^{-1}$, with $\tilde{V}$ the potential defined in Ref. [23]). The differential equation associated with the constraint is now of hyperbolic form:

$$\frac{\partial^2 \Psi}{\partial Q^2} + Q\Psi = 0. \tag{35}$$

As this equation is of second order, it has two independent solutions, which are the Airy functions $Ai(-Q)$ and $Bi(-Q)$. The central point is that while $Bi(-Q)$ diverges as $Q \to -\infty$, $Ai(-Q)$ is well-behaved (in fact, it vanishes) in this limit, and it is a Fourier transform of the solution of Eq. (34). This provides a rule for selecting solutions of the hyperbolic equation: physical solutions are those which are in correspondence with the solutions of the Schrödinger equation.

This line is then followed in [18] for quantizing the Taub universe, which is a particular case of the Bianchi type IX model [49, 55]. In the absence of matter, its Hamiltonian constraint reads

$$H = p_+^2 - p_\Omega^2 + \frac{1}{3} \mathrm{e}^{4\Omega} (\mathrm{e}^{-8\beta_+} - 4\mathrm{e}^{-2\beta_+}) = 0, \tag{36}$$

where β_+ determines the degree of anisotropy. The Taub universe involves a potential which vanishes for finite values of the coordinates, so making impossible the definition of an intrinsic time in terms of the original variables. By defining $x = \Omega - 2\beta_+$, $y = 2\Omega - \beta_+$ the constraint can be put in the form

$$H = p_x^2 - p_y^2 + \frac{1}{9} (\mathrm{e}^{4x} - 4\mathrm{e}^{2y}) = 0 \tag{37}$$

(the authors work with a different choice of the constants); then the corresponding WDW equation

$$\left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{1}{9} \mathrm{e}^{4x} + \frac{4}{9} \mathrm{e}^{2y} \right) \Psi(x, y) = 0 \tag{38}$$

is solved as was done by Moncrief and Ryan. The authors obtain the solutions

$$\Psi_\omega(x, y) = \left[a(\omega) I_{i\omega} \left(\frac{2}{3} \mathrm{e}^y \right) + b(\omega) K_{i\omega} \left(\frac{2}{3} \mathrm{e}^y \right) \right] \times \left[c(\omega) I_{i\omega/2} \left(\frac{1}{6} \mathrm{e}^{2x} \right) + d(\omega) K_{i\omega/2} \left(\frac{1}{6} \mathrm{e}^{2x} \right) \right], \tag{39}$$

with I and K modified Bessel functions. Then they consider a canonical transformation generated by

$$\Phi_1(y, s) = -\frac{2}{3} \mathrm{e}^y \sinh s, \tag{40}$$

leading to the following form of the Hamiltonian constraint:

$$H(s, x, \pi_s, \pi_x) = -p_s^2 + p_x^2 + \frac{1}{9}\mathrm{e}^{4x} = 0, \tag{41}$$

so that the momentum p_s is negative-definite, and the time is $t = s$; hence the constraint is written as a product of two factors linear in p_s, the first one positivee-definite, and the second one a constraint including a true Hamiltonian $h = \sqrt{p_x^2 + (1/9)\mathrm{e}^{4x}}$ which is time-independent (as we have already remarked, this makes possible an equivalence of the linear constraint and the original quadratic one). This constraint then leads to the Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(x, t) = \left(-\frac{\partial^2}{\partial x^2} + \frac{1}{9}\mathrm{e}^{4x}\right)^{1/2}\Psi(x, t). \tag{42}$$

It is necessary to have a prescription to give a precise meaning to the Hamiltonian operator; the square root containing the derivative operator must be understood as its binomial expansion, which allows one to propose solutions of the form $\sim \phi(x)\mathrm{e}^{-i\omega t}$. According to this interpretation, the contribution of the functions $I_{i\omega/2}((1/6)\mathrm{e}^{2x})$ is discarded because they diverge in the classically forbidden region associated with the exponential potential $\frac{1}{9}\mathrm{e}^{4x}$; the functions $I_{i\omega}((2/3)\mathrm{e}^{y})$, instead, are not discarded, because in this picture the coordinate y is associated with the definition of time. In fact, by transforming the solutions of the WDW equation, it is shown that those corresponding to the solutions of the Schrödinger equation are precisely the functions $I_{i\omega}((2/3)\mathrm{e}^{y})$, while the functions $K_{i\omega}((2/3)\mathrm{e}^{y})$ must be ruled out because they cannot be associated with definite energy states of the true Hamiltonian h. It is remarkable that the functions in the selected subspace do not decay in what was previously considered a classically forbidden zone; note then the central difference with the result of the preceding subsection.

3.6. WDW equation with extrinsic time

A possible deparametrization and canonical quantization programme can start from a form of the Hamiltonian constraint such that a global phase time is easily identified as one of the canonical coordinates (in the general case, this could require a preliminary canonical transformation); this is reflected in the corresponding WDW equation, and hence the resulting wave function has an evolutionary form. If the reduced Hamiltonian does not depend on time, the wave function may be interpreted as it is in ordinary quantum mechanics. We shall illustrate this line of work with a solution for the Taub universe [35].

If we admit a double sign in the generating function for the canonical transformation, leading to a constraint with a non-vanishing potential, then the Hamiltonian (41) allows one to immediately define time as

$$t = -s \ \mathrm{sign}(p_s).$$

As we shall see in Part II, this time can be obtained by choosing a simple canonical gauge condition, which, in the variables $\tilde{q}^i$ including a global time, has the form $s = \eta T(\tau)$, $\eta = \pm 1$. The corresponding WDW equation is

$$\left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial s^2} - \frac{1}{9}\mathrm{e}^{4x}\right)\Psi(x, s) = 0. \tag{43}$$

This equation has the set of solutions [35]

$$\Psi_\omega(x, s) = \left[a(\omega)\mathrm{e}^{i\omega s} + b(\omega)\mathrm{e}^{-i\omega s}\right] \times \left[c(\omega)I_{i\omega/2}\left(\frac{1}{6}\mathrm{e}^{2x}\right) + d(\omega)K_{i\omega/2}\left(\frac{1}{6}\mathrm{e}^{2x}\right)\right], \tag{44}$$

where $\pm s$ is a global phase time. The contribution of the functions $I_{i\omega/2}$ should be discarded since they are not well-behaved for large values of x; now this is completely justified, since the exponential $\sim \mathrm{e}^{4x}$ is the potential of a true Hamiltonian. Then, recalling that $t = \pm s$, the wave function can be given in terms of a set of definite-energy solutions:

$$\Psi_\omega(x, t) = a(\omega)\mathrm{e}^{-i\omega t}K_{i\omega/2}\left(\frac{1}{6}\mathrm{e}^{2x}\right). \tag{45}$$

This reflects that the two theories, corresponding to two sheets (in terms of the new variables) of the constraint surface, are equivalent [65].

The solutions of this WDW equation correspond to those of the Schrödinger equation of the preceding section. This procedure allows one to obtain them without the necessity of defining a prescription for the square root operator, but only by choosing trivial factor ordering; differing from the previous treatment, now these solutions are not merely considered as a tool for imposing boundary conditions, but are understood as the wave function of the model. A point to be remarked is that in this description the role of the original momenta, though unavoidably provided the topology of the constraint surface in the original variables, is restricted to the global phase time $s = \pm\mathrm{arcsinh}\left(\frac{1}{2}(p_\Omega + p_+)\mathrm{e}^{(-2\Omega+\beta_+)}\right)$; another coordinate entering into the wave function is a simple function of only the original coordinates.

Though this procedure is the most straightforward, including a correct notion of time, an unsatisfactory point is that the resulting wave function can be interpreted in terms of probabilities because the constraint of the model considered here leads to the same solutions for both the WDW and the Schrödinger equations; hence we can define the probability by means of the ordinary Schrödinger inner product, which is conserved and positive-definite. In the case of a model with a time-depending potential, this would not be possible, and though we could isolate time and obtain an evolutionary wave function, its meaning would not at all be clear (see, however, Sec. 3.8 for a possible solution for a restricted class of models).

3.7. Gauge fixing and Schrödinger equation for isotropic models

As we have already pointed out, a close relation existing between the identification of time and gauge fixing suggests a possible way of solving the problem of time in quantum cosmology. This was strongly supported by, e.g., Barvinsky [8] (see below), and we have developed the idea for its application in the path integral for homogeneous cosmologies (see below and [66]). An interesting development of this line of work within the canonical formalism is that by Cavaglià, De Alfaro and Filippov in [20]. In their proposal, canonical gauge fixing is used to reduce the system: one degree of freedom is given as a function of the remaining ones and the time parameter τ, and a true (called "effective" by the authors) Hamiltonian is obtained; this Hamiltonian may in general depend on the time parameter. The gauge choice is dictated by the simplicity of the Hamiltonian for the reduced system. Once the reduction is performed, the system is quantized in reduced canonical phase space; this is achieved by writing a Schrödinger equation which is in general τ-dependent. In a given gauge, the time parameter is connected with the canonical degree of freedom that has been eliminated.

The authors illustrate their proposal studying a Friedmann–Robertson–Walker universe with matter in the form of a conformal scalar field (CS) and of a SU(2) Yang–Mills field (YM) [19]. The corresponding Hamiltonian constraint is

$$-H_{GR} + H_{CS} + H_{YM} = 0, \qquad (46)$$

where H_{GR} is the pure gravitation Hamiltonian and

$$\begin{aligned} H_{CS} &= \frac{1}{2}\left(p_\chi^2 + V(\chi)\right), \\ H_{YM} &= \frac{1}{3}\left(\frac{1}{2}p_\xi^2 + V(\xi)\right). \end{aligned}$$

Different gauge choices and the resulting Schrödinger equations are explored. For a gauge condition in terms of the gravitational degree of freedom like [31], $p_\Omega + \frac{1}{12}\mathrm{e}^\Omega \cot\tau = 0$, the equation

$$i\frac{\partial}{\partial\tau}\Psi(\xi,\chi,\tau) = (H_{CS} + H_{YM})\Psi(\xi,\chi,\tau) \qquad (47)$$

is obtained; its solution gives a wave function for both matter fields. Rather a different choice connects the conformal field with the time parameter: $p_\chi - \chi\cot\tau = 0$. This gauge leads to a Schrödinger equation for the metric and the Yang–Mills field:

$$i\frac{\partial}{\partial\tau}\Psi(\xi,\Omega,\tau) = (H_{YM} - H_{GR})\Psi(\xi,\Omega,\tau). \qquad (48)$$

An explicit solution is given for the simple case of a closed universe with a scalar field ϕ with $V(\phi) = 0$. The gauge condition $p_\Omega - 12\mathrm{e}^\Omega \sinh\left(\frac{\tau}{\sqrt{3}}\right) = 0$ yields the equation

$$\left(\frac{\partial}{\partial\tau} \mp \frac{\partial}{\partial\phi}\right)\Psi(\phi,\tau) = 0 \qquad (49)$$

for the only physical degree of freedom ϕ. The solutions are of the form

$$\Psi(\phi,\tau) = f(\phi \pm \tau). \qquad (50)$$

A particular solution is $\Psi(\phi,\tau)\mathrm{o}^{-(\phi\pm\tau)^2/2\sigma}$, which represents a universe whose maximum probability follows the classical path $\phi = \pm\tau$.

Apart from the usual problem of possibly non-equivalent quantizations related to different gauge choices, this procedure has the advantage that, instead of a WDW equation (even one with time among the coordinates), a Schrödinger equation is obtained. Hence the wave function has the same properties of that in ordinary quantum mechanics: an evolutionary form, a conserved current and positive density. Note that the price for this achievement has been the choice of gauges in terms of not only the coordinates but also the momenta, so that the resulting time is in general extrinsic.

3.8. Avoiding non-equivalent formulations

As we have seen, the central obstruction for the existence of a trivial correspondence between the WDW and Schrödinger solutions for minisuperspaces is a constraint with a time-dependent potential. For a class of models including some of those studied in the preceding sections, a coordinate choice avoiding the decision between inequivalent quantum theories can be introduced [67]. Consider the constraint (22) and define

$$\begin{aligned} u &= \alpha\exp\left(\frac{a\tilde{q}^1 + b\tilde{q}^2}{2}\right)\cosh\left(\frac{b\tilde{q}^1 + a\tilde{q}^2}{2}\right), \\ v &= \alpha\exp\left(\frac{a\tilde{q}^1 + b\tilde{q}^2}{2}\right)\sinh\left(\frac{b\tilde{q}^1 + a\tilde{q}^2}{2}\right), \end{aligned} \qquad (51)$$

with $\alpha = \sqrt{|A|}$. These coordinates allow one to write the constraint in the equivalent (scaled) form

$$H - p_u^2 + p_v^2 + \eta m^2 = 0, \qquad (52)$$

with $\eta = \mathrm{sign}(A)$ and $m^2 = 4/|a^2 - b^2|$. It is clear that commutators cannot appear now; hence the WDW equation is equivalent to two Schrödinger equations. The time is u or v, depending on η. The double sign given by η corresponds to both possible sheets of the constraint surface where the evolution can take place.

Let us illustrate this coordinate choice with some simple dilatonic cosmologies (see [66] and references therein); consider the scaled constraint

$$H = -p_\Omega^2 + p_\phi^2 + 2c\mathrm{e}^{6\Omega+\phi} = 0.$$

which corresponds to a flat model with the dilaton field ϕ. For $c < 0$ we have $t = \pm v$, while for $c > 0$ we obtain $t = \pm u$. In case $c < 0$ (for which the dilaton ϕ itself is a globally good time as $p_\phi \neq 0$), we obtain $-\infty < t < \infty$ on both sheets of the constraint determined by the sign of p_v; in case $c > 0$ (which admits Ω as a global time), instead, we have that t goes from $-\infty$ to 0 on the sheet $p_u > 0$ and from 0 to ∞ on the sheet $p_u < 0$, with

$t \to 0$ corresponding to the singularity $\Omega \to -\infty$. If we include in the model a non-vanishing antisymmetric field $B_{\mu\nu}$ coming from the NS-NS sector of effective string theory, the constraint turns to

$$H = -p_\Omega^2 + p_\phi^2 + 2c\mathrm{e}^{6\Omega+\phi} + \lambda^2 \mathrm{e}^{-2\phi} = 0.$$

which in principle does not admit the proposed coordinate change. Moreover, in case $c < 0$ the model does not admit an intrinsic time. However, because these models come from the low energy string theory, which makes sense in the limit $\phi \to -\infty$, the $\mathrm{e}^\phi \equiv V(\phi)$ factor in the first term of the potential satisfies $V(\phi) = V'(\phi) \ll 1$, and we can replace $c\mathrm{e}^\phi$ with the constant $\overline{c} \ll c$. We can then perform the canonical transformation introduced for the Taub universe to obtain a constraint with only one term in the potential:

$$H = -p_\Omega^2 + p_s^2 + 2\overline{c}\mathrm{e}^{6\Omega} = 0,$$

and we can apply our procedure starting from this constraint. As before, for $\overline{c} < 0$ we obtain $t = \pm v$, while for $\overline{c} > 0$ we obtain $t = \pm u$. Now, because both u and v depend on the coordinate s which involves in its definition the original momenta, the time is extrinsic (note that in case $\overline{c} < 0$ an intrinsic time does not exist). However, in case $\overline{c} > 0$, t behaves with Ω as it did in the absence of the antisymmetric field; t goes from $-\infty$ to 0 on the sheet $p_u > 0$ of the constraint surface and from 0 to ∞ on the other sheet, while $t \to 0$ for the singularity $\Omega \to -\infty$.

3.9. Two-component wave function

A two-component formulation is a possible way to associate a set of differential equations which are first-order in the time derivative with a Klein–Gordon type equation, as is the WDW one. Hence a Schrödinger equation is obtained, to which the well-known resolution procedures can be applied and an interpretation in terms of a well-defined inner product can be given. As was recently shown in Refs. [51, 52, 53], such an idea can be effectively carried out for some minisuperspace models. The procedure reduces resolution of the WDW equation to an eigenvalue problem analogous to that of a non-relativistic harmonic oscillator and a series of algebraic equations which can be solved by iteration. Application of the theory of pseudo-Hermitian operators [53] allows one to solve the problem of constructing an invariant positive-definite inner product on the space of solutions of the WDW equation.

The method has been exemplified with a Friedmann–Robertson–Walker universe with matter in the form of a massive scalar field ϕ. The corresponding second-order equation is reduced by identifying the logarithm of the scale factor Ω as a time variable, and defining the wave function

$$\Psi = \frac{1}{\sqrt{2}} \begin{pmatrix} \psi + i\dot{\psi} \\ \psi - i\dot{\psi} \end{pmatrix}, \tag{53}$$

where dots mean derivatives with respect to Ω, and the time-dependent Hamiltonian operator

$$H = \frac{1}{2} \begin{pmatrix} 1 + D & -1 + D \\ 1 - D & -1 - D \end{pmatrix}, \tag{54}$$

where $D - \partial^2/\partial\phi^2 - k\mathrm{e}^{4\Omega} + m^2\phi^2\mathrm{e}^{6\Omega}$. This leads to the Schrödinger equation

$$i\dot{\Psi} = H\Psi \tag{55}$$

which is solved by finding solutions to the eigenvalue problem $H\Psi_n = E_n\Psi_n$ (see Ref. [52] for details). For the closed ($k = 1$) model, imaginary eigenvalues are obtained for $\mathrm{e}^\Omega > m$; the corresponding eigenvectors are null. The not completely satisfactory feature of imaginary eigenvalues is associated with the fact that the scale factor is really not a global time for a closed Friedmann–Robertson–Walker universe.

4. Beyond the minisuperspace approximation

In this section we shall review two approaches dealing with the full theory: the first one consists in a proposal of Brown and Kuchař [11] for using dust as time within the canonical formalism; this leads to a constraint linear in the momentum conjugated to the corresponding field, and therefore to a Schrödinger equation; the second one is Barvinsky's programme [4, 5, 6, 8], presented both in the canonical and path integral formalisms; this contains the basic ideas underlying any deparametrization procedure.

4.1. Dust as time

The proposal presented by Brown and Kuchař in Ref. [11] is to find a medium which, when quantizing the system in the Dirac formulation for constrained systems, leads to a Schrödinger equation — a functional one, because the proposal is presented at the general superspace level.

It is found that incoherent dust, that is, dust which interacts only gravitationally, is a good choice for a time variable. A central feature of dust is that the Hamiltonian in the resulting Schrödinger equation does not depend on the dust variables. Hence the Hamiltonian density commutes (then allowing for a simultaneous definition by spectral analysis), and the equation can be solved by separating dust (time) from the gravitational degrees of freedom.

The Hamiltonian and momentum constraints, resulting when adding the dust contribution in the action, can be put in such a form that they can be solved in the dust momentum field. This leads to the new constraints $H_\uparrow(X)$ and $H_{\uparrow k}(X)$, the first one generating dynamics along the dust flow lines, and the others inducing motion on the surfaces of constant proper time of dust. The true Hamiltonian associated with the choice of dust as time is a square root $G(X)$ depending only on the gravitational degrees of freedom.

The variables T, Z^k and their conjugate quantities M, W_k $(k = 1, 2, 3)$ are introduced, such that the values of Z^k are the comoving coordinates of dust particles, while T is the proper time along the particle flow lines. In terms of these new variables, the Hamiltonian and momentum constraints of the whole system read

$$H_\uparrow = P(X) + h(X, g_{ab}, p^{ab}) = 0, \tag{56}$$
$$H_{\uparrow k} = P_k(X) + h_k(X, T, Z^k, g_{ab}, p^{ab}) = 0 \tag{57}$$

where

$$\begin{aligned} h(X) &= -\sqrt{G(X)}, \\ G(X) &= (H^G)^2 - g^{ab} H_a^G H_b^G, \\ h_k(X) &= Z_k^a H_a^G + \sqrt{G(X)} T_{,a} Z_k^a; \end{aligned}$$

here H^G and H_a^G are the usual Hamiltonian and momentum constraints of pure gravitation, and P is the projection of the rest mass current of dust onto the four-velocity of Eulerian observers, while $P_k = -PW_k$. Note that the Hamiltonian $h(X)$ does not depend on the dust variables. To proceed with the canonical quantization, a new set of variables $\mathbf{T}(z), \mathbf{P}(z), \mathbf{g}_{kl}(z), \mathbf{p}^{kl}(z)$ is introduced with the following meaning: $\mathbf{T}$ is the proper time along the dust worldline whose Lagrangian coordinate is z^k, $\mathbf{P}$ is the dust rest mass per unit coordinate cell, and $\mathbf{g}_{kl}$ is the metric giving the proper distance between nearby particles with coordinates z^k and $z^k + dz^k$. This yields the Hamiltonian constraint

$$\mathbf{H}_\uparrow = \mathbf{P}(z) + \mathbf{h}(z, \mathbf{g}_{kl}, \mathbf{p}^{kl}) = 0. \tag{58}$$

Hence the resulting Schrödinger equation for the wave functional $\Psi(Z, \mathbf{T}, \mathbf{g})$ is

$$i\frac{\delta\Psi(Z, \mathbf{T}, \mathbf{g})}{\delta\mathbf{T}} = \mathbf{h}(z, \mathbf{g}, \mathbf{p})\Psi(Z, \mathbf{T}, \mathbf{g}). \tag{59}$$

But since the wave functional must satisfy the momentum constraints which, as operators, are functional derivatives with respect to the canonical coordinates Z^k, Ψ does not depend on Z^k and hence one obtains

$$i\frac{\delta\Psi(\mathbf{T}, \mathbf{g})}{\delta\mathbf{T}} = \mathbf{h}(z, \mathbf{g}, \mathbf{p})\Psi(\mathbf{T}, \mathbf{g}). \tag{60}$$

Replacement of the WDW equation with this functional Schrödinger equation thus allows one to define a conserved positive-definite inner product. (To be precise, to obtain a self-adjoint new physical Hamiltonian $\mathbf{h}$, the theory must be restricted to the subspace given by the positive eigenvalues of the operator $\hat{\mathbf{G}}$ associated with G defined above). It is interesting to note that the idea of Brown and Kuchař has been recently applied by A. Sen [56] to string cosmology, with a tachyon playing the same role as dust, that is, as a time variable for the system and leading to a Schrödinger equation.

4.2. Reduction to true degrees of freedom as a way to unitary quantum cosmology

A central contribution to the search for a unitary quantum theory of gravity has been that of Barvinsky [1, 3, 4, 5, 6, 8]. It is clearly beyond the scope of these notes to give a thorough review of his seminal works — moreover, they are mostly devoted to the full theory rather than to the minisuperspace approximation — but since most of our own contributions have largely drawn on them, here we shall briefly comment some of their central aspects.

The programme starts from reduction of gravity theory to true physical variables ζ by means of gauge fixing, which appears natural after the following considerations. The dynamical evolution, which includes the problem of the multiplicity of times associated with the fact that separation between successive three-hypersurfaces is arbitrary, can be reproduced by gauge transformations [8]. The extremal condition $\delta S = 0$ gives the canonical equations

$$\frac{dq^i}{d\tau} = N_\mu[q^i, \mathcal{H}^\mu], \qquad \frac{dp_i}{d\tau} = N_\mu[p_i, \mathcal{H}^\mu]. \tag{61}$$

A solution of these equations describes the evolution of a spacelike hypersurface along the timelike direction, and the presence of the multiplier N introduces arbitrariness in the evolution, which is related to the multiplicity of times. From a different point of view, the constraint $\mathcal{H} = 0$ acts as a generator of gauge transformations which can be written as

$$\begin{aligned} \delta_\epsilon q^i &= \epsilon_\mu(\tau)[q^i, \mathcal{H}^\mu], \\ \delta_\epsilon p_i &= \epsilon_\mu(\tau)[p_i, \mathcal{H}^\mu], \\ \delta_\epsilon N_\mu &= \frac{\partial\epsilon_\mu(\tau)}{\partial\tau} - u_\mu^{\nu\rho}\epsilon_\rho N_\nu, \end{aligned} \tag{62}$$

where $u_\mu^{\nu\rho}$ are the structure functions of the constraints algebra. Then, from (61) and (62), we see that the dynamical evolution can be reproduced by a gauge transformation progressing with time, that is, any two successive points on each classical trajectory are connected by a gauge transformation; this leads to the idea of identifying time and true degrees of freedom by fixing the gauge.

Once the gauge is fixed, the constraints are solved, then yielding a true non-vanishing Hamiltonian and a physical time. The reduced system is then quantized, and the theory is reformulated in terms of the initial superspace variables q (that is, in terms of the canonical variables including spurious degrees of freedom). This procedure allows one to obtain a wave function $\Psi(q)$ solving the operator form of the constraints and including the central feature of a precise inner product allowing for a clear probabilistic interpretation.

After reduction of the classical theory, quantization follows the usual path integral procedure; and the subsequent reformulation in terms of the original variables gives a unitary gauge-independent superspace propagator which allows one to evolve the initial conditions on a given Cauchy surface, that is, to evolve from a given subspace in superspace. This allows for obtention of a wave function $\Psi(q)$ for which the measure is well defined in the sense that the probability amplitude is conserved in the superspace theory including a multiplicity of times.

Within this context, Barvinsky has also analysed the generalized Batalin–Fradkin–Vilkovisky (BFV) canonical quantization and has shown that the superspace wave function $\Psi(q)$ is an intermediate step between the wave function for the physical degrees of freedom $\psi(\zeta)$ and the quantum states in the extended BFV Hilbert space. Also, a definite operator ordering, and the corresponding quantum corrections, are given which ensure the closure of the constraint algebra and their hermiticity properties resulting from the BFV formalism.

Some points of Barvinsky's proposal can be outlined: 1) The absence of an asymptotically free limit in gravity theory forces the choice of a coordinate representation; this implies the restriction to systems which admit an intrinsic time, which appears in the reduction procedure as a result of imposing gauges not involving the momenta. 2) To avoid a frozen formalism, the appropriate gauge conditions must be explicitly time-dependent:

$$\chi(q,\tau) = 0. \tag{63}$$

3) Because of the form of the Hamiltonian constraint, which is quadratic in the momenta, the theory in the reduced space described by the set of canonical variables (ζ^A, π_a) includes *two* physical Hamiltonians $H_\pm$ satisfying

$$H_-(\zeta, -\pi, \tau) = -H_+(\zeta, \pi, \tau), \tag{64}$$

corresponding to two disjoint theories. 4) It is assumed that the quantum description in terms of the physical degrees of freedom (ζ^A, π_a) is a gauge-invariant quantum theory for the original variables (q^i, p_i, N^μ). 5) The theory in the physical subspace is given by the commutation relations

$$[\zeta^A, \pi_A] = i\delta^A_B \tag{65}$$

and the Schrödinger equation

$$i\frac{\partial}{\partial\tau}\psi(\zeta,\tau) = H(\zeta,\pi,\tau)\psi(\zeta,\tau) \tag{66}$$

with the inner product

$$\langle\tilde{\psi}|\psi\rangle = \int d\zeta\, \tilde{\psi}^*\psi, \tag{67}$$

or, in the path integral formulation, by the propagator

$$K(\zeta_2,\tau_2|\zeta_1,\tau_1) = \int D\zeta\, D\pi\, \exp\left(iS[\zeta,\pi]\right). \tag{68}$$

6) Once the reduced theory has been constructed, so ensuring unitarity of the quantum description, a reformulation in terms of the original variables is performed. This means obtaining a wave function $\Psi(q)$ and gauge fixing in superspace, establishing a correspondence between $\Psi(q)$ and $\psi(\zeta)$, and definition of a conserved inner product in the Hilbert space associated with superspace, as well as a proof of consistency of different gauge choices. The existence of two disjoint theories at the level of the true degrees of freedom is reflected in the fact that *two* superspace propagators

$$\mathbf{K}^+(q_2|q_1), \qquad \mathbf{K}^-(q_2|q_1)$$

are obtained. Since these propagators are gauge-independent, after transition from a theory for true degrees of freedom to a unitary theory in superspace one obtains a wave function $\Psi(q)$ which depends only on the initial gauge conditions, included in the initial-value data for it (see Ref. [8] for detail).

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