Singularity avoidance in anisotropic quantum cosmology

Claus Kiefer and Nick Kwidzinski
Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

Abstract. We discuss the fate of the classical singularities in quantum cosmological models. We state our criteria of singularity avoidance and apply them to Friedmann-Lemaître models models as well as, in more detail, to the anisotropic case of a Bianchi I universe. We find that the classical singularities are generally avoided in these cases.

1. Introduction
A major issue in any quantum theory is the fate of the classical singularities. Since so far no final theory of quantum gravity exists, this problem can only be addressed within particular approaches [1]. In our contribution, we shall address singularity avoidance in the framework of canonical (metrical) quantum general relativity (quantum geometrodynamics).

In Section 2, we state and discuss our general criteria for singularity avoidance. We employ a generalization of the DeWitt criterion that demands the quantum gravitational state to approach zero in the region of the classical singularity. In Section 3, we briefly review the situation for Friedmann-Lemaître models. In Section 4, we extend the discussion to an anisotropic model – the Bianchi I universe. Sections 2 and 4 are based on our recent paper [2]. Section 5 contains our conclusions and an outlook.

2. Criteria for singularity avoidance
It is well known that singularities are ubiquitous in general relativity. In their general form, the singularity theorems do not display the physical nature of singularity. They usually state incompleteness for timelike or null geodesics. Since cases of physical importance mostly deal with curvature singularities, it seems appropriate to include them explicitly in the definition. In the words of Ellis et al. ([3], p. 145):

We shall define a singularity as a boundary of spacetime where either the curvatures diverges . . . or geodesic incompleteness occurs.

We shall adopt this definition here. (Scalar) curvature singularities are either Ricci tensor divergences or Weyl tensor divergences or a mixture of the two. The first are related to unbounded matter (or field) densities, while the second are related to gravitational field divergences in the vacuum. Both cases will be of relevance here.

In general relativity, singularity theorems can be formulated and proved in a mathematically rigorous manner. This is possible because the theory itself has a sound mathematical foundation. This is not the case in quantum gravity. First, there exist various approaches to such a theory, without any consensus so far [1]. Second, even within particular approaches, the mathematical foundation is limited. Nevertheless, it is of importance to study the fate of classical singularities in quantum gravity approaches, even if this is only possible heuristically. The reason for this is to gain hints on the viability of approaches and to get an idea about the conceptual nature of singularity avoidance.
Our approach here is quantum geometrodynamics. This is, in a sense, the most conservative approach, because its central equations (Wheeler-DeWitt equation and quantum momentum constraints) are obtained by formulating quantum wave equations that lead to the Einstein equations\(^1\) in the semiclassical (WKB) limit. The kinematic quantity here is the wave functional of all three-geometries (and non-gravitational fields). This configuration space is called superspace.

In his pioneering paper on canonical quantum gravity, DeWitt came up with a heuristic proposal for singularity avoidance\([4]\). Assuming that the wave functional \(\Psi\) in quantum gravity is at least loosely related to the probability interpretation in ordinary quantum theory, he suggested to demand that \(\Psi = 0\) in regions where classical singularities are situated. He writes ([4], p. 1129):

\[
\text{Provided it does not turn out to be ultimately inconsistent, this condition,}^2 \ldots \text{yields two important results. Firstly, it makes the probability amplitude for catastrophic 3-geometries vanish, and hence gets the physicist out of his classical predicament. Secondly, it may permit the Cauchy problem for the “wave equation” \ldots to be handled in a manner very similar to that of the ordinary Schrödinger equation.}
\]

In his second point, DeWitt expresses the hope that \(\Psi = 0\) together with the specification of \(\Psi\) on one three-geometry (instead of two, as is natural for a second-order equation) suffices to determine \(\Psi\) for all three-geometries. This is, however, mathematically far from clear. It is even imaginable that only the trivial solutions remain from these two boundary conditions. The specification of \(\Psi\) on one boundary only is related, in spirit, to the no-boundary proposal by Hartle and Hawking (see e.g. [1], p. 279).

The DeWitt condition has frequently been used in the context of Friedmann-Lemaître cosmology, where the configuration space is finite-dimensional and called minisuperspace\([1, 6]\). It also arises as a consequence of unitary evolution for quantum collapsing dust shells; see, for example, [5] in which it is shown how a wave packet representing a collapsing shell will develop into a superposition of collapsing and expanding shell, thereby avoiding the black and white hole singularities.

In the rest of this section, we shall formulate the DeWitt criterion for a general anisotropic model in quantum cosmology. In this, we make use of the fact that the quantum cosmological wave function is, in fact, defined over a conformal manifold, which leads us to a generalization of the original DeWitt criterion\([2]\). This generalization becomes relevant for models with dimension of configuration space greater than two; see below the example for a Bianchi I universe.

To be specific, let us consider the action for general (diagonal) Bianchi class A models with unspecified matter part (see for the following [2] and the references therein):

\[
S_{\text{EH}} + S_m = \int dt \ N e^{3\alpha} \left[ -\dot{\alpha}^2 + \beta_+^2 + \beta_-^2 + \frac{(3)^R}{12} \right] + S_m. \tag{1}
\]

The minisuperspace, \(\mathcal{M}\), of these models is parametrized here by the coordinates \(q = \{\alpha, \beta_+, \beta_-, \phi\}\), where \(\alpha \equiv \ln a\), \(\beta_+, \text{ and } \beta_-\) are the ‘Misner variables’, and \(\phi\) denotes matter field degrees of freedom; \((3)^R\) denotes the three-dimensional Ricci scalar. Units are chosen such that \(3c^6 V_0/4\pi G = 1\), where \(V_0\) is the volume of three-dimensional space (assumed to be compact here).

The central equation of the canonical theory is the Hamiltonian constraint, which follows from (1) by variation with respect to the lapse function \(N\):

\[
\mathcal{H} = \frac{1}{2} G_{IJ} p_I p_J + V = 0. \tag{2}
\]

Here, \(G_{IJ}\) are the components of the DeWitt metric, \(G^{IJ}\) the components of its inverse, and \(V\) is the minisuperspace potential which contains contributions from the three-curvature and from the matter part. The \(p_I\) are the momenta canonically conjugate to the \(q\) above.

\(^1\) More precisely, the four Einsteins equations which are constraints.

\(^2\) He refers to \(\Psi = 0\).
Under a re-scaling of the lapse, $N \rightarrow \tilde{N} = \Omega^2 N$, the transformation of the Hamiltonian constraint follows from the invariance of the total Hamiltonian $H$,

$$H = N\mathcal{H} = \tilde{N}\tilde{\mathcal{H}} = \tilde{N} \left(\frac{1}{2} \Omega^{-2} \mathcal{G}^{IJ}_{pI} p_{pJ} + \Omega^{-2} \mathcal{V}\right) \equiv \tilde{N} \left(\frac{1}{2} \tilde{\mathcal{G}}^{IJ}_{pI} p_{pJ} + \tilde{\mathcal{V}}\right).$$

(3)

For this reason, we can interpret the minisuperspace as a conformal manifold $\left(\mathcal{M}, \left[\mathcal{G}_{IJ} dq^I \otimes dq^J\right]\right)$. This conformal structure motivates the choice of a factor ordering that renders the Wheeler–DeWitt equation conformally covariant. Explicitly,

$$\left[-\frac{\hbar^2}{2} \left(\Box - \xi \mathcal{R}\right) + \mathcal{V}\right] \Psi = 0,$$

(4)

where $\mathcal{R}$ denotes the Ricci scalar constructed from $\mathcal{G}_{II}$ and $\xi = \frac{d-2}{d(d-1)}$, with $d = \dim(\mathcal{M})$. For the equation to be conformally covariant the wave function has to transform as $\Psi \rightarrow \tilde{\Psi} = \Omega^{-\frac{d-2}{2}} \Psi$. This is why the original DeWitt criterion ($\Psi \rightarrow 0$) is only a good criterion when dealing with two-dimensional minisuperspaces.

We are now interested in the formulation of a conformally invariant DeWitt criterion. For this we note that the following scalar density is invariant under a conformal transformation in minisuperspace:

$$\star |\Psi|^{2d} = |\Psi|^{2d} \text{dvol}.$$

(5)

Here, dvol contains the square root of the (absolute value of the) determinant of the DeWitt metric, and $\star$ denotes the Hodge star. The generalized DeWitt criterion then reads:

A singularity is said to be avoided if $\star |\Psi|^{2d} \rightarrow 0$ in the vicinity of the singularity.

We emphasize that this criterion, as the original one, is a sufficient criterion only, not a necessary one. As one knows from quantum mechanics (e.g. from the solutions for the energy eigenstates of the hydrogen atom from the Dirac equation), one can have singularity avoidance even for diverging wave functions.

One can think of other criteria. In the first paper along this direction, [7], singularity avoidance was inferred from the breakdown of the semiclassical approximation when approaching the region of the singularity. Then, the notion of a classical trajectory loses its meaning and the classical theorems cannot be applied. In a sense, the DeWitt criterion also obeys this criterion, because the vanishing of the wave function signals the breakdown of the semiclassical approximation.

In [2], we have also applied the criterion that implies singularity avoidance if the Klein-Gordon flux vanishes in the vicinity of the classical singularity\footnote{This was motivated by the fact that the Klein-Gordon current is a conformally invariant $(d-1)$-form.}. In the explicit examples discussed there, this leads in general to results different from the DeWitt criterion. Because some aspects of the Klein-Gordon flux are problematic in this context (e.g. it is not positive definite), we shall not consider this criterion here. It must, however, be remarked that the validity of the DeWitt criterion usually demands the superposition of different semiclassical components for the Klein-Gordon current (see Eq. (6.29) in [4]).

3. Singularity avoidance in Friedmann-Lemaître cosmology

Friedmann-Lemaître models are homogeneous and isotropic. From the gravitational side, the scale factor $a(t)$ is the only dynamical quantity. In order to represent matter and render the model non-trivial, usually a scalar field $\phi(t)$ with an appropriate potential $V(\phi)$ is added. We thus have a two-dimensional minisuperspace. The metric is given by

$$\text{d}s^2 = -N^2(t)\text{d}t^2 + a^2(t)\text{d}\Omega^2_3,$$

(6)
where $d\Omega^2_3$ is the three-dimensional spatial line element (here chosen to be the three-sphere). After quantization, the Wheeler-DeWitt equation reads

$$\frac{1}{2} \left( \frac{\hbar^2}{a^2} \frac{\partial^2}{\partial a^2} \left( a \frac{\partial}{\partial a} \right) - \frac{\hbar^2}{a^3} \frac{\partial^2}{\partial \phi^2} - a + \frac{\Lambda a^3}{3} + 2a^3 V(\phi) \right) \Psi(a, \phi) = 0.$$  \hspace{1cm} (7)

Here, the Laplace-Beltrami factor ordering is chosen, which for a two-dimensional configuration space is equivalent to the above conformal factor ordering.

The standard singularities in general relativity are big bang and (for a recollapsing universe) big crunch. Motivated by the observation of a currently accelerating universe, one can introduce a scalar field with a suitable potential as the origin of such an acceleration. The presence of such a ‘dark energy’ can lead to further singularities, such as big rip, big brake, big freeze, and others; see, for example, [8] and the references therein. In a series of papers (see e.g. [9] and the references therein) it was possible to investigate the applicability of the DeWitt criterion in detail. The main result is that this is in generally possible: the Wheeler-DeWitt equation possesses solutions with $\Psi = 0$ in the region of the classical singularity. Let us quote one specific example. In [10], the avoidance of a classical big-brake singularity\(^4\) was demonstrated. The result is illustrated in Figure 1.

![Classical trajectory and wave packet](image)

(a) Classical trajectory. From [10].

(b) Wave packet; here, $\tau = a^6$. From [10].

Figure 1: The avoidance of a classical singularity in quantum cosmology.

The left part (a) shows the classical trajectory $\phi(a)$ in configuration space. The big brake occurs at $\phi = 0$. The right part b) shows a plot of an exact solution of the Wheeler-DeWitt equation close to $\phi = 0$; this solution goes to zero there and thus satisfies the DeWitt criterion.

### 4. Singularity avoidance in Bianchi I quantum cosmology

The simplest anisotropic model is the vacuum Bianchi I model, also called Kasner universe. The metric can be written as

$$ds^2 = -dt^2 + t^{2p_x} dx^2 + t^{2p_y} dy^2 + t^{2p_z} dz^2 \quad \text{with} \quad p_x^2 + p_y^2 + p_z^2 = 1 \quad \text{and} \quad p_x + p_y + p_z = 1.$$  \hspace{1cm} (8)

\(^4\) In a big-brake singularity the universe comes to an abrupt halt in the future, with the density $\rho$ finite, but the pressure $p$ diverging.
Details on this model (and other anisotropic models) can be found, for example, in [3]. In the Kasner universe one has a singularity which can be described by the divergence of the Weyl squared scalar. After quantization, one obtains the Wheeler-DeWitt equation, which in the above conformal factor ordering reads (with $\hbar = 1$),

$$\left[-\frac{\partial^2}{\partial \alpha^2} + \frac{\partial^2}{\partial \beta_+^2} + \frac{\partial^2}{\partial \beta_-^2}\right] \Psi(\alpha, \beta_+, \beta_-) = 0.$$  \hspace{1cm} (10)

This is identical, in its form, to the classical wave equation in $d = 1 + 2$ dimensions. Using decay rate estimates for such an equation, one finds that the DeWitt criterion is fulfilled for a small universe ($\alpha \to -\infty$) as well as for a big universe ($\alpha \to +\infty$):

$$|\Psi|^6 \to 0 \text{ as } \alpha \to \pm \infty.$$  \hspace{1cm} (11)

The initial singularity is thus avoided by this criterion. The decay of the amplitude $|\Psi|$ is induced by a spreading of the wave packet as shown in Figure 2. It is at first glance surprising that this criterion applies to the future evolution, too: whereas classically the universe expands forever, quantum cosmologically the wave packets cease to evolve, and the semiclassical approximation breaks down. This demonstrates that quantum effects can, in principle, occur at any scale, as a mere consequence of the superposition principle. Other examples are the above mentioned quantum effects near the big brake as well as quantum effects near the turning point of a classically recollapsing universe [11].

Let us now add matter to this model. The simplest way is to treat matter by an effective potential only, without considering a kinetic term for it [2]. Using the ansatz for a barotropic fluid, one finds that the situation for a small universe is similar to the quantum Kasner model, and that the DeWitt criterion holds as before: the initial singularity is avoided. For a big universe, one can have classically an ever expanding universe or a big-rip singularity, depending on the exact form of the equation of state. In both cases, the DeWitt criterion holds, so the wave packets do not reflect either of these two cases. A plot of a corresponding wave packet is shown in Figure 3.

At a fundamental level, matter should be described dynamically, for example by using a scalar field. Let us here only address the case of a phantom field, that is, a field with negative kinetic term that can mimic dark energy [2]. Classically, this leads to a big-rip singularity in the future (universe expanding...
Figure 3: Plot of equipotential surfaces of $|D^{-1/2}\psi|$ for a wave packet $\psi$ solving the Wheeler-DeWitt equation with an effective dust potential. The factor $D^{-1/2}$ provides a suitable rescaling for the purpose of visualization. The thin black line is the classical trajectory, which describes an isotropizing Bianchi I universe. The wave packet spreads in the region close to the big-bang singularity similarly to the Kasner model.

to infinity in a finite time). Unlike the situation shown in Figure 1, the field $\phi$ diverges in this limit. The conformally covariant Wheeler–DeWitt equation in the limit approaching the big rip is found to read

$$\left[ \frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \beta_+^2} - \frac{\partial^2}{\partial \beta_-^2} + \frac{\partial^2}{\partial \phi^2} + V_0 e^{6(\alpha + |\phi|)} \right] \Psi(\alpha, \beta_+, \beta_-, \phi) = 0. \quad (12)$$

A detailed analysis of this equation and its solutions reveals that the DeWitt criterion is fulfilled and the big rip is thus avoided [2].

Figure 4 shows a plot of a wave packet using numerical integration. It gives the results for $\alpha = 10$ and increasing values of $|\phi|$. For increasing $|\phi|$, the wave packet assumes an annular shape and propagates outwards with decreasing amplitude; it is peaked in the direction of negative $\beta_\pm$.

5. Conclusion and Outlook

In this contribution, we have discussed the fate of classical singularities in Friedmann-Lemaître as well as Bianchi I models of quantum cosmology. Employing a generalized form of the DeWitt criterion, we have seen that these singularities can generally be avoided.

Singularity avoidance is also discussed in other approaches such as loop quantum cosmology. There, the resolution is usually treated as a non-singular bounce in quantum-corrected cosmological models; see, for example, the recent discussion of Bianchi models in [12]. It would, of course, be of great interest to perform a detailed comparison of this approach with the present one.

Future work should address the issue of singularity avoidance for models of increasing complexity. The Bianchi I models discussed here belong to the class of asymptotically velocity dominated (AVTD) models, for which the kinetic terms become dominant in the vicinity of the initial singularity. Our results for these models should thus be representative for more general models which admit such an AVTD behaviour.

The general approach to a classical spacelike singularity is been assumed to be of the Belinsky-Khalatnikov-Lifshits (BKL) type; see, for example, [13] for a recent discussion. This corresponds to
\[ \phi = 10.75, \quad \phi = 14.25, \quad \phi = 18, \quad \phi = 18, \times 10 \]

Figure 4: Density plot for \(|\Psi|e^{\frac{3}{2}(\alpha + |\phi|)}\), showing the position of the wave packet for different values of \(|\phi|\), each with a different scaling to visualize the decaying wave in a single graphic. From [2].

an evolution that behaves as if a separate mixmaster model were attached to each spatial point. The discussion of the Wheeler-DeWitt equation for such a situation should give a quantum picture of the BKL behaviour and should answer the question whether the singularities are avoided in the generic case. If this could be achieved, one would have gained a complete picture of the situation in quantum geometrodynamics, given our present level of understanding.

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