

On the Avoidance of Classical Singularities in Quantum Cosmology

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Abstract.

Many cosmological models based on general relativity contain singularities. I address here the question whether consistent models without singularities can exist in quantum cosmology. The discussion is based on the Wheeler–DeWitt equation of quantum geometrodynamics. The models under consideration are partly motivated by recent discussions of dark energy. Natural criteria of singularity avoidance in the quantum theory are the vanishing of the wave function at the classical singularity or the breakdown of the semiclassical approximation upon approaching the region of the singularity. I show that singularity avoidance in this sense can happen in the models under consideration.

1. Introduction

The search for a quantum theory of gravity belongs to the most important tasks in fundamental physics [1]. Whilst such a theory is not yet available in final form, it is more or less obvious which expectations it should fulfill. Among them is the fate of the classical singularities in quantum gravity: a reasonable theory of quantum gravity should predict their avoidance.

Given the incomplete understanding of quantum gravity, it is obvious that general conclusions cannot yet be drawn. However, the issue of singularity avoidance may be addressed within the context of simple models. This is the topic of my contribution. I shall restrict myself to singularities for homogeneous and isotropic cosmological models. For such models, the quantization can be performed and the question can be investigated whether singularity-free solutions exist and whether they are natural.

My paper is organized as follows. In section 2, I shall quote one of the famous singularity theorems and give an overview of cosmological singularities in Friedmann models; here, one does not only have the standard big-bang and big-crunch singularities, but also more exotic ones such as a big rip or a big brake. Section 3 presents the general framework of my discussion, quantum geometrodynamics and the Wheeler–DeWitt equation, as well as arguments why this framework is an appropriate one for the issue under investigation. In section 4, then, I review the quantum cosmology of some of these models and show that there, indeed, singularities can be avoided in a natural way. One could imagine that singularity avoidance is similarly implementable in full quantum gravity. I end with some brief conclusions.

My contribution here is closely related to a similar contribution for another conference [2].

2. Classical singularities in cosmology

We call a spacetime singular if it is incomplete with respect to a timelike or null geodesic and if it cannot be embedded in a bigger spacetime. There exists a variety of theorems which postulate the existence of singularities in general relativity [3]. Typically, they involve an energy condition, a condition on the

global structure, and the condition that gravitation be strong enough to lead to the existence of a closed trapped surface. Let me quote one of the famous theorems proved by Hawking and Penrose in 1970 [4]:

A spacetime M cannot satisfy causal geodesic completeness if, together with Einstein's equations, the following four conditions hold:

- (i) M contains no closed timelike curves.
- (ii) The strong energy condition is satisfied at every point.
- (iii) The generality condition (...) is satisfied for every causal geodesic.
- (iv) M contains either a trapped surface, or a point P for which the convergence of all the null geodesics through P changes sign somewhere to the past of P , or a compact spacelike hypersurface

If we take an ideal fluid as a model for matter, with ρ as the energy density and p_i ($i = 1, 2, 3$) as the principal pressures, the strong energy condition used in this theorem reads as

$$\rho + \sum_i p_i \geq 0, \quad \rho + p_i \geq 0, \quad i = 1, 2, 3. \quad (1)$$

In fact, as was already shown in [4] and discussed in [3], the observation of the Cosmic Microwave Background Radiation indicates that there is enough matter on the past light-cone of our present location P to imply that the divergence of this cone changes somewhere to the past of P . Thus, if in addition the strong energy condition is fulfilled, the conditions stated in the above theorem will apply and the origin of our Universe cannot be described within general relativity.

Modern cosmology entertains the idea that a period of quasi-exponential acceleration ("inflation") took place in the very early Universe. Since such an inflationary phase may violate the strong energy conditions, it has been speculated that the singularity can thereby be avoided. Is this true? There are two aspects of this. On the one hand, it was shown by Börde *et al.* in [5] that singularities are not avoided by an inflationary phase if the universe has open spatial sections or if the Hubble expansion rate is bounded away from zero in the past. On the other hand, Ellis *et al.* have presented an example of a singularity-free inflationary model with closed spatial sections [6]. Thus, independent of what describes more precisely the real conditions in the early Universe, one should at least envisage the possibility that the classical solution describing it is singular.

Cosmological singularities cannot only happen in the past. There is the option (presently not supported by observations) that the Universe will recollapse in the future and encounter a big-crunch singularity. But even if the Universe continues to expand, it can encounter singularities in the future for non-vanishing scale factor. This can happen for various equations of state which can describe a form of dark energy. (Such singularities may also occur at a finite value $a > 0$ in the past). In fact, present observations still allow the possibility of an equation of state leading to such "exotic" singularities, cf. [7] and the references therein. In the light of the above-quoted singularity theorem it is of interest to remark that these exotic singularities may or may not violate energy conditions, so this theorem is not directly applicable and one has to explore additional options for relevant energy conditions.

One can classify cosmological singularities for homogeneous and isotropic spacetimes following the schemes proposed in [7, 9]. Different singularities can be distinguished according to the behaviour of scale factor a , energy density ρ , and pressure p . The classification is

Big Bang/Crunch $a = 0$ at finite proper time, but ρ diverges.

Type I (Big Rip) a diverges in finite proper time, and both ρ and p diverge. A big rip is obtained from phantom dark energy, that is, matter with an equation of state $p = w\rho$, $w < -1$. Phantoms not only violate the strong energy condition (cf. the theorem quoted above), but also all the other energy conditions.

Type II (Sudden singularity) a and ρ remain finite, p diverges, but the Hubble parameter stays finite (\dot{H} diverges). Sudden singularities only violate the dominant energy condition. Special cases

are the big-brake singularity in the future and the big-démarrage singularity in the past; these are characterized as sudden singularities arising from a generalized Chaplygin equation of state, $p = -A/\rho^\beta$. For sudden singularities, geodesics can be continued through these singularities, but tidal forces diverge. Sudden singularities can appear as close as 8.7 million years in the future [7]. There exist also generalized sudden singularities, which are singularities of pressure derivatives and which fulfill all energy conditions.

Type III (Finite scale factor singularity) a remains finite, but both ρ and p diverge (as well as H and \dot{H}); particular examples are the “big-freeze” singularities (both in the past and the future), which are characterized by a generalized Chaplygin equation of state.

Type IV (Big Separation) a , ρ , and p remain finite, but the r th derivative of a and the $(r - 1)$ th derivative of H diverge ($r \geq 3$).

w -singularity The only singularity here is in the barotropic index w [8].

In extension of the Type I to IV classification, one could call big bang/big crunch Type 0 and the w -singularity Type V.

It is now of interest to see whether some or all of these singularities can be avoided in quantum gravity. We have investigated the quantum theory for some of these models [10, 11, 12], and some of the results will be discussed below. Before that, however, I shall briefly introduce the framework on which the investigation is based.

3. Quantum geometrodynamics

A full quantum theory of gravity remains elusive [1]. Can one nevertheless say something reliable about quantum gravity without knowing the exact theory? In [13] I have made the point that this is indeed possible. The situation is analogous to the role of the quantum mechanical Schrödinger equation. Although this equation is not fundamental (it is non-relativistic, it is not field-theoretic, and so on), important insights can be drawn from it. For example, in the case of the hydrogen atom, one has to impose boundary conditions for the wave function at the origin $r \rightarrow 0$, that is, at the centre of the atom. This is certainly not a region where one would expect non-relativistic quantum mechanics to be exactly valid, but its consequences, in particular the resulting spectrum, are empirically correct to an excellent approximation.

Erwin Schrödinger has found his equation by “guessing” a wave equation from which the Hamilton–Jacobi equation of classical mechanics can be recovered in the limit of small wavelengths, in analogy to the limit of geometric optics from wave optics. The same approach can be applied to general relativity. One can start from the Hamilton–Jacobi version of Einstein’s equations and “guess” a wave equation from which it can be recovered in the classical limit. The only assumption that is required is the universal validity of quantum theory, that is, its linear structure. It is not yet needed for this step to impose a Hilbert-space structure. Such a structure is employed in quantum mechanics because of the probability interpretation for which one needs a scalar product and its conservation in time (unitarity). Its status in quantum gravity remains open.

The Hamilton–Jacobi equation for general relativity was formulated by Peres [14]. In the vacuum case, it reads (we set $c = 1$ in the following)

$$16\pi G G_{abcd} \frac{\delta S}{\delta h_{ab}} \frac{\delta S}{\delta h_{cd}} - \frac{\sqrt{h}}{16\pi G} ({}^{(3)}R - 2\Lambda) = 0. \quad (2)$$

The functional $S[h_{ab}]$ depends on the three-dimensional metric, h_{ab} . It also obeys the equation

$$D_a \frac{\delta S}{\delta h_{ab}} = 0, \quad (3)$$

which guarantees that $S[h_{ab}]$ is invariant under three-dimensional coordinate transformations.

The task is now to find a wave equation which yields the Hamilton–Jacobi equation (2) as well as Eq. (3) in the semiclassical limit (“WKB approximation”) where the wave functional reads

$$\Psi[h_{ab}] = C[h_{ab}] \exp\left(\frac{i}{\hbar} S[h_{ab}]\right) \quad (4)$$

with a rapidly varying phase and a slowly varying amplitude. In the vacuum case, one then finds from (2) and (3) the equations

$$\hat{H}\Psi \equiv \left(-16\pi G\hbar^2 G_{abcd} \frac{\delta^2}{\delta h_{ab}\delta h_{cd}} - (16\pi G)^{-1} \sqrt{h} ({}^3R - 2\Lambda)\right) \Psi = 0, \quad (5)$$

and

$$\hat{D}^a\Psi \equiv -2\nabla_b \frac{\hbar}{i} \frac{\delta\Psi}{\delta h_{ab}} = 0. \quad (6)$$

The first equation is called the Wheeler–DeWitt equation, the second one – which guarantees the invariance of the wave functional under three-dimensional coordinate transformations – is called the quantum diffeomorphism (momentum) constraint. Whether these equations hold at the most fundamental level or not, they should approximately be valid away from the Planck scale, provided that quantum theory is universally valid.

We recognize from (5) and (6) that no external time is present anymore – spacetime has *disappeared* and only space remains [1]. Nevertheless, a local *intrinsic time* can be defined through the local hyperbolic structure of the Wheeler–DeWitt equation. This intrinsic time is solely constructed from the three-geometry (and matter degrees of freedom, if present).

If non-gravitational degrees of freedom are present, the equations (5) and (6) have to be augmented by the corresponding terms. For the semiclassical approximation one then makes the following “Born–Oppenheimer”-type of ansatz [1]

$$|\Psi[h_{ab}]\rangle = C[h_{ab}] e^{im_P^2 S[h_{ab}]} |\psi[h_{ab}]\rangle, \quad (7)$$

where the *bra* and *ket* notation refers to non-gravitational fields, for which we can assume that a standard Hilbert-space is at our disposal (m_P denotes the Planck length).

One then evaluates the wave functional $|\psi[h_{ab}]\rangle$ along a solution of the classical Einstein equations, $h_{ab}(\mathbf{x}, t)$, corresponding to a solution, $S[h_{ab}]$, of Equations (2) and (3); this solution is obtained from

$$\dot{h}_{ab} = NG_{abcd} \frac{\delta S}{\delta h_{cd}} + 2D_{(a} N_{b)} , \quad (8)$$

where N and N_b denote the lapse function and the shift vector, respectively [1]. Employing in the semiclassical limit the following definition of an *approximate* time parameter t ,

$$\frac{\partial}{\partial t} |\psi(t)\rangle = \int d^3x \dot{h}_{ab}(\mathbf{x}, t) \frac{\delta}{\delta h_{ab}(\mathbf{x})} |\psi[h_{ab}]\rangle,$$

one obtains a functional Schrödinger equation for quantized matter fields in the chosen external classical gravitational field:

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle &= \hat{H}^m |\psi(t)\rangle, \\ \hat{H}^m &\equiv \int d^3x \left\{ N(\mathbf{x}) \hat{\mathcal{H}}_+^m(\mathbf{x}) + N^a(\mathbf{x}) \hat{\mathcal{H}}_a^m(\mathbf{x}) \right\}. \end{aligned} \quad (9)$$

Here, \hat{H}^m denotes the matter-field Hamiltonian in the Schrödinger picture, parametrically depending on the (generally non-static) metric coefficients of the curved space-time background; the “WKB time” t controls the dynamics in this approximation.

The special ansatz (7) can be justified through the process of decoherence [15]. Unobserved degrees of freedom such as tiny gravitational waves or small density fluctuations interact with the relevant degrees of freedom (e.g. the volume of the three-dimensional space) in such a way that, for example, the superposition of (7) with its complex conjugate cannot be distinguished from a corresponding mixture; the state (7) can thus be treated separately. This is analogous to the emergence of the chiral structure for certain molecules [15].

The semiclassical approximation and the ensuing time parameter exist, of course, only under special conditions. Only then can the notions of spacetime and geodesics, needed for the application of the classical singularity theorems, be employed. In the quantum case we have to think first about the meaning of singularities and singularity avoidance.

4. Quantum avoidance of singularities

There does not yet exist any general agreement on the necessary criteria for quantum avoidance of singularities. I shall not attempt here to provide such necessary criteria either, but shall focus instead on two sufficient criteria which have turned out to be useful in the discussion of the models presented below. The first criterium dates back to the pioneering work of Bryce DeWitt on canonical quantum gravity [16]. He has suggested that the wave function should vanish at the point of the classical singularity. We shall thus interpret the vanishing of the wave function in the region of the classical singularity as singularity avoidance. As a second criterium we shall adopt the spreading of wave packets when approaching the region of the classical singularity: the semiclassical approximation discussed above breaks down in this case and no classical time parameter is available. The classical singularity theorems can then no longer be applied.

It must be emphasized that $\Psi \rightarrow 0$ is really only a sufficient, but by no means a necessary criterium for singularity avoidance. Consider, for example, the solution of the Dirac equation for the ground state of hydrogen-like atoms (in standard notation). This solution diverges at the origin,

$$\psi_0(r) \propto (2mZ\alpha r)^{\sqrt{1-Z^2\alpha^2}-1} e^{-mZ\alpha r} \xrightarrow{r \rightarrow 0} \infty ,$$

but $\int dr r^2 |\psi_0|^2$ remains finite. So the important quantity is, in fact, the inner product. As already mentioned, there is no general consensus about the role of the inner product in quantum cosmology, but the situation could be analogous to the hydrogen atom. In the case of the Wheeler–DeWitt equation for a Friedmann universe with a massless scalar field, for example, the simplest solution diverges for scale factor $a \rightarrow 0$,

$$\Psi \propto K_0(a^2/2) \xrightarrow{a \rightarrow 0} c \ln a ,$$

but nevertheless the integral $\int da d\phi \sqrt{|G|} |\psi(a, \phi)|^2$, where G here denotes the determinant of the DeWitt metric, may be finite.

For a closed Friedmann–Lemaître universe with scale factor a , containing a homogeneous scalar field ϕ with potential $V(\phi)$, that is, a two-dimensional *minisuperspace*, the classical line element is

$$ds^2 = -N^2(t)dt^2 + a^2(t)d\Omega_3^2 .$$

The Wheeler–DeWitt equation reads (with units $2G/3\pi = 1$)

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

where the factor ordering has been chosen in order to achieve covariance in minisuperspace; this is the Laplace–Beltrami factor ordering. (For a general overview of quantum cosmology, see, for example, [1, 17] and the references therein.)

Let us consider now various models with classical singularities. The first one is a model with “phantoms”. These are fields with negative kinetic energy, which are certainly very exotic but which cannot yet be excluded on the basis of supernova data. Classically, the ensuing dynamics develops a “big-rip singularity”, that is, ρ and p diverge as a goes to infinity at a *finite time* (see above). The corresponding quantization was discussed in [10]. It was found that wave-packet solutions of the Wheeler–DeWitt equation necessarily disperse in the region of the classical big-rip singularity; time and the classical evolution thus come to an end and only a stationary quantum state is left. Quantum effects thus become important for a big universe, not only for a small Planck-size universe. Interestingly, it was shown that an alternative quantization, employing the Bohm interpretation of quantum theory, cannot avoid the big-rip singularity [18].

Another model is cosmology with a big brake [11]. We take an equation of state of the form $p = A/\rho$, $A > 0$, that is, an “Anti-Chaplygin gas”. For a Friedmann universe with scale factor $a(t)$ and a scalar field $\phi(t)$, this equation of state can be realized by the potential

$$V(\phi) = V_0 \left(\sinh \left(\sqrt{3\kappa^2} |\phi| \right) - \frac{1}{\sinh \left(\sqrt{3\kappa^2} |\phi| \right)} \right); \quad V_0 = \sqrt{A/4},$$

where $\kappa^2 = 8\pi G$. The classical dynamics develops a pressure singularity (only $\ddot{a}(t)$ becomes singular) and comes to an abrupt halt in the future.

The Wheeler–DeWitt equation for this model reads

$$\frac{\hbar^2}{2} \left(\frac{\kappa^2}{6} \frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \phi^2} \right) \Psi(\alpha, \phi) + V_0 e^{6\alpha} \left(\sinh \left(\sqrt{3\kappa^2} |\phi| \right) - \frac{1}{\sinh \left(\sqrt{3\kappa^2} |\phi| \right)} \right) \Psi(\alpha, \phi) = 0, \quad (10)$$

where $\alpha = \ln a$, and Laplace–Beltrami factor ordering has again been used. The vicinity of the big-brake singularity is the region of small ϕ ; we can therefore use the approximation

$$\frac{\hbar^2}{2} \left(\frac{\kappa^2}{6} \frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \phi^2} \right) \Psi(\alpha, \phi) - \frac{\tilde{V}_0}{|\phi|} e^{6\alpha} \Psi(\alpha, \phi) = 0,$$

where $\tilde{V}_0 = V_0/3\kappa^2$.

It was shown in [11] that all normalizable solutions read

$$\Psi(\alpha, \phi) = \sum_{k=1}^{\infty} A(k) k^{-3/2} K_0 \left(\frac{1}{\sqrt{6}} \frac{V_\alpha}{\hbar^2 k \kappa} \right) \times \left(2 \frac{V_\alpha}{k} |\phi| \right) e^{-\frac{V_\alpha}{k|\phi|}} L_{k-1}^1 \left(2 \frac{V_\alpha}{k} |\phi| \right), \quad (11)$$

where K_0 is a Bessel function, L_{k-1}^1 are Laguerre polynomials, and $V_\alpha \equiv \tilde{V}_0 e^{6\alpha}$. They all *vanish* at the classical singularity. This model therefore implements our other criterium above: the vanishing of the wave function in the spirit of DeWitt. A similar result holds for the corresponding loop quantum cosmology. Interestingly, the solutions also implement the avoidance of the big-bang singularity, $\Psi \rightarrow 0$ for $\alpha \rightarrow -\infty$.

The big-brake singularity is an example of type-II singularities. A more general class of type-II and type-III singularities was discussed in [12]. The equation of state in this class is chosen to be that of a generalized Chaplygin gas:

$$p = -\frac{A}{\rho^\beta}$$

with general real parameters A and β . For example, in the big-freeze (type III) singularity, both H and \dot{H} blow up at a finite value of the scale factor in the past. The big-freeze singularity occurs in the past at a

minimal scale factor $a_{\min} > 0$; there are thus no classical solutions in the limit $\alpha \rightarrow -\infty$. For this reason we have to demand that the wave function go to zero in the classically forbidden region, $\Psi \xrightarrow{\alpha \rightarrow -\infty} 0$, because otherwise one would not obtain the correct classical limit.

The class of solutions then reads

$$\Psi_k(\alpha, \phi) \propto \sqrt{|\phi|} J_\nu(k|\phi|) \left[b_1 e^{i \frac{\sqrt{6}k}{\kappa} \alpha} + b_2 e^{-i \frac{\sqrt{6}k}{\kappa} \alpha} \right],$$

with ν as a function of α . These solutions obey, in fact, DeWitt's boundary condition at the singularity, $\Psi_k(0, 0) = 0$. The same also holds for the other cases discussed in [12].

The vanishing of the wave function at the classical singularity plays also a key role in other approaches. An especially interesting example are the supersymmetric quantum cosmological billiards discussed in [19]. In $D = 11$ supergravity, one can employ near a spacelike singularity a cosmological billiard description based on the Kac–Moody group E_{10} and address the corresponding Wheeler–DeWitt equation. It was found there, too, that $\Psi \rightarrow 0$ near the singularity. Such a behaviour also occurs in a model with null dust shells where the classical black-hole and white-hole singularities are thereby avoided in the quantum theory [20]. DeWitt's criterium of singularity avoidance may thus be a viable criterium implementable in a wide range of quantum cosmological models.

5. Conclusion

I have shown that the classical cosmological singularities of various models can be avoided in quantum cosmology. Two sufficient (but by no means necessary) criteria have been employed for this purpose: unavoidable spreading of the wave function when approaching the singular region and vanishing of the wave function at the singularity itself.

The models discussed here can have (in the classical theory) singularities at large values of the scale factor, that is, far away from the Planck length. The corresponding quantum avoidance thus means that quantum gravitational effects can occur for large universes – an intriguing thought. Such macroscopic quantum effects have hitherto only been envisaged near the turning point of a classically recollapsing universe [21, 22]. It is clear that these scenarios have also consequences for the arrow of time in the universe [21, 23].

Singularity avoidance also occurs in the framework of loop quantum cosmology, although in a somewhat different way, see [24]. The big-bang singularity can be avoided by solutions of the difference equation which there replaces the Wheeler–DeWitt equation. The avoidance can also be achieved by the occurrence of a bounce in the effective Friedmann equations. For the singularities at large scale factors of the big-rip or big-brake type, the mechanism of avoidance is similar to the one discussed above for the Wheeler–DeWitt equation, but there are other sudden singularities that do not seem to be avoided [25].

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