Some remarks on singularities in quantum cosmology

Mark J. Gotay and Jacques Demaret

1. INTRODUCTION

The question of whether classical singularities persist in quantum cosmology remains a fascinating one. In [1], we conjectured that (F) self-adjoint quantum dynamics in a fast-time gauge is singular, whereas (S) self-adjoint quantum dynamics in a slow-time gauge is always nonsingular. By a “fast-time gauge” we mean a choice of time \( t \) such that the classical singularities occur at \( t = \pm \infty \) or \( t = -\infty \). A time \( t \) is “slow” if the singularities occur when \( |t| < \infty \).

In this paper, we verify Conjecture (F) for a \( k = 0 \) Robertson-Walker cosmology containing a massless scalar field \( \phi \). Detailed discussions of these “RW(\phi)” models can be found in [4, 5, 6]; the background we need can be summarized as follows. Upon making an ADM reduction by choosing the intrinsic-time gauge \( t = \phi \), the dynamics of this model can be described in terms of the canonical variables \((R, \pi_R)\), where \( R > 0 \) is the classical radius and \( \pi_R \neq 0 \). (The reason why \( \pi_R \neq 0 \) when \( k \leq 0 \) is explained in [4].) The phase space thus has two components, \((0, \infty) \times (-\infty, 0)\) and \((0, \infty) \times (0, \infty)\), and the Hamiltonian is

\[
H(R, \pi_R) = \frac{1}{\sqrt{12}} R |\pi_R|.
\]

When \( \pi_R > 0 \), the model has an initial singularity at \( t = -\infty \) and expands thereafter. The situation is time-reversed when \( \pi_R < 0 \). Thus \( t = \phi \) is fast.

The quantum dynamics of the RW(\phi) models in various fast-time gauges have been extensively studied [5, 6, 7]. In all cases the quantized models were found to be singular. We will prove that the quantized \( k = 0 \) model with \( t = \phi \) is singular as well, contrary to the assertion in [4].

2. RW(\phi) MODELS

We start with a \( k = 0 \) Robertson-Walker cosmology filled with a massless scalar field \( \phi \). Detailed discussions of these “RW(\phi)” models can be found in [4, 5, 6]; the background we need can be summarized as follows. Upon making an ADM reduction by choosing the intrinsic-time gauge \( t = \phi \), the dynamics of this model can be described in terms of the canonical variables \((R, \pi_R)\), where \( R > 0 \) is the classical radius and \( \pi_R \neq 0 \). (The reason why \( \pi_R \neq 0 \) when \( k \leq 0 \) is explained in [4].) The phase space thus has two components, \((0, \infty) \times (-\infty, 0)\) and \((0, \infty) \times (0, \infty)\), and the Hamiltonian is

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2.1. Canonical Quantization

Canonically quantizing, we take the Hilbert space to be the orthogonal direct sum \( L^2(0, \infty) \oplus L^2(0, \infty) \), corresponding to the two components of the phase space. The quantum Hamiltonian is \( \hat{H} = \hat{H}_- \oplus \hat{H}_+ \) acting on the first and second summands, respectively, where

\[
\hat{H}_\pm = \mp \frac{i \hbar}{\sqrt{12}} \left( R \frac{d}{dR} + \frac{1}{2} \right).
\]

Note that as \( \hat{H} \) is linear in the momentum on each component, it is (unambiguously) quantized according to the “product \( \rightarrow \) anticommutator” rule. Now \( \hat{H} \) commutes with the projectors onto each summand, whence the two halves of the Hilbert
space are dynamically decoupled, i.e., there can be no tunneling between states in them. It therefore suffices to study the quantum dynamics on each summand individually.\footnote{1} We will accordingly restrict attention to the first \((-\) one; the other can be handled analogously.

It is useful to make the unitary transformation $U : L^2(0, \infty) \to L^2(\mathbb{R})$ given by $(U\psi)(y) = e^{-y/2}\psi(e^{-y})$, corresponding to the classical rescaling $R = e^{-y}$. Then (2) becomes

$$\hat{H}_- = -\frac{i\hbar}{\sqrt{12}} \frac{d}{dy},$$

and the quantum evolution is

$$\psi(y, t) = \psi(y - t/\sqrt{12}).$$

Thus evolving states in the first summand represent purely contracting quantum universes; initial states do not split up into peaks corresponding to contracting and expanding universes as happens, e.g., in \cite{1} and \cite{3}. This is \textit{not} because the Hilbert space is an orthogonal direct sum\footnote{That the first summand arises from quantizing the component of phase space corresponding to classically contracting models does not \textit{ab initio} mean that evolving states belonging to this summand will contract quantum mechanically. Indeed, this is what we wish to determine.}, rather, it reflects the fact that Hamiltonian (2) is a first order differential operator. (Compare \cite{1} and \cite{3}, where the evolution was generated by second order Hamiltonians.)

To check for quantum collapse, we compute the expectation value of the radius operator $\hat{R} = e^{-y}$ on $L^2(\mathbb{R})$. Evidently

$$\langle \hat{R} \rangle_t = e^{-t/\sqrt{12}} \langle \hat{R} \rangle_0,$$

whence $\langle \hat{R} \rangle_t \to 0$ as $t \to \infty$. Thus any initial state $\psi$ with a well-defined radius must collapse, at least in the sense that $\lim_{t \to \infty} \langle \hat{R} \rangle_t = 0$.

On the other hand, this quantization is to a certain extent defective, due to the non-positivity of $\hat{H}$. (Compare the classical Hamiltonian \cite{1}, which is a positive function.)\footnote{This phenomenon can be traced to the geometric fact that the vertical polarization is not complete, cf. \cite{1}} In an effort to get around this, in \cite{4} the positive square root of the positive self-adjoint operator

$$\hat{H}^2 = -\frac{\hbar^2}{12} \frac{d^2}{dy^2},$$

was used as the quantum Hamiltonian instead of (3). With this modification a “contradiction” to Conjecture (F) was derived, by exhibiting a wave packet which does not collapse as $t \to \infty$ relative to the one-parameter unitary group $V_t$ generated by this operator. Specifically, it was shown that for an initial Gaussian $\psi$,

$$\lim_{t \to \infty} \langle V_t\psi| \hat{R} |V_t\psi \rangle \geq \frac{1}{2} \langle \hat{R} \rangle_0. \quad (4)$$

But this result is physically flawed: Indeed, \cite{4} prohibits any (Gaussian) universe from contracting to less than half its initial radius, even when $\langle \hat{R} \rangle_0$ is arbitrarily large, i.e., for a very classical initial state. Since under such circumstances quantum effects should be negligible, it follows that the evolution generated by $V_t$ does not have the correct classical limit.

Thus $\sqrt{\hat{H}^2}$ cannot serve as the quantum Hamiltonian (which, in any case, is given unambiguously by (4)), and this renders the assertions in \cite{1,4} invalid. In fact, we have already proven that relative to the genuine quantum Hamiltonian, Conjecture (F) is true.

If one regards positivity is a kinematical requirement that must be preserved by the quantization procedure, then the proper way to circumvent this problem is to construct an alternate quantization in such a manner that the resulting Hamiltonian operator is positive. This we do in the next section. Of course, this alternate quantization cannot be unitarily equivalent to the quantization presented above. Regardless, it is a rigorous quantization for which, as we will show, the collapse Conjecture (F) is \textit{still} valid.

\subsection*{2.2. An Alternate Quantization}

We make the canonical change of coordinates

$$q = R\pi_R, \quad p = \frac{1}{2} \log (|\pi_R|/R),$$

so that the phase space becomes the union of $(-\infty, 0) \times \mathbb{R}$ with $(0, \infty) \times \mathbb{R}$. We quantize in the $q$-coordinate representation, whence the Hilbert
space is $L^2(-\infty, 0) \oplus L^2(0, \infty) \cong L^2(\mathbb{R})$ with respect to Lebesgue measure $dq$. (Note, by means of this isomorphism, that we “simultaneously” quantize classically contracting and expanding models.) Then

$$\hat{H} = \frac{1}{\sqrt{12}} |q|$$

is self-adjoint (on the appropriate domain) and manifestly positive. The resulting quantum evolution is given by

$$\psi(q, t) = e^{-i|q|t/\sqrt{12}} \psi(q).$$

To check for quantum collapse, we consider the classical observable $f = 2p - \log |q| = -2 \log R$, since $f \to \infty$ iff $R \to 0$. Then

$$\hat{f} = -\left(2\hbar \frac{d}{dq} + \log |q| \right)$$

is essentially self-adjoint on the domain consisting of smooth functions compactly supported away from zero. As before, it suffices to consider the dynamics in each summand separately. For an initial state $\psi$ with $\text{supp} \psi \subset (-\infty, 0)$, we calculate

$$\langle \hat{f} \rangle_t = \langle \hat{f} \rangle_0 + \frac{2t}{\sqrt{12}}.$$

This implies that $\langle \hat{f} \rangle_t \to \infty$ as $t \to \infty$. Similarly, $\langle \hat{f} \rangle_t \to -\infty$ as $t \to -\infty$ for an initial $\psi$ with $\text{supp} \psi \subset (0, \infty)$. Thus in this quantization the quantum collapse Conjecture (F) is also valid.

3. FRW MODELS

Next we consider a dust-filled Friedmann-Robertson-Walker (“FRW”) cosmology. We refer the reader to [1, 3, 9] for background on this model.

Prior to an ADM reduction, canonical coordinates are $(R, \pi_R)$ and $(\varphi, \pi_\varphi)$, where $\varphi$ is the only nonzero Seliger-Whitham-Schutz velocity potential for dust and $\pi_\varphi > 0$. The superHamiltonian constraint is

$$\pi_\varphi - \frac{\pi_R^2}{24R} - 6kR = 0. \tag{5}$$

Now suppose $k = -1$. (The analysis for $k = 0$ is similar.) Since $\pi_\varphi > 0$, [3] requires $|\pi_R| > 12R$.

When $\pi_R > 12R$ the model expands from an initial singularity, and when $\pi_R < -12R$ it collapses to a final one.

Choosing the slow time $t = \pi_R$ and performing an ADM reduction, the Hamiltonian is

$$R(\varphi, \pi_\varphi, t) = \frac{1}{12} \left( \sqrt{\pi_\varphi^2 + t^2} - \pi_\varphi \right).$$

In [3] this model is canonically quantized in the momentum representation and it is shown that $\hat{R}(0) = 0$. From this it is concluded that the $k = -1$ FRW model is singular in this slow-time gauge, despite the fact that $\hat{R}(t)$ is self-adjoint for all $t$.

However, the gauge $t = \pi_R$, while acceptable classically when suitably restricted, is not permissible quantum mechanically. The catch is that the reduced phase space is again disconnected into two components, corresponding to whether $\pi_R > 12R$ or $\pi_R < -12R$. Fixing one of these components (say the second, corresponding to a collapsing universe), we see that $\pi_R$ is a priori bounded above by zero. Thus a classical model with $\pi_R < 0$ initially can never evolve to a state for which $\pi_R > 0$, since this entails collapsing through an infinite density singularity where one necessarily loses all predictive power. In fact, for such a model, it does not even make sense to speak of $\pi_R > 0$. But quantum mechanically the Hamiltonian $\hat{R}(t)$ is self-adjoint for all times, so that the evolution is defined for all $t$. The quantized model therefore transits through the classical singularity and emerges into an expansion phase. While the quantized model certainly cannot be said to avoid the singularity at $R = 0$ (as $\hat{R}(0) = 0$), it suffers no apparent “damage”—there is no loss of predictability, or other pathology—as it collapses. Thus it is unclear as to whether the quantum model is actually singular in any sense.

To avoid this sort of conundrum, in [3] such choices of time were specifically excluded. (According to the terminology there, the gauge $t = \pi_R$ is not “dynamically admissible.”) The sine qua non is that if the time variable does not range

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4 Again see [3, §6.4.3].
over all of $(-\infty, \infty)$ classically, then it is unreasonable to expect it to do so quantum mechanically, which is what the self-adjointness of the Hamiltonian requires. Since it is explicitly stated as part of our conjectures in [1, p. 2404] that the choice of time must be dynamically admissible, these models do not qualify as counterexamples to Conjecture (S).

We remark that there do exist dynamically admissible slow-time gauges for the FRW models, e.g., $t = -\varphi$. The corresponding quantized models have been shown to be nonsingular [1, 3, 4, 5], in accordance with Conjecture (S).

In [3], a similar analysis of a $k = 0$ model in the slow-time gauge $t = \pi \mu$, where $\mu = \log R$, is performed. This choice of time is likewise dynamically inadmissible.

4. CONCLUSIONS

Our calculations show unequivocally that the $k = 0$ RW\(\phi\) models collapse quantum mechanically, at least according to the (standard) criteria we have employed [1, 3]. Of course, which of the two inequivalent quantizations presented in §2 is physically correct (if either!) is a matter for speculation. But an essential point is that whether the quantized models collapse does not depend upon the positivity of the quantum Hamiltonian. In this regard, we contend that the alternate quantization in §2.2 is a completely rigorous and systematic way of dealing with problems like non-positivity, as opposed to making ad hoc modifications to the quantum dynamics. We also draw attention to the treatment of the subtleties arising from the disconnectedness of the classical phase space in both the RW\(\phi\) and FRW models.

It will likely require an analysis of more realistic cosmologies to make sense of the behavior of the quantized FRW models. Regardless, these examples illustrate the difficulties that arise when the classical choice of time is ab initio incompatible with the requirement that the quantum dynamics be generated by a self-adjoint Hamiltonian.

For an entirely different approach to these issues, we refer the reader to the recent paper [12].

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