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Conservation of probability and quantum cosmological singularities

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By taking as a counterexample a spatially flat Friedmann-Robertson-Walker universe filled with a massless scalar field, we show that conservation of probability does not rule out singularities in quantum cosmology. Consequently, it is unnecessary to resort to contractive quantum dynamics in order to permit singularities in "slow-time gauges."

I. INTRODUCTION

There is a continuing debate among physicists on the nature and physical meaning of cosmological singularities, as well as on their inevitability. There are many widely different points of view on this subject, ranging from the contention that loss of predictive power is unacceptable[1] to Misner's position[2] that singularities should be treated as an essential element of cosmology, an absolute zero of time one cannot do without.

One interesting and feasible approach to the study of quantum properties of the gravitational field is afforded by the so-called quantum cosmological models, initiated by DeWitt[3] and followed up by many others[4] in the last few years. According to DeWitt, if the universal wave function vanishes at classically singular metrics for all time then there is no singularity. Otherwise, the state described by the universal wave function develops a singularity for some time t. This criterion has often been used to characterize the nonsingular nature of some quantum cosmological models,[5] but its status has been criticized by several authors,[6-8] and in the case of quantum mechanics in curved spacetime, an explicit counterexample has been found[9] to the effect that DeWitt's proposal actually is not a valid criterion for the existence or absence of a singularity. Criteria based on the vanishing of expectation values of positive operators associated with classical quantities which vanish at the classical singularity have been proposed[8] and seem to be much more reliable. Therefore, this is the sort of criterion we shall be considering from now on.

Recently, Gotay and Demaret[8] proved that unitary evolution and strongly suggested that conservation of probability rule out quantum singularities in the case of what they call "slow-time gauges." This led them to investigate non-self-adjoint Hamiltonian operators and their accompanying contractive quantum dynamics in order to make singularities possible whenever one has chosen a "slow" time to implement the quantization procedure. Again, in the context of quantum mechanics in curved spacetime we have been able to establish[9] that conservation of probability alone does not prevent quantum singularities. In the present paper we produce an explicit counterexample to Gotay and Demaret's intimation in the cadre of quantum cosmology proper, and so prove that conservation of probability is not powerful enough to forbid quantum cosmological singularities.

II. THE COUNTEREXAMPLE

Let us reexamine the model discussed by Blyth and Isham[6] which consists of a Friedmann-Robertson-Walker universe with a scalar field acting as the source of the gravitational field. Let R be the scale factor and suppose one chooses the time variable in such a way that $t=R$, from which it follows that $t\in[0,\infty)$. In this case, they have shown that a suitable Hamiltonian for the classical theory is

$$H=\pm\sqrt{24}\left[-6Kt^2+t^4\frac{m^2}{2}\phi^2+\frac{\pi_\phi{}^2}{2t^2}\right]^{1/2}, \tag{1}$$

where $K=1$, 0, or -1 according to whether the geometry of the three-space is that of a three-sphere, flat, or hyperbolic, ϕ is the scalar field of mass m, and π_ϕ is the canonical momentum conjugate to ϕ. The plus or minus sign in Eq. (1) is chosen depending on whether the model corresponds to an expanding or a contracting universe. We shall study the simplest case of a massless scalar field ($m=0$) in a spatially flat universe ($K=0$). Furthermore, we shall take the plus sign in the Hamiltonian since taking $t=R$ is actually appropriate only for an expanding universe. In view of the previous choices, the Hamiltonian takes the form

$$H=\sqrt{12}\frac{p}{t}, \tag{2}$$

where, for the sake of notational simplicity, we write $p\equiv\pi_\phi$. From now on we shall also write x for the canonical variable conjugate to p, that is, $x\equiv\phi$. As shown by Blyth and Isham, for $K=0$ the scale factor is given as a function of x as

$$R(x)=e^{x/\sqrt{12}}, \tag{3}$$

where, without loss of generality, we have picked out the constants R_0 and ϕ_0 that appear in Ref. 6 in such a way that

$$R_0\exp(-\phi_0/\sqrt{12})=1 .$$

As a check, let us analyze the equation of motion for x which follows from the Hamiltonian (2). We have

$$\dot{x}=\frac{\partial H}{\partial p}=\frac{\sqrt{12}}{t} \tag{4}$$

with a solution

$$x(t)=\sqrt{12}\ln t \ . \tag{5}$$

Inserting this result into Eq. (3) one gets

$$R(t)=t \ , \tag{6}$$

and this is just the expected correct result. [Had we chosen the minus sign in Eq. (1) we would have been led to a contracting cosmological model.]

We now turn to our main interest: namely, the quantum theory of the cosmological model with which we are dealing. The Hamiltonian operator is

$$\hat{H}(t)=\sqrt{12}\frac{\hat{p}}{t} \ , \tag{7}$$

where $\hat{x}$ and $\hat{p}$ obey the standard canonical commutation relations (we set $\hbar=1$). Inasmuch as

$$[\hat{H}(t),\hat{H}(t')]=0 \tag{8}$$

for all t,t', the time-evolution operator is readily given by

$$\hat{U}(t,t_0)=\exp\left[-i\int_{t_0}^{t}\hat{H}(t')dt'\right] = \exp[-i\sqrt{12}\ln(t/t_0)\hat{p}] \ . \tag{9}$$

The propagator is defined by means of

$$G(x,t;x_0,t_0)=\langle x \mid \hat{U}(t,t_0) \mid x_0\rangle \ , \tag{10}$$

and by inserting the completeness relation expressed in the momentum basis $\{\,|p\rangle\}$ one easily finds

$$G(x,t;x_0,t_0)=\int_{-\infty}^{\infty}\frac{dp}{2\pi}\exp\{i[x-x_0-\sqrt{12}\ln(t/t_0)]p\} \ . \tag{11}$$

Since we shall always regard t_0 as a fixed instant, it will be useful to introduce a function $\xi(t)$ defined as

$$\xi(t)=\sqrt{12}\ln(t/t_0) \ . \tag{12}$$

With this definition the propagator may be written in the extremely simple form

$$G(x,t;x_0,t_0)=\delta(x-x_0-\xi(t)) \ . \tag{13}$$

Let $\psi_0(x)$ be the normalized wave function at $t=t_0$. Then the state of the system at time t is described by

$$\psi(x,t)=\int_{-\infty}^{\infty}G(x,t;x_0,t_0)\psi_0(x_0)dx_0=\psi_0(x-\xi(t)) \tag{14}$$

because of Eq. (13). Notice that

$$\|\psi(t)\|^2=\int_{-\infty}^{\infty}|\psi(x,t)|^2dx = \int_{-\infty}^{\infty}|\psi_0(x-\xi(t))|^2dx = \int_{-\infty}^{\infty}|\psi_0(x)|^2dx=1 \ , \tag{15}$$

so that probability is strictly conserved for all t, even in the limit $t\rightarrow 0$. By taking advantage of Eqs. (3) and (14) we are in a position to calculate the expectation value of the scale factor R. It is given by

$$\langle R\rangle_t=\int_{-\infty}^{\infty}e^{x/\sqrt{12}}|\psi_0(x-\xi(t))|^2dx \ . \tag{16}$$

If ψ_0 is such that

$$\int_{-\infty}^{\infty}e^{x/\sqrt{12}}|\psi_0(x)|^2dx<\infty \ , \tag{17}$$

then the simple shift of the integration variable $y=x-\xi(t)$ casts Eq. (16) into the form

$$\langle R\rangle_t=e^{\xi(t)/\sqrt{12}}\int_{-\infty}^{\infty}e^{y/\sqrt{12}}|\psi_0(y)|^2dy \ . \tag{18}$$

Since from Eq. (12) it follows that $\xi(t)\rightarrow-\infty$ as $t\rightarrow 0$, one concludes that

$$\lim_{t\rightarrow 0}\langle R\rangle_t=0 \ . \tag{19}$$

Therefore, our quantum cosmological model is undeniably singular at $t=0$ according to the criterion proposed by Gotay and Demaret. Of course there are infinitely many wave functions for which Eq. (17) holds. Perhaps the simplest examples are wave functions of the Gaussian-type:

$$\psi_0(x)=(\sigma\sqrt{\pi})^{-1/2}e^{-x^2/2\sigma^2} \tag{20}$$

with $\sigma>0$ being a constant. Note further that either $\langle R\rangle_t$ is finite for all t or it is infinite for all t. In other words, *all* states for which $\langle R\rangle$ is defined, unavoidably collapse into a singularity at $t=0$.

It is worthwhile to investigate somewhat more deeply the behavior of the time-evolution operator as $t\rightarrow 0$. With the purpose of making our analysis as simple as possible, let us consider the wave functions as given in the momentum representation, which will be typically denoted by $\tilde{\psi}(p)$. Let $\tilde{\psi}_1(p)$ and $\tilde{\psi}_2(p)$ be any two such wave functions. As long as in the momentum representation $\hat{p}$ is nothing but multiplication by p, we can write

$$(\tilde{\psi}_1,\hat{U}(t,t_0)\tilde{\psi}_2)=\int_{-\infty}^{\infty}dp\, e^{-ip\xi(t)}\tilde{\psi}_1^*(p)\tilde{\psi}_2(p) \ . \tag{21}$$

If one lets $t\rightarrow 0$, then $\xi(t)\rightarrow-\infty$, and as $\tilde{\psi}_1^*\tilde{\psi}_2\in L^1(\mathbb{R})$ the Riemann-Lebesgue lemma[10] ascertains that

$$\lim_{t\rightarrow 0}(\tilde{\psi}_1,\hat{U}(t,t_0)\tilde{\psi}_2)=0 \tag{22}$$

for all $\tilde{\psi}_1,\tilde{\psi}_2\in L^2(\mathbb{R})$. Thus, we conclude that

$$\hat{U}(t,t_0)\xrightarrow[t\rightarrow 0]{}0 \tag{23}$$

in the sense of weak convergence,[11] even though for any $t>0$ one has

$$\|\hat{U}(t,t_0)\|=1 \ . \tag{24}$$

Of course the time-evolution operator can converge neither strongly nor uniformly to zero owing to the last equation above. However, weak convergence to zero is all that should be demanded[12] to make any scalar product vanish at the instant corresponding to the singularity. Since the criterion proposed by Gotay and Demaret involves only expectation values, that is, scalar products, weak convergence of $\hat{U}(t,t_0)$ to zero is sufficient to give rise to a singularity, as in the example we have just discussed.

III. CONCLUDING REMARKS

In the previous section we have shown unequivocally, by means of an explicit example, that it is possible to construct quantum cosmological models whose dynamics rigorously conserve probability, but at the same time possess states that are singular at a certain instant. It is clear, therefore, that by slightly relaxing the requirement of self-adjointness of $\hat{H}(t)$, that is, by allowing that $\hat{H}(t)$ may not be self-adjoint at a particular instant but still keeping probability strictly conserved, one can make room for singular states in "slow-time gauges," contrary to the strong indication advanced by Gotay and Demaret. Moreover, it is quite unnecessary to introduce artificially Hamiltonian operators which are everywhere (with respect to t) non-self-adjoint and lead to contractive dynamics in order to open the possibility for singularities in those gauges. As to the failure of Gotay and Demaret's reasoning as applied to our example, notice that an initial wave function of the form (20), for instance, is peaked at $x=0$ at instant $t=t_0$. According to Eq. (14), at any other instant t its peak occurs at $x=\xi(t)$. Thus, as $t\to 0$ the time evolution described by Eq. (9) is such that the peak of the wave function moves away to $x=-\infty$. As an immediate consequence, there exists no square-integrable function that uniformly bounds $\psi(x,t)$ for all t. Therefore, Lebesgue's dominated convergence theorem is unapplicable and this explains why Gotay and Demaret's argument suggesting that probability conservation forbids singular states breaks down in the present circumstances.

Our last remark concerns a point that is usually overlooked when dealing with time-dependent Hamiltonian operators. Consider, for instance, a Hamiltonian of the form

$$\hat{H}(t)=\frac{\hat{\mathcal{O}}}{2\sqrt{t}}\ , \tag{25}$$

where $\hat{\mathcal{O}}$ is a time-independent self-adjoint operator and $t\in[0,\infty)$. It is clear that the time-evolution operator associated with the above Hamiltonian is simply

$$\hat{U}(t,t_0)=\exp[-i(\sqrt{t}-\sqrt{t_0})\hat{\mathcal{O}}]\ . \tag{26}$$

Clearly $\hat{U}(t,t_0)$ is unitary for all $t,t_0\in[0,\infty)$ although $\hat{H}(t)$ is not self-adjoint at $t=0$ because it is not even defined at that instant. Different from the usual case, for systems which are not homogeneous in time the dynamics is not given by a one-parameter unitary group of operators.[13] If, in addition, the domain of the time variable is restricted for physical reasons, we conclude from the above example that self-adjointness of the Hamiltonian is a sufficient but not at all necessary condition to make sure that the time evolution is unitary, in the sense of being characterized by a family of operators $\hat{U}(t,s)$ which are unitary for all values of t,s belonging to the restricted domain allowed to the time variable. It is remarkable, therefore, that in such circumstances and in the sense just explained, self-adjoint dynamics is not always the same thing as unitary dynamics. On the other hand, a singularity in $\hat{H}(t)$ at some instant is a necessary but by no means sufficient condition to give rise to singular dynamics. In spite of appearing here as a mere curiosity, this kind of peculiar behavior may be of some relevance in concrete quantum cosmological models.

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[1] For efforts in constructing physical mechanisms to eliminate singularities, see N. D. Birrell and P. C. W. Davies, *Quantum Fields in Curved Space* (Cambridge University Press, Cambridge, England, 1982), Sec. 7.4, and references therein.

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[9] N. A. Lemos (unpublished).

[10] E. Prugovečki, *Quantum Mechanics in Hilbert Space*, 2nd ed. (Academic, New York, 1981), pp. 216–217.

[11] Prugovečki (Ref. 10), Chap. III, Sec. 5.3.

[12] This requires some qualifications, as the attentive reader has certainly noticed that $\hat{U}(t,t_0)$ also converges weakly to zero as $t\to\infty$, but Eq. (18) shows that in spite of this $\lim_{t\to\infty}\langle R\rangle_t=\infty$. Consider $\langle R\rangle_t=(\psi(t),\hat{R}\psi(t))$ and suppose

$$\hat{R}\psi(t)\xrightarrow[t\to 0]{}\psi_1\in\mathcal{H}=L^2(\mathbb{R})\ .$$

Then,

$$|(\psi(t),\hat{R}\psi(t))-(\psi(t),\psi_1)|\le\|\psi(t)\|\,\|\hat{R}\psi(t)-\psi_1\|$$
$$=\|\hat{R}\psi(t)-\psi_1\|\xrightarrow[t\to 0]{}0\ ,$$

where we have used Schwarz's inequality. Therefore,

$$\lim_{t\to 0}\langle R\rangle_t=\lim_{t\to 0}(\psi(t),\psi_1)$$
$$=\lim_{t\to 0}(\hat{U}(t,t_0)\psi_0,\psi_1)=0\ ,$$

whenever $\hat{U}(t,t_0)$ converges weakly to zero as $t\rightarrow 0$. In our particular model this reasoning applies with $\psi_1=0$. As to the limit $t\rightarrow\infty$, it is easy to see that $\hat{R}\psi(t)$ does not converge to an element of the Hilbert space $\mathcal{H}$ because $\|\hat{R}\hat{U}(t,t_0)\psi_0\|\rightarrow\infty$ as $t\rightarrow\infty$, as one can readily verify, so that the previous argument breaks down.

[13]J. M. Jauch, *Foundations of Quantum Mechanics* (Addison-Wesley, Reading, MA, 1968), p. 159.