Quantum resolution of the cosmological singularity

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We study a quantum Hot Big Bang with matter characterized by a constant of motion \( m \), whose conjugate defines time. A superposition in \( m \) suggests a natural, conserved inner product. For two quantum theories in connection and metric variables, unitarity resolves the classical singularity. For connection variables, the most likely value for the curvature saturates at a finite maximum, followed by a regular transition between contraction and expansion. In metric variables, unitarity implies a boundary condition reflecting a contracting Universe into an expanding one. No appeal to new physics is needed.

Spacetime singularities are among the most troubling features of classical General Relativity (GR). In particular, the standard Big Bang model of cosmology implies that our Universe itself began at a singularity, a rather unsatisfactory situation to be in. In this Letter, we will consider the simplest approximation to the early Universe: dominated by radiation and homogeneous, isotropic and spatially flat. In such a model any observer would have encountered a singularity at a finite time in the past \([1]\).

A possible alternative to the singularity is a quantum “bounce” from a contracting into our current expanding phase. Most bounce models rely on physics beyond GR, such as string theory or loop quantum gravity \([2]\). Here we will instead revisit an older question: are the principles of quantum mechanics and GR enough to resolve the Big Bang singularity? This is a long-standing question in quantum cosmology going back over 50 years \([3]\). There is no consensus on its answer, with ambiguities both in the definition of quantum cosmology models and in criteria for singularity resolution \([4]\).

The classical history of the Universe has only had a finite time in the past, but standard unitarity demands that a quantum state can be translated arbitrarily far into the past by a time-evolution operator. This already seems to imply that the quantum evolution must deviate from the classical Big Bang, making it non-singular. There are, however, many subtleties. Foremost, the “timelessness” of the Wheeler–DeWitt equation forces us to define “quantum time” in a relational sense from the dynamical degrees of freedom \([5]\). The relational time distance to the Big Bang may or may not be finite. If it is finite, one would expect singularity resolution by quantum effects, whereas if it is infinite the quantum theory could still be singular \([6]\).

Although the general idea that unitarity may lead to singularity resolution is not new \([7]\), here we add a twist: we examine the issue in the connection representation. The Big Bang singularity occurs at zero scale factor (metric), and at infinite extrinsic curvature (connection). For both, the singularity is at finite time in our past, in terms of the time associated to the total matter in the Universe. We will show that unitarity does indeed imply that the quantum state is regular and well-defined across the classical singularity, replacing it by a quantum bounce. The two representations lead to different quantum theories, and it is only in the connection representation that this is achieved without supplementary boundary conditions. Unitarity alone suffices. Our solution to the singularity problem is minimalistic, and does not need new or unconventional physics.

**Required theoretical tools.** — In a wide class of cosmological models one can identify quantities \( \alpha_i \) that classically appear as either conserved quantities \([7]\), or as fundamental parameters of Nature. They can be put on an equal footing by elevating the latter to dynamical quantities subject to a conservation law. The prime example is the redesignation of the cosmological constant, \( \Lambda \), as an integration constant in unitary modular gravity \([8, 9]\), but the recipe in \([9]\) can be extended to Newton’s constant, spatial curvature, or the Planck mass \([10–14]\). Whatever their origin, upon quantization these conserved quantities can play the role of “energy”, and their conjugate variables that of time.

In such a theory, if \( q \) are other degrees of freedom of geometry and matter, the Hamiltonian constraint can either be written in terms of \( \alpha_i \) (resulting in the standard Wheeler–DeWitt equation for timeless \( \psi_s(q, \alpha_i) \)) or in terms of their conjugate “times” \( T_i \) (leading to a Schrödinger-like equation for \( \psi(q, T_i) \)) \([7, 12, 14]\). We are interested in the case of a single \( \alpha \) where \( \psi_s \) is such that the general solution is

\[
\psi(q, T) = \int \frac{d\alpha}{\sqrt{2\pi\hbar}} A(\alpha) \exp \left[ \frac{i}{\hbar} \alpha(X - T) \right] \tag{1}
\]

with \( X(q) \) independent of \( \alpha \) and \( \hbar \) an “effective Planck constant” (defined shortly). In these cases minisuperspace behaves like a dispersive medium \([13]\), with packets changing their shape (in \( q \)) as they propagate. \( \alpha, X \) and \( T \) are the medium’s linearizing variables: they remove dispersion when waves are written in terms of them \([14, 15]\).
A central aspect of this approach is that a natural inner product can be defined as an integral in terms of the progenitor constant and the amplitudes \[14\] \[16\],

\[
\langle \psi_1 | \psi_2 \rangle = \int d\alpha \ A_1^\dagger (\alpha) A_2 (\alpha).
\]

(2)

This inner product is automatically conserved. Inserting \[11\] in (2) leads to

\[
\langle \psi_1 | \psi_2 \rangle = \int dX \psi_1^\dagger (X, T) \psi_2 (X, T)
\]

(3)

if \(\alpha, X\) vary over all of \(\mathbb{R}\), which is a condition for the unitarity of \[3\]. Note that whereas replacing \(\alpha\) by \(\beta = \beta(\alpha)\) leads to classically equivalent theories (with new conjugate \(T_\beta = T_\alpha / \beta'(\alpha)\)), the corresponding quantum theories are not equivalent. Their inner products are different, since \(A(\alpha) d\alpha = A(\beta) d\beta\) implies

\[
\int d\alpha \ A_1^\dagger (\alpha) A_2 (\alpha) = \int d\beta \ A_1^\dagger (\beta) A_2 (\beta) \beta'(\alpha).
\]

(4)

Their time evolution is different: generally \(\alpha \cdot T_\alpha \neq \beta \cdot T_\beta\); cf. Eq. \[1\]. States coherent in \(\alpha\), with Gaussian \(A(\alpha)\), are generally not coherent in \(\beta\).

We now specify the dynamics of the model. At high energies, matter has equation of state \(w = 1/3\). Our action for GR with matter is

\[
S = \frac{3V_c}{8\pi G} \int dt \left( \dot{b} a^2 + \dot{m} T - Na \left( -(\dot{b}^2 + k) + \frac{m}{a^2} \right) \right)
\]

(5)

where \(a\) is the cosmological scale factor, \(b\) represents the connection (on-shell the inverse Hubble length, \(b = \dot{a}/N\)), \(k\) is spatial curvature, and \(m\) is a quantity associated to matter whose conservation is enforced by the second term. \(V_c\) is the coordinate volume of space. Variation with respect to the lapse \(N\) enforces the standard Hamiltonian constraint

\[
- (\dot{b}^2 + k) a^2 + m = 0.
\]

(6)

Below we comment on how the \(m\) terms in Eq. \[5\] can be derived from different starting points, but what follows does not depend on these discussions.

**Singularity resolution in the connection representation.** — Action \[5\] suggests canonical pairs

\[
\{ b, a^2 \} = \{ m, T \} = \frac{8\pi G}{3V_c},
\]

(7)

so that upon quantization \(\{ b, a^2 \} = \{ m, T \} = \hbar \) := \(8\pi G \hbar / 3V_c\). With suitable ordering, Eq. \[6\] becomes

\[
\frac{\partial}{\partial T} \psi(b, T) = -i\hbar (b^2 + k) \frac{\partial}{\partial b} \psi(b, T),
\]

(8)

the promised Schrödinger equation. Its solutions are of the form \[4\], with

\[
\alpha_b = m, \quad X_b = \int_b^\infty \frac{db}{(b^2 + k)}
\]

(9)

or \(X_b = -1/b\) for \(k = 0\), which we now assume. These solutions are nothing but an adaptation for radiation of a generalized Chern–Simons state for \(\Lambda \) \[14\].

Several states are possible, with some disabusing the constant \(m\) of its name. Our Universe happens to have reasonably sharp “constants”; this is related to the existence of a semiclassical limit at late times. We choose \(A(m) = \sqrt{N(m_0, \sigma_m)}\), where \(N(m_0, \sigma_m)\) is a (normalized) normal distribution with mean \(m_0\) and standard deviation \(\sigma_m\). Integrating \[1\] we obtain a squeezed-coherent state in \(X_b\) (not in \(b\), we stress),

\[
\psi(b, T) = e^{\frac{i}{2}\frac{m_0}{N}} \frac{\exp \left[-\frac{(X_b - T)^2}{2\sigma^2} \right]}{(2\pi \sigma T)^{1/4}}
\]

(10)

with \(\sigma_T = b/2\sigma_m\) saturating the Heisenberg relation. Using Eq. \[3\] we find the probability for a given \(b\) at time \(T\):

\[
P(b, T) = \left| \frac{dX_b}{db} \right| |\psi|^2 = \frac{1}{b^2} \frac{\exp \left[-\frac{(\dot{T} + \dot{b})^2}{2\sigma^2} \right]}{\sqrt{2\pi \sigma T}^2}.
\]

(11)

While \(\sigma_T\) is a free parameter (which one may think of as related to the Planck time), most importantly it is constant in \(T\). Classically \(\dot{T} = -\frac{N}{a}\) so, within the conditions of Ehrenfest’s theorem, \(T\) is minus conformal time \(\eta\).

Eq. \[1\] illustrates the dispersive nature of the medium, essential for the solution of the singularity problem. Wave packets sharpen up for increasing \(|T| \gg \sigma_T\), but lose their WKB shape and become fully quantum as \(|T| \ll \sigma_T\). We display the former behavior in Fig. \[4\] for an expanding Universe (\(T < 0\), \(\eta > 0\)). We can use the relation \(T = -\eta\) because \(\sigma(T)/|T| = \sigma_T/|T| \ll 1\). The peak moves along the classical trajectory \(b = 1/\eta\) with ever tinier fractional standard deviation \(\sigma(b)/b\) (since \(\sigma_T = \sigma(X_b)\) implies \(\sigma_b \approx \sigma(X_b)/|X_b'| = b^2 \sigma_T\)). The state therefore is near-coherent (indeed delta-like) in \(b\):

\[
P(b, \eta) \approx \frac{\exp \left[-\frac{(b - \frac{1}{2\sigma^2})^2}{2\sigma^2} \right]}{\sqrt{2\pi \sigma b}^2}, \quad \sigma_b \approx \sigma_T/\eta^2.
\]

(12)

In contrast, for \(|T| \lesssim \sigma_T\) the dispersive nature of the medium is all-important, as shown in Fig. \[2\]. The packet widens and becomes grossly distorted, disallowing a WKB approximation. In addition the probability peak gets stuck at \(b \approx b_p = 1/(\sqrt{2\sigma_T}) = \sqrt{2\sigma_m/\hbar}\), instead of going to infinity, as expected from the singular classical trajectory. The distribution is very skewed, with a tail that is more prominent for smaller \(|T|\), whilst the height of the peak decreases. Meanwhile, a contracting peak emerges at \(b \approx -b_p < 0\), its height increasing in tandem with the first peak’s lowering. The wavefunction is always regular, and indeed at \(T = 0\) it is symmetric with

\[
P(b, T = 0) = \frac{1}{b^2} \frac{\exp \left[-\frac{(\dot{T} + \dot{b})^2}{2\sigma^2} \right]}{\sqrt{2\pi \sigma T}^2}.
\]

(13)
revealing a perfectly balanced quantum superposition of a contracting and expanding Universe. For \( T > 0 \) the situation reverses, the peak at \( b = -b_P \) now growing at the expense of that at \( b = b_P \), until for \( T \gg \sigma_T \) we link up with a semi-classical contracting Universe. These results can be derived directly from Eq. (11) and they are due to the form of \( \psi \) (and \( X(b) \)) and the measure \( d\mu(b) \).

We therefore have a quantum model for a non-singular bouncing Universe. It avoids the singularity because time around the classical singularity is smeared by quantum uncertainty. It results directly from the fact that unitarity requires \( X \) (and so \( b \)) not to be constrained (it must cover the whole real line, so that \( \sigma \) is conserved). Hence, \( b \) should not be constrained to an expanding Universe. Unitarity forces a bounce directly, precisely by ruling out any constraints on \( b \) and the need for any associated boundary conditions. This is to be contrasted with the picture to emerge from the more familiar metric formulation, as we now show.

**Singularity resolution in metric variables.** — An alternative way of achieving singularity resolution is in the metric representation, based on the pair \( \{ a, p_a \} \) with \( p_a := -2ha \). The constraint \( (6) \) becomes \( m = \frac{a^2}{2} \alpha \) leading to the Schrödinger equation

\[
\frac{i}{2} \frac{\partial}{\partial T} \psi(a, T) = -\frac{1}{4} \hbar^2 \frac{\partial^2}{\partial a^2} \psi(a, T)
\]

given that \( [a, p_a] = i\hbar \). This fits into the general formalism based on Eq. (1), with linearizing variables \( X_a = a, \alpha_a \) satisfying \( \sigma_a^2 = 4m \) (where \( m \geq 0 \) but \( \alpha_a \) is unrestricted) and \( T_a = T/\alpha_a^2(m) \). Eq. (3) is then simply

\[
\langle \psi_1 | \psi_2 \rangle = \int da \, \psi_1^*(a, T) \psi_2(a, T).
\]

This inner product differs from the one in the connection representation since \( \alpha_a = \pm 2\sqrt{m} \) and \( \alpha_b = m \) are different.

A priori \( a \) could take any real value, but it is common to restrict \( a \geq 0 \). The operator on the right-hand side of Eq. (14) is then no longer self-adjoint. Instead, demanding \( \langle \psi_1 | \psi_2 \rangle = \langle \psi_2 | \psi_1 \rangle \) on \([0, \infty)\) requires a Robin boundary condition

\[
\frac{\partial \psi}{\partial a}(0, T) = \gamma \psi(0, T)
\]

where \( \gamma \) is a free parameter (which can be \( \infty \) if we demand \( \psi(0, T) = 0 \)). The operator \( \partial^2 / \partial a^2 \) has a one-parameter family of self-adjoint extensions corresponding to different \( \gamma \).

Hence, unitarity with a non-negative scale factor leads to a reflecting boundary condition: rather than “disappearing” through \( a = 0 \) as the classical solutions, the quantum state is reflected back to positive \( a \). Inserting (14) into (16) leads to

\[
A(\pm|\alpha_a|) = B(|\alpha_a|) \left( 1 \mp \frac{\gamma \hbar}{\alpha_a} \right)
\]

for some function \( B \) on the positive half-line. Eq. (1) becomes

\[
\psi(a, T) = \int_0^\infty \frac{dm}{\sqrt{2\pi \hbar}} C(m) \exp \left( \frac{1}{\hbar} mT \right) \times \left( \cos \left( \frac{\sqrt{2m}}{\hbar} \left( a + \frac{\gamma \hbar}{2m} \sin \left( \frac{2\sqrt{m}}{\hbar} \right) \right) \right) \right)
\]

where \( C(m) = 2B(m)/\sqrt{m} \). Values at \( a < 0 \) would be determined by those at \( a > 0 \), as in the method of images for reflections. Eliminating the spurious \( a < 0 \) domain, Eqs. (2)–(3) become the time-independent

\[
\int_0^\infty da \, |\psi|^2 = \int_0^\infty dm \, |C(m)|^2 \left( \frac{\sqrt{m}}{4} + \frac{\gamma^2 \hbar^2}{16m} \right).
\]
The theory is now unitary at the cost of introducing boundary conditions dependent on the parameter $\gamma$.

Choosing again $C(m) = \sqrt{N(m_0, \sigma_m)}$, in Fig. 3 we show how the boundary condition leads to quantum departures from the classical solution, with a contracting solution matched to an expanding one. The full quantum state is a superposition of the two, and fluctuations over the expectation value are large; see Fig. 4 for the probability distribution $|\psi|^2$. Near $T = 0$ the distribution has several peaks, one at $a = 0$ and others at a finite $a$, as a result of the interference between contracting and expanding solution. The expectation value is largely determined by the relative heights of these peaks.

Again this behavior follows from the quantum nature of time for small $|T|$, together with unitary dynamics, here enforced by suitable boundary conditions. By setting these boundary conditions (and even explicitly eliminating $a = 0$) one has, in a way, reverse-engineered this solution. This is to be contrasted with results in the connection representation. In addition, as the wave packets move out of the Planck epoch they spread out in time in the metric representation, another significant difference between the two inequivalent theories.

**Discussion.** — The origin of our results is manifold (choice of inner product, existence of relational time, etc). But foremost, the time variable $T$ we use is conjugate to a classical constant of motion that is not infinitely sharp, but also not entirely undefined. Hence, $T$ must have a complementary uncertainty $\sigma_T$. As we plunge into the classical singularity at $T = 0$, $|T| \sim \sigma_T$: quantum fluctuations become significant, leading to deviations from the classical trajectory. In the connection representation the spread in $T$ is translated into a smearing of $b$ from $b_T$ (where the probability peak gets stuck) to infinity. The probability of infinite $b$ is always zero, even as $T \to 0$. The wavefunction then develops non-negligible support at $b < 0$, so that $|b|$ and its sign are undefined: at the “Big Bang” the Universe is in a superposition of contracting and expanding phases. There is no reflection or interference (“ringing”), simply a regular quantum transition through the classical Big Bang, transferring the probability peak from contraction to expansion at finite curvature.

In contrast, in the metric representation there is a reflection from $a = 0$ because $a \geq 0$ is imposed, and unitarity forces a reflection. Near the Big Bang, contracting and expanding universes form two packets moving in opposite directions, one being the reflection of the other. They interfere near the reflection point, leading to ringing: the internal beats of the packets appear in the probability (e.g. $18, 19$; see Fig. 4). However different these two phenomenologies may appear, in fact something similar happens in any quantum bounce when seen in position and in momentum space $20$. Nonetheless these are different quantum theories, with different requirements and achievements, as we explained throughout.

Given that we are dealing with the Planck epoch, one may wonder how fundamental the theory we have used is. Several theories lead to Eq. (5), some blatantly “effective”, others with “fundamental” pretensions, but always well-defined beyond minisuperspace. We may frame our model as a GR (isentropic) fluid, with action

$$S_R = \int d^4x \left[ -\sqrt{-g} \rho \left( \frac{|J|}{\sqrt{-g}} \right) + J^\mu \left( \partial_\mu \phi + \beta_A \partial_\mu \alpha^A \right) \right]$$

(20)

where $J^\mu$ is a vector density representing the densitized particle number flux, $|J| = \sqrt{-g_{\mu\nu} J^\mu J^\nu}$ and $\varphi, \beta_A$ and $\alpha^A$ are suitable Lagrange multipliers $21$. Choosing the appropriate function $\rho$ for radiation, $\rho(n) \propto n^{4/3}$, and reducing the action to minisuperspace would lead to Eq. (5), as in (22). This is conservative, but conversely one may question the validity of using a perfect fluid description in the Planckian regime.

Alternatively, we may derive (5) from a theory of constants of Nature $10, 12, 14$ carbon-copied from the covariant formulation of unimodular gravity $9$. In such theories, after
where $\alpha$ is a scalar and $T^\mu_\alpha$ again a vector density, so the added term is diffeomorphism invariant. $\alpha$ becomes a constant-on-shell-only ($\partial_\mu \alpha = 0$ is an equation of motion), with conjugate “time” $T^\alpha_\alpha$ (for $\Lambda$, this time is proportional to the spacetime volume to the observer’s past). Applications of this approach may be found in [10] for the Planck mass, and [11, 13] for the gravitational coupling. The latter would lead to Eq. (5). All these approaches have in common that they “deconstantize” the conserved quantity $m$, which is all we require.

They may differ, however, regarding the robustness of our results, in particular regarding the threat of anisotropy. The classical anisotropy instability is not an issue because we do not follow the classical trajectory where it would hurt us. However, we may ask what happens to the wavefunction once anisotropic degrees of freedom are inserted. In this respect [20] and [21] may be very different: gravity is always isotropic even if its solutions are not. Given the solutions’ $T \to -T$ symmetry, our general results regarding singularity resolution remain valid, as long as anisotropies have not dominated while the Universe is still semiclassical.

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