

Singularities in a scalar field quantum cosmology

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The quantum theory of a spatially flat Friedmann-Robertson-Walker universe with a massless scalar field as the source is further investigated. The classical model is singular and in the framework of a genuine canonical quantization (Arnold-Deser-Misner formalism) a discussion is made of the cosmic evolution, particularly of the quantum gravitational collapse problem. It is shown that in a matter-time gauge such that time is identified with the scalar field the classical model is singular either at $t = -\infty$ or at $t = +\infty$, but the quantum model is nonsingular. The latter behavior disproves a conjecture according to which quantum cosmological singularities are predetermined on the classical level by the choice of time.

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I. INTRODUCTION

The problem of constructing a consistent quantum theory of the gravitational field and its sources remains unsolved, in spite of great efforts of several decades. Since the standard perturbative techniques applied to quantum gravity appear to lead to a nonrenormalizable theory [1], other lines of attack have been attempted. It is true that there has been significant progress on nonperturbative canonical quantization of the full gravitational field [2–5], but the enormous complexity of the problem calls for manageable approximation schemes, one of the most attractive and fascinating of which is quantum cosmology, initiated by DeWitt [6] nearly 30 years ago.

The essential idea of quantum cosmology [7] is to freeze out all but a finite number of degrees of freedom of the system, the gravitational field plus its sources, and then quantize the remaining ones. This procedure is known as “minisuperspace quantization,” and although it cannot be strictly valid and is open to criticism [8], it is expected to provide some general insights on what an acceptable quantum theory of gravity should be like. This method has been put to work for quantizing Friedmann-Robertson-Walker (FRW) universes with varying matter content such as a scalar field [9–11], a spinor field [12], dust [13–16], or a Rarita-Schwinger field [17].

A fundamental issue of quantum cosmology is that of boundary or initial conditions on the wave function of the universe [18], a subject that will not be discussed here. Another outstanding problem is that of gravitational collapse or quantum cosmological singularities. On the classical domain the celebrated theorems of Hawking and Penrose assert that singularities inevitably occur in any spacetime obeying reasonable conditions on the causal structure and matter content. At the quantum level the situation is not so neat. The canonical quantization method developed by Arnould, Deser, and Misner [19] seems to provide suitable means for studying quantum cosmological singularities. This approach

consists of performing quantization in a reduced phase space spanned by independent canonical variables, and demands a definite choice of time. Although often leading to complicated and time-dependent Hamiltonians, this formalism has the great advantage of reducing the problem to one of standard quantum mechanics, enabling one to make full use of the powerful theory of linear operators in Hilbert space. In so doing, at least for FRW models one can define a quantum cosmological singularity with mathematical precision and analyze in a satisfactorily rigorous fashion the influence of quantum effects upon gravitational collapse.

It turns out that the issue of time in quantum cosmology (see [7] for references in this connection) is entangled with the problem of quantum gravitational collapse. Within the framework of the Arnould-Deser-Misner (ADM) genuine canonical quantization, Gotay and Demaret [13] made a fairly general inquiry into quantum cosmological singularities. They classify the time variable t of a classically singular model as either “slow,” if the classical singularity occurs at a finite value of t , or “fast,” if the classical singularity occurs at $t = \pm\infty$. According to them, the existence of quantum gravitational collapse is predetermined at the classical level by the choice of time, the crucial distinction being between times that give rise to complete or incomplete classical evolution. Basing their contentions on their own findings concerning dust-filled FRW models and on the models encountered in the literature until that date, they summarized their analysis by conjecturing that “self-adjoint quantum dynamics in a fast-time gauge is always singular.”

The first part of the above conjecture was disproved a few years ago by exhibiting singular unitary [15] and strictly self-adjoint [16] quantum cosmological models in a slow-time gauge. At that time no evidence was known against the second part of the conjecture.

In this paper we further study the quantum theory of a spatially flat FRW model with a massless scalar field as source, originally introduced by Blyth and Isham [9]. We find that for the choice of time $t = \phi$, where ϕ is the scalar field, the classical model is singular either at $t = -\infty$ or at $t = +\infty$, but the quantized model is self-adjoint and nonsingular. Thus the second part of the conjecture is disproved.

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This paper is organized as follows. In Sec. II the classical model is specified and the solution to the equations of motion found originally in [9] is reviewed. In Sec. III the ADM reduction of phase space is discussed for the choice of time referred to in the previous paragraph. In Sec. IV the model is quantized in the matter-time gauge $t = \phi$ and shown to be self-adjoint and free of singularity. Section V is devoted to final remarks and a general conclusion.

II. DESCRIPTION OF THE CLASSICAL MODEL

We shall be interested in homogeneous and isotropic universes described by the FRW metrics

$$ds^2 = g_{\mu\nu} dx^\mu dx^\nu = -N(t)^2 dt^2 + R(t)^2 \sigma_{ij} dx^i dx^j, \quad (1)$$

where σ_{ij} is the metric for a three-space of constant curvature $k = +1, 0,$ or -1 , corresponding to spherical, flat, or hyperbolic spacelike sections, respectively.

The classical action (in units such that $c = 16\pi G = 1$) is

$$S = - \int_M d^4x \sqrt{-g^{(4)}} R - 2 \int_{\partial M} d^3x \sqrt{h} h_{ij} K^{ij} + \frac{1}{2} \int_M d^4x \sqrt{-g} \partial_\mu \phi \partial^\mu \phi, \quad (2)$$

where ϕ is a massless scalar field, ${}^{(4)}R$ is the scalar curvature derived from the spacetime metric $g_{\mu\nu}$, h_{ij} is the metric on the boundary ∂M , and K^{ij} is the second fundamental form of the boundary [20]. The surface term is necessary in the path-integral formulation of quantum gravity in order to rid the Einstein-Hilbert Lagrangian of second-order derivatives. Compatibility with the homogeneous spacetime metric requires a space-independent scalar field, that is, $\phi = \phi(t)$.

In the geometry characterized by (1) the appropriate boundary condition for the action principle is to fix the initial and final hypersurfaces of constant time. The second fundamental form of the boundary becomes $K_{ij} = -\dot{h}_{ij}/2N$. From now on an overall factor of the spatial integral of $(\det\sigma)^{1/2}$ will be discarded, since it has no effect on the equations of motion. Insertion of the metric (1) and of the homogeneous scalar field into (2) yields the reduced action

$$S_r = \int dt L \quad (3)$$

with the Lagrangian

$$L = \frac{6R}{N} \dot{R}^2 - 6kNR - \frac{1}{2} \frac{R^3}{N} \dot{\phi}^2. \quad (4)$$

The canonical momentum conjugate to R is

$$p_R = \frac{\partial L}{\partial \dot{R}} = 12 \frac{R \dot{R}}{N}, \quad (5)$$

whereas the momentum conjugate to ϕ is

$$p_\phi = \frac{\partial L}{\partial \dot{\phi}} = - \frac{R^3}{N} \dot{\phi}, \quad (6)$$

so that the classical action can be recast in the Hamiltonian form

$$S_r = \int dt \left\{ \dot{R} p_R + \dot{\phi} p_\phi - N \left(\frac{p_R^2}{24R} - \frac{p_\phi^2}{2R^3} + 6kR \right) \right\}. \quad (7)$$

If one inserts the metric (1) and the homogeneous scalar field $\phi(t)$ into the field equations derived from the full action (2), the resulting equations of motion are identical to those that follow from the reduced action (7) under variation of R , ϕ , and N . These classical equations of motion were explicitly solved in [9] for closed or open models. For the purpose of quantization we shall direct our attention only to the simplest case $k=0$, for which Einstein's " G_{00} equation" is

$$3 \frac{\dot{R}^2}{R^2} = \frac{1}{4} \dot{\phi}^2. \quad (8)$$

In the gauge $t = \phi$ the above equation is equivalent to

$$\dot{R} = \begin{cases} R/\sqrt{12} & \text{if } \dot{R} > 0, \\ -R/\sqrt{12} & \text{if } \dot{R} < 0. \end{cases} \quad (9)$$

The field equations allow for expanding or contracting universes, that is, $R(t) = R_0 \exp(\pm t/\sqrt{12})$, where R_0 is an arbitrary positive constant. These are mutually exclusive solutions, depending on the initial conditions. The model is singular at $t = -\infty$ in the expanding case or at $t = +\infty$ in the contracting case. As will be seen, although classically the existence of one of these solutions automatically precludes the existence of the other, at the quantum level they not only coexist but also interfere with each other.

The form (7) of the reduced action shows clearly that the lapse function N plays the role of a Lagrange multiplier. Variation with respect to N leads to the super-Hamiltonian constraint

$$\frac{p_R^2}{24R} - \frac{p_\phi^2}{2R^3} + 6kR = 0, \quad (10)$$

which for $k=0$ and with the use of (5) and (6) is easily seen to be identical to Eq. (8). This constraint reveals that the phase space (R, ϕ, p_R, p_ϕ) is too large, so that a bona fide canonical quantization can only be performed after going over to a reduced phase space spanned by independent canonical variables alone. This can be achieved by first making a choice of time and then solving the constraint equation (9) for the canonical variable conjugate to the time chosen in the first step. This ensures that the final action preserves its canonical form, with a Hamiltonian identical to the variable whose Poisson bracket is unity with whatever was chosen as time, but now expressed as a function of the remaining independent canonical variables [19]. This is the essence of the ADM formalism, which will be illustrated below for a specific choice of time.

III. MATTER-TIME GAUGE AND ADM REDUCTION

For the sake of simplicity, from now on our attention will be focused solely on the spatially flat case, that is, $k=0$. Let

us make the choice of time $t = \phi$, the matter field itself providing a clock by means of which the evolution of the system can be followed. According to the ADM prescription, the Hamiltonian in the reduced phase space is $H = -p_\phi$. Now, solving Eq. (10) for p_ϕ and picking up the negative square root gives rise to the reduced Hamiltonian

$$H = -p_\phi = \frac{1}{\sqrt{12}} R |p_R|. \tag{11}$$

It is important to notice that in the gauge $t = \phi$ it follows from Eq. (6) that $p_\phi < 0$ since $R > 0$ and $N > 0$ by definition. This is the reason why the positive solution for p_ϕ was abandoned. One sees, therefore, that the Hamiltonian (11) is positive. Hamilton’s equation of motion for R in the reduced phase space is

$$\dot{R} = \frac{\partial H}{\partial p_R} = \begin{cases} R/\sqrt{12} & \text{if } p_R > 0, \\ -R/\sqrt{12} & \text{if } p_R < 0. \end{cases} \tag{12}$$

Because $R > 0$ and $N > 0$ by definition, it is a consequence of Eq. (5) that p_R and \dot{R} have the same sign, so that Eqs. (9) and (12) are identical. This completes the verification that the equations of motion generated by the reduced Hamiltonian (11) are the same as those that arise from variation of the action (7) in the extended phase space.

The reduced phase space $\mathcal{P} = (R, p_R)$ is the union $\mathcal{P} = \mathcal{P}_+ \cup \mathcal{P}_-$ of the two disjoint sets $\mathcal{P}_+ = (0, \infty) \times (0, \infty)$ and $\mathcal{P}_- = (0, \infty) \times (-\infty, 0)$. From Eq. (8) in the gauge $t = \phi$ it follows that \dot{R} can never vanish, so that the line $p_R = 0$ does not belong to the reduced phase space. The sets \mathcal{P}_+ and \mathcal{P}_- are disconnected in the sense that the dynamical trajectories remain entirely confined to one of them, selected according to the initial conditions, and cannot cross the border $p_R = 0$ between them.

As remarked previously, for the present choice of time the scale factor vanishes and Riemann tensor invariants such as ${}^{(4)}R$ become infinite either when $t = -\infty$ or when $t = +\infty$. Therefore the classical model is singular and $t = \phi$ is a “fast” time in accordance with the terminology introduced in [13].

IV. QUANTIZATION IN THE MATTER-TIME GAUGE

As discussed above, in the gauge $t = \phi$ the classical Hamiltonian function is (11). An operator corresponding to $R |p_R|$ can be naturally defined as the positive square root of an operator corresponding to $R^2 p_R^2$. Thus, we look for a positive Hamiltonian operator whose square has as classical counterpart the square of the Hamiltonian function (11). Following Blyth and Isham [9], such a positive self-adjoint Hamiltonian can be constructed as the square root of the positive self-adjoint operator

$$\hat{\mathcal{C}} = -\frac{1}{12} R^\nu \frac{d}{dR} R^{2-2\nu} \frac{d}{dR} R^\nu \tag{13}$$

with a suitable domain of definition, where the parameter ν reflects factor-ordering ambiguities. In Ref. [9] the choice $\nu = 0$ was made, but it turns out, as will be shown below, that

there is a better choice of the parameter ν that makes easier the analysis of the quantum dynamics. Therefore we take

$$\hat{H}^2 = -\frac{1}{12} R^\nu \frac{d}{dR} R^{2-2\nu} \frac{d}{dR} R^\nu = -\frac{1}{12} \left[\frac{d}{dR} R^2 \frac{d}{dR} + \nu(1-\nu) \right] \tag{14}$$

acting on $L^2(0, \infty)$. A great deal of simplification is achieved by means of the unitary mapping from $\mathcal{H} = L^2(0, \infty)$ onto $\tilde{\mathcal{H}} = L^2(-\infty, \infty)$ defined by [9]

$$\tilde{\psi}(y) = e^{-y/2} \psi(e^{-y}), \tag{15}$$

which is tantamount to the change of variable $R = e^{-y}$. Indeed, the expectation value

$$\langle \hat{R} \rangle_\psi = \langle \psi | \hat{R} | \psi \rangle = \int_0^\infty R |\psi(R)|^2 dR \tag{16}$$

becomes

$$\begin{aligned} \langle \hat{R} \rangle_\psi &= \int_{-\infty}^\infty e^{-y} |\psi(e^{-y})|^2 e^{-y} dy \\ &= \int_{-\infty}^\infty e^{-y} |\tilde{\psi}(y)|^2 dy = \langle e^{-\hat{y}} \rangle_{\tilde{\psi}}. \end{aligned} \tag{17}$$

The transformed Hamiltonian squared is easily obtained by demanding that its expectation value in a state $\tilde{\psi} \in L^2(-\infty, \infty)$ be equal to the expectation value of (14) calculated in the state $\psi \in L^2(0, \infty)$ with ψ and $\tilde{\psi}$ related by Eq. (15). The result is

$$\hat{H}^2 = \frac{1}{12} \left[-\frac{d^2}{dy^2} + \frac{1}{4} + \nu(\nu-1) \right], \tag{18}$$

which, with the choice $\nu = 1/2$, reduces to the simple form

$$\hat{H}^2 = -\frac{1}{12} \frac{d^2}{dy^2}. \tag{19}$$

It is very convenient to investigate the quantum dynamics in the momentum representation in the transformed Hilbert space $\tilde{\mathcal{H}}$. Then $-id/dy$ becomes the operator of multiplication by p and the positive square root of (19) is such that

$$(\hat{H} \tilde{\psi})(p) = \frac{1}{\sqrt{12}} |p| \tilde{\psi}(p) \tag{20}$$

on the dense domain

$$\mathcal{D} = \left\{ \tilde{\psi} \in L^2(-\infty, \infty) \mid \int_{-\infty}^\infty p^2 |\tilde{\psi}(p)|^2 dp < \infty \right\}. \tag{21}$$

Given an initial wave function $\tilde{\psi}_0(p)$ at $t = t_0$, one finds that, at time t ,

$$\tilde{\psi}(p, t) = (\exp[-i(t-t_0)\hat{H}]\tilde{\psi}_0)(p) = e^{-i(t-t_0)|p|/\sqrt{12}} \tilde{\psi}_0(p). \tag{22}$$

The singularity criterion to be adopted here is the following [13,21]: the quantum system is singular at a certain instant if $\langle \psi | \hat{f} | \psi \rangle = 0$ for any quantum observable \hat{f} whose classical counterpart f vanishes at the classical singularity, ψ being any state of the system at the instant under consideration. For models of the FRW type the relevant quantum observable is $\hat{f} = \hat{R}$, since $R=0$ defines the classical singularity. This criterion is in agreement with the usage in quantum cosmology. Indeed, since \hat{R} is a positive operator on $L^2(0, \infty)$, if $\langle \hat{R} \rangle_t = 0$ then $\psi(t)$ is sharply peaked at $R=0$, and a strong peak in the wave function at a certain classical configuration is regarded in quantum cosmology as a prediction of the occurrence of such a configuration [7].

Accordingly, if $\langle \psi(t) | \hat{R} | \psi(t) \rangle$ never vanishes for some evolving state $\psi(t)$ then the model is nonsingular. Let us take as the initial state the Gaussian wave packet

$$\tilde{\psi}_0(p) = \pi^{-1/4} e^{-p^2/2}, \tag{23}$$

from which one finds

$$\begin{aligned} \tilde{\psi}(y, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\psi}(p, t) e^{ipy} dp \\ &= \frac{\pi^{-1/4}}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left[\frac{i}{\sqrt{12}}(t-t_0)|p| - \frac{p^2}{2} + ipy\right] dp. \end{aligned} \tag{24}$$

In terms of the convenient quantities

$$\xi_{\pm}(y, t) = y \pm \frac{t-t_0}{\sqrt{12}} \tag{25}$$

one can reexpress Eq. (24) as

$$\begin{aligned} \tilde{\psi}(y, t) &= \frac{\pi^{-1/4}}{\sqrt{2\pi}} \left\{ \int_0^{\infty} \cos[p\xi_+(y, t)] e^{-p^2/2} dp \right. \\ &\quad - i \int_0^{\infty} \sin[p\xi_+(y, t)] e^{-p^2/2} dp \\ &\quad + \int_0^{\infty} \cos[p\xi_-(y, t)] e^{-p^2/2} dp \\ &\quad \left. + i \int_0^{\infty} \sin[p\xi_-(y, t)] e^{-p^2/2} dp \right\}. \end{aligned} \tag{26}$$

These integrals can be explicitly evaluated to yield [22]

$$\begin{aligned} \tilde{\psi}(y, t) &= \frac{\pi^{-1/4}}{\sqrt{2\pi}} \left\{ \frac{\sqrt{2\pi}}{2} e^{-\xi_+(y, t)^2/2} \right. \\ &\quad \left. - i \xi_+(y, t) {}_1F_1\left(1, \frac{3}{2}; -\frac{\xi_+(y, t)^2}{2}\right) + (\xi_+ \leftrightarrow \xi_-)^* \right\}, \end{aligned} \tag{27}$$

where ${}_1F_1$ denotes a degenerate (confluent) hypergeometric function and the asterisk stands for complex conjugate. The above wave function is the superposition of two wave packets, one centered on $y = -(t-t_0)\sqrt{12}$ and the other on $y = +(t-t_0)/\sqrt{12}$. The first packet corresponds to an expanding universe, while the second one describes a contracting universe.

The initial expectation value of \hat{R} is finite and can be computed once $\tilde{\psi}_0(y)$ has been found. We have

$$\tilde{\psi}_0(y) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\psi}_0(p) e^{ipy} dy = \pi^{-1/4} e^{-y^2/2}, \tag{28}$$

hence,

$$\langle \hat{R} \rangle_{t_0} = \int_{-\infty}^{\infty} e^{-y} \pi^{-1/2} e^{-y^2} dy = e^{1/4}. \tag{29}$$

The general structure of Eq. (27) is

$$\tilde{\psi}(y, t) = \tilde{\psi}_1(\xi_+) - i\tilde{\psi}_2(\xi_+) + \tilde{\psi}_1(\xi_-) + i\tilde{\psi}_2(\xi_-) \tag{30}$$

with $\tilde{\psi}_1, \tilde{\psi}_2$ real functions, and, in particular,

$$\tilde{\psi}_1(x) = \frac{\pi^{-1/4}}{2} e^{-x^2/2}. \tag{31}$$

Therefore, since $\tilde{\psi}_1$ is a positive function,

$$\begin{aligned} |\tilde{\psi}(y, t)|^2 &\geq |\tilde{\psi}_1(\xi_+) + \tilde{\psi}_1(\xi_-)|^2 \\ &\geq |\tilde{\psi}_1(\xi_+)|^2 + |\tilde{\psi}_1(\xi_-)|^2, \end{aligned} \tag{32}$$

whence

$$\begin{aligned} \langle \hat{R} \rangle_t &\geq \int_{-\infty}^{\infty} e^{-y} |\tilde{\psi}_1(\xi_+(y, t))|^2 dy \\ &\quad + \int_{-\infty}^{\infty} e^{-y} |\tilde{\psi}_1(\xi_-(y, t))|^2 dy. \end{aligned} \tag{33}$$

A straightforward evaluation of the above integrals with the help of (25) and (31) furnishes

$$\langle \hat{R} \rangle_t \geq \frac{\langle \hat{R} \rangle_{t_0}}{2} \cosh\left(\frac{t-t_0}{\sqrt{12}}\right) \geq \frac{\langle \hat{R} \rangle_{t_0}}{2}. \tag{34}$$

It is thus established that the expectation value $\langle \hat{R} \rangle_t$ never vanishes, and, in particular, $\langle \hat{R} \rangle_t$ tends to infinity as $t \rightarrow \pm \infty$ (classical singularity). This constitutes an example of a nonsingular self-adjoint quantum cosmological model in a fast-time gauge, and allows us to conclude that the second part of the conjecture advanced by Gotay and Demaret [13] is not true. We remark that the special choice $\nu = 1/2$ is not a weak point of our argument. The conjecture asserts that *all* self-adjoint quantum cosmological models in a fast-time gauge are singular. Here a particular counterexample (with $\nu = 1/2$) has been exhibited of a nonsingular self-adjoint quantum cosmological model in a fast-time gauge.

V. CONCLUSION

The main finding of this paper is that, contrary to a plausible belief, quantum cosmological models in fast-time gauges are not necessarily singular. Combined with the results obtained in [15,16], our present investigation reveals that the occurrence of gravitational collapse at the quantum level is not classically predetermined by the choice of a “fast” or “slow” time, such a classification not being very relevant to the problem of quantum gravitational collapse. It thus appears that the issue of time in quantum cosmology and quantum gravity is actually deeper and more complicated than was guessed hitherto. The apparent absence of an intrinsic time variable in the general theory of relativity, and

the physical inequivalence of different choices of time in quantum cosmology remain as challenges to be met by any candidate to a viable quantum theory of the gravitational field.

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