On the avoidance of classical singularities in quantum cosmology

Claus Kiefer

Institut für Theoretische Physik
Universität zu Köln
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Definition of a singularity
A spacetime is singular if it is incomplete with respect to a timelike or null geodesic and if it cannot be embedded in a bigger spacetime.

- Energy condition
- Condition on the global structure
- Gravitation strong enough to lead to the existence of a closed trapped surface
Theorem (Hawking and Penrose 1970)

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

1. \( M \) contains no closed timelike curves.
2. The strong energy condition is satisfied at every point.
3. The generality condition (\ldots) is satisfied for every causal geodesic.
4. \( M \) 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

Strong energy condition:

\[
\rho + \sum_i p_i \geq 0, \quad \rho + p_i \geq 0, \quad i = 1, 2, 3
\]
Cosmological singularities for homogeneous and isotropic spacetimes

Classified by behaviour of scale factor $a$, energy density $\rho$, pressure $p$:

**Big Bang/Crunch**  $a = 0$ at finite proper time, $\rho$ diverges

**Type I (Big Rip)**  $a$ diverges in finite proper time, $\rho$ and $p$ diverge

**Type II or “sudden” (Big Brake/Big Démarrage)**  $a$ finite, $\rho$ finite, $p$ diverges, Hubble parameter finite

**Type III (Big Freeze)**  $a$ finite, both $\rho$ and $p$ diverge

**Type IV**  $a$ finite, both $\rho$ and $p$ finite, but curvature derivatives diverge
Relation to observations

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 $p$.

but: inflationary phase in the early Universe may violate the strong-energy condition $\rightarrow$ singularity avoidance?
What about inflation?

- Borde et al. (2003): Singularities are not avoided by an inflationary phase if the universe has open spatial sections or the Hubble expansion rate is bounded away from zero in the past;
- Ellis et al. (2004): There exist singularity-free inflationary models for closed spatial sections

moreover: observation of “dark energy” suggests the possibility of a future singularity at a finite $a$ in the future (e.g. Big Rip/Big Brake)

Quantum gravitational avoidance of the classical singularity?
Main Approaches to Quantum Gravity

No question about quantum gravity is more difficult than the question, “What is the question?” (John Wheeler 1984)

- Quantum general relativity
  - Covariant approaches (perturbation theory, path integrals, …)
  - Canonical approaches (geometrodynamics, connection dynamics, loop dynamics, …)

- String theory

- Other approaches
  (Quantization of topology, causal sets . . .)

Topic here: Canonical quantum geometrodynamics

(more details on all approaches e.g. in C. K., Quantum Gravity (Oxford 2007))
Erwin Schrödinger 1926:

*We know today, in fact, that our classical mechanics fails for very small dimensions of the path and for very great curvatures.* Perhaps this failure is in strict analogy with the failure of geometrical optics . . . that becomes evident as soon as the obstacles or apertures are no longer great compared with the real, finite, wavelength. . . . Then it becomes a question of searching for an undulatory mechanics, and the most obvious way is by an elaboration of the Hamiltonian analogy on the lines of undulatory optics.¹

¹*Wir wissen doch heute, daß unsere klassische Mechanik bei sehr kleinen Bahndimensionen und sehr starken Bahnkrümmungen versagt.* Vielleicht ist dieses Versagen eine volle Analogie zum Versagen der geometrischen Optik . . . , das bekanntlich eintritt, sobald die ‘Hindernisse’ oder ‘Öffnungen’ nicht mehr groß sind gegen die wirkliche, endliche Wellenlänge. . . . Dann gilt es, eine ‘undulatorische Mechanik’ zu suchen – und der nächstliegende Weg dazu ist wohl die wellentheoretische Ausgestaltung des Hamiltonschen Bildes.
Hamilton–Jacobi equation

In the vacuum case, one has

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

\[ D_a \frac{\delta S}{\delta h_{ab}} = 0 \]

(Peres 1962)

Find wave equation which yields the Hamilton–Jacobi equation in the semiclassical limit

**WKB approximation:**

\[ \Psi[h_{ab}] = C[h_{ab}] \exp \left( \frac{i}{\hbar} S[h_{ab}] \right) \]
Quantum equations

In the vacuum case, one has

\[ \hat{H} \Psi \equiv \left( -2\kappa \hbar^2 G_{abcd} \frac{\delta^2}{\delta h_{ab} \delta h_{cd}} - (2\kappa)^{-1} \sqrt{h} \left( \frac{3}{2} R - 2\Lambda \right) \right) \Psi = 0, \]

\[ \kappa = \frac{8\pi G}{c^4} \]

Wheeler–DeWitt equation

\[ \hat{D}^a \Psi \equiv -2\nabla_b \frac{\hbar}{i} \frac{\delta \Psi}{\delta h_{ab}} = 0 \]

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 (if quantum theory is universally valid)
Problem of time

- no external time present; spacetime has disappeared!
- local intrinsic time can be defined through local hyperbolic structure of Wheeler–DeWitt equation (‘wave equation’)
- related problem: Hilbert-space problem – which inner product, if any, to choose between wave functionals?
  - Schrödinger inner product?
  - Klein–Gordon inner product?
- Problem of observables
Standard approach: \( 3 + 1 \)-decomposition

\[
\dot{X}^\nu = N n^\nu + N^a X_{,a}^\nu
\]

\[
ds^2 = g_{\mu\nu} dx^\mu dx^\nu = -N^2 dt^2 + h_{ab}(dx^a + N^a dt)(dx^b + N^b dt)
\]

configuration variable: three-metric \( h_{ab} \)

quantum theory: Wheeler–DeWitt equation
Semiclassical approximation

Ansatz:

$$|\Psi[h_{ab}]\rangle = C[h_{ab}] e^{im_P^2 S[h_{ab}]} |\psi[h_{ab}]\rangle$$

(bra and ket notation refers to non-gravitational fields)

One evaluates $|\psi[h_{ab}]\rangle$ along a solution of the classical Einstein equations, $h_{ab}(x, t)$, corresponding to a solution, $S[h_{ab}]$, of the Hamilton–Jacobi equations; this solution is obtained from

$$\dot{h}_{ab} = N G_{abcd} \frac{\delta S}{\delta h_{cd}} + 2 D_{(a} N_{b)}$$
\[
\frac{\partial}{\partial t} |\psi(t)\rangle = \int d^3x \dot{h}_{ab}(x, t) \frac{\delta}{\delta h_{ab}(x)} |\psi[h_{ab}]\rangle
\]

→ functional Schrödinger equation for quantized matter fields in the chosen external classical gravitational field:

\[
i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}^m |\psi(t)\rangle
\]

\[
\hat{H}^m \equiv \int d^3x \left\{ N(x) \hat{H}^m_\perp(x) + N^a(x) \hat{H}^m_a(x) \right\}
\]

\(\hat{H}^m\): matter-field Hamiltonian in the Schrödinger picture, parametrically depending on (generally non-static) metric coefficients of the curved space–time background.

WKB time \(t\) controls the dynamics in this approximation
Time from symmetry breaking

Analogy from molecular physics: emergence of chirality

\[ V(z) \]

\[ |1\rangle \quad |2\rangle \]

Dynamical origin: decoherence due to scattering with light or air molecules

Quantum cosmology: decoherence between \( \exp(iS_0/\hbar) \) and \( \exp(-iS_0/\hbar) \)-part of wave function through interaction with multipoles

One example for decoherence factor:

\[ \exp \left( -\frac{\pi m H_0^2 a^3}{128\hbar} \right) \sim \exp \left( -10^{43} \right) \quad (\text{C. K. 1992}) \]
Criteria for quantum avoidance of singularities

No general agreement!

Sufficient criteria in quantum geometrodynamics:

- Vanishing of the wave function at the point of the classical singularity (dating back to DeWitt 1967)
- Spreading of wave packets when approaching the region of the classical singularity

Concerning the second criterium: only in the semiclassical regime (narrow wave packets following the classical trajectories) do we have an approximate notion of geodesics → only in this regime can we apply the classical singularity theorems
$\Psi \rightarrow 0$ is a sufficient, but not a necessary criterium for singularity avoidance!

**Example in quantum mechanics:** Solution of the Dirac equation for the ground state of hydrogen-like atoms:

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

but \( \int dr \, r^2 |\psi_0|^2 < \infty \)

**Example in quantum cosmology:** Wheeler–DeWitt equation for a Friedmann universe with a massless scalar field: simplest solution is \( \propto K_0(a^2/2) \quad \rightarrow \quad e \ln a , \)

but \( \int da \, d\phi \sqrt{|G|} |\psi(a, \phi)|^2 \) may be finite
Closed Friedmann–Lemaître universe with scale factor $a$, containing a homogeneous scalar field $\phi$ with potential $V(\phi)$ (two-dimensional *minisuperspace*)

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

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

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

*Factor ordering* chosen in order to achieve covariance in *minisuperspace*
Quantum phantom cosmology

**Classical model**: Friedmann universe with scale factor $a(t)$ containing a scalar field with negative kinetic term (‘phantom’) → develops a **big-rip singularity** ($\rho$ and $p$ diverge as $a$ goes to infinity at a *finite time*).

**Quantum model**: Wave-packet solutions of the Wheeler–DeWitt equation disperse in the region of the classical big-rip singularity → time and the classical evolution come to an end; only a stationary quantum state is left.

**Exhibition of quantum effects at large scales!**

(Dąbrowski, C. K., Sandhöfer 2006)
Big-brake cosmology: Classical model

Equation of state $p = A/\rho$, $A > 0$, for a Friedmann universe with scale factor $a(t)$ and scalar field $\phi(t)$ with potential $(24\pi G = 1)$

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

develops pressure singularity (only $\ddot{a}(t)$ becomes singular)

▶ total lifetime: $t_0 \approx 7 \times 10^2 \frac{1}{\sqrt{V_0 \left[ \frac{\text{g}}{\text{cm}^3} \right]}}$ s

▶ lifetime much bigger than current age of our Universe for

$$V_0 \ll 2.6 \times 10^{-30} \frac{\text{g}}{\text{cm}^3}$$

(is not a model for dark energy)
Figure: Classical trajectory in configuration space.
Wheeler–DeWitt equation:

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

(\(\kappa^2 = 8\pi G\), \(\alpha = \ln a\), Laplace–Beltrami factor ordering)

vicinity of big-brake singularity: region of small \(\phi\); therefore use

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

where \(\tilde{V}_0 = V_0 / 3\kappa^2\).
Normalizable solutions read

\[ \Psi(\alpha, \phi) = \sum_{k=1}^{\infty} A(k) k^{-3/2} K_0 \left( \frac{1}{\sqrt{6}} \frac{V_\alpha}{\hbar^2 k \kappa} \right) \]

\[ \times \left( 2 \frac{V_\alpha}{k} |\phi| \right) e^{-\frac{V_\alpha}{k} |\phi|} L_{k-1}^{1} \left( 2 \frac{V_\alpha}{k} |\phi| \right) . \]

\(K_0: \text{Bessel function; } L_{k-1}^{1}: \text{Laguerre polynomials; } V_\alpha \equiv \tilde{V}_0 e^{6\alpha}\)

\[\rightarrow \text{construction of wave packets}\]
Normalizable solutions of the Wheeler–DeWitt equation vanish at the classical singularity.

Similar result for the corresponding loop quantum cosmology.

(Kamenshchik, C. K., Sandhöfer 2007)
Intuitive explanation of the singularity avoidance

Analogously to the Coulomb potential in ordinary quantum mechanics, the energy of the matter component is also bounded from below. The minimal energy corresponds to a minimal value of $|\phi|$, similar to the ‘minimal radius’ in quantum mechanics.

The normalization condition also leads to the avoidance of the classical big-bang singularity: $\Psi \to 0$ for $\alpha \to -\infty$. 
Other type-III singularities

Consider a generalized Chaplygin gas:

\[ p = -\frac{A}{\rho^\beta} \]

e.g. big-freeze singularity (type III): both \( H \) and \( \dot{H} \) blow up

\[ \alpha = \ln\left(\frac{a}{a_0}\right), \quad \kappa^2 = 8\pi G \]

(Bouhmadi-López, C. K., Sandhöfer, Moniz 2009)
Important boundary condition: wave function go to zero in the classically forbidden region, $\Psi \xrightarrow{\alpha \to \infty} 0$

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 $\nu$ as a function of $\alpha$)

Obeys DeWitt’s boundary condition at the singularity:

$$\Psi_k(0, 0) = 0$$

(holds also for the other cases)
Supersymmetric quantum cosmological billiards

$D = 11$ supergravity: near spacelike singularity cosmological billiard description based on the Kac–Moody group $E_{10} \rightarrow$ discussion of Wheeler–DeWitt equation

- $\Psi \rightarrow 0$ near the singularity
- $\Psi$ is generically complex and oscillating

(Kleinschmidt, Koehn, Nicolai 2009)
Criteria in loop quantum cosmology

- difference equation $\rightarrow$ deterministic evolution of wave packet across the singularity
- occurrence of a “bounce” in the effective dynamics
- boundedness of the expectation value of the operator corresponding to the inverse scale factor

(cf. papers by M. Bojowald)
Effective equations in loop quantum cosmology

Effective Hamiltonian constraint reads

$$H_{\text{eff}} = -\frac{3}{8\pi G \beta^2} \frac{\sin^2(\lambda p)}{\lambda^2} a^3 + H_m,$$

where $$\lambda = 2(\sqrt{3\pi\beta})^{1/2} l_P$$

This leads to a modified Hubble rate:

$$H^2 = \frac{8\pi G}{3} \rho \left(1 - \frac{\rho}{\rho_c}\right),$$

where $$\rho_c = \frac{3}{(8\pi G \beta^2 \lambda^2)} \approx 0.41\rho_P$$

→ **bounces** which may prevent singularities

(P. Singh, arXiv:0901.2750: “All strong singularities are generically resolved in loop quantum cosmology.”)

Corresponds to the second of the criteria above (breakdown of semiclassical approximation near the classical singularity)
**Null dust shells**

A quantum theory for a lightlike shell leading to a singularity-free situation can be rigorously constructed; this is a consequence of the unitary dynamics.

(P. Hájíček 2001, P. Hájíček and C.K. 2001)

**Figure:** Penrose diagramme for the outgoing shell in the classical theory. The shell is at $U = u$. 

On the avoidance of black-hole singularities
Initial state (wave packet) at $t = 0$:

$$
\psi_{\kappa \lambda}(0, p) = \frac{(2\lambda)^{\kappa+1/2}}{\sqrt{(2\kappa)!}} p^{\kappa+1/2} e^{-\lambda p}
$$

($\lambda$ and $\kappa$ are free positive parameters)

Exact state for later times:

$$
\Psi_{\kappa \lambda}(t, r) = \frac{1}{\sqrt{2\pi}} \frac{\kappa!(2\lambda)^{\kappa+1/2}}{\sqrt{(2\kappa)!}} \left[ \frac{i}{(\lambda + it + ir)^{\kappa+1}} - \frac{i}{(\lambda + it - ir)^{\kappa+1}} \right]
$$

fulfills

$$
\lim_{r \to 0} \Psi_{\kappa \lambda}(t, r) = 0
$$

No singularity! The ingoing quantum shell develops into a superposition of ingoing and outgoing shell if the region is reached where in the classical theory a singularity would form.
At least for certain models, and under some conditions, quantum geometrodynamics predicts the avoidance of classical singularities. It is not clear how generic this is.