Superpositions of the cosmological constant allow for singularity resolution and unitary evolution in quantum cosmology

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A novel approach to quantization is shown to allow for superpositions of the cosmological constant in isotropic and homogeneous mini-superspace models. Generic solutions featuring such superpositions display: i) a unitary evolution equation; ii) singularity resolution; iii) a cosmic bounce. Explicit cosmological solutions are constructed. These exhibit characteristic bounce features including a 'super-inflation' regime with universal phenomenology that can naturally be made to be insensitive to Planck-scale physics.

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Introduction The 'big bang' singularity and the cosmological constant are well established features of classical cosmological models [1]. In the context of quantum cosmology, the singularity is typically understood as a pathology that can be expected to be 'resolved' by Planck-scale effects. Most contemporary approaches to resolving the singularity are based upon cosmic bounce scenarios [2]. In contrast, the cosmological constant receives very much the same treatment in classical and quantum cosmological models: it is a constant of nature classically, and thus quantum solutions are supersselected to eigenstates labelled by its classical value. Cosmological time evolution is unlike either the singularity or cosmological constant. Whereas, its classical treatment is relatively unproblematic, quantum cosmologies based upon the standard Dirac quantization techniques are described by a 'frozen formalism' that lacks a fundamental evolution equation [3–5]. In this letter we use a simple model to demonstrate that by treating the cosmological constant differently in quantum cosmological models, there is a prospect to produce a bounce scenario that simultaneously resolves the classical singularity and restores fundamental quantum time evolution.

In the following sections we apply a novel quantization scheme [6–8] to a class of isotropic and homogeneous mini-superspace models. For these models our scheme is demonstrated to allow for a superpositions of the cosmological constant in a manner connected to the unimodular approach to gravity [9, 10]. Three particularly noteworthy features result directly from including solutions with superposition of cosmological constant. First, our model features an evolution equation for the entire quantum state that is guaranteed to be unitary. This is in contrast to internal time approaches to representing evolution in quantum cosmology [11–18]. Second, the mechanism for singularity avoidance obtained does not involve the introduction of a Planck-scale cutoff [19]. Rather, observable operators evolve unitarily and remain finite because they are 'protected' by the uncertainty principle. Third, characteristic features of the cosmological bounce persist into a 'super-inflation' regime that contains universal phenomenology that can be rendered insensitive to the underlying Planck-scale physics in very nature way. In particular, the model displays a 'cosmic beat' phenomenon and associated 'bouncing envelope'. The cosmic beats can be identified with Planck-scale effects and, under certain parameter constraints, are negligible compared with the effective envelope physics. Under these same constraints, the bouncing envelope persists into the super-inflation regime where it is insensitive to the beat effects in a manner that is closely analogous to *Rayleigh scattering*. Significantly, this 'Rayleigh' limit is only available when superpositions of the cosmological constant are allowed. This behaviour constitutes a remarkable unique feature of the bouncing unitary cosmologies identified. Two companion papers provide further, more detailed, interpretation and analysis of both general and particular cosmological solutions. [20, 21]

Model and Observables Consider an homogeneous and isotropic FLRW universe with zero spatial curvature ($k = 0$); scale factor, a; massless free scalar field, ϕ; and cosmological constant, Λ. The field redefinitions

$$v = \sqrt{\frac{2}{3}} a^3 \qquad\qquad \varphi = \sqrt{\frac{3\kappa}{2}} \phi \,, \tag{1}$$

where $\kappa = 8\pi G$, give a convenient parameterization of the configuration space, $\mathcal{C}(v, \varphi)$, in terms of relative spatial volumes, v, and the dimensionless scalar field, φ. The time evolution of the system is given in terms of coordinate time, t, related to the proper time, τ, via the *lapse* function $\mathrm{d}\tau = N\mathrm{d}t$. The dimensionless lapse, $\tilde{N}$, and cosmological constant, $\tilde{\Lambda}$, can be defined as

$$\tilde{N} = \sqrt{\frac{3}{2}} \frac{\kappa \hbar^2 v N}{V_0} \qquad\qquad \tilde{\Lambda} = \frac{V_0^2}{\kappa^2 \hbar^2} \Lambda \,, \tag{2}$$

using the reference volume V_0 of some fiducial cell and the (at this point) arbitrary angular momentum scale $\hbar$.

In terms of these variables, the mini-superspace Hamiltonian is

$$H = \tilde{N}\left[\frac{1}{2\hbar^2}\left(-\pi_v^2 + \frac{1}{v^2}\pi_\varphi^2\right) + \tilde{\Lambda}\right], \qquad (3)$$

where π_v and π_φ are the momenta conjugate to v and φ respectively. The utility of these variables is revealed by their suggestion of a coordinate-independent formulation of H in terms of the Rindler metric $\eta_{AB} = \hbar^2 \mathrm{diag}(-1, v^2)$, where $A, B = 1, 2$. Using generalized coordinates, q^A, and momenta, p^A, the Hamiltonian can be expressed as

$$H = \tilde{N}\left[\frac{1}{2}\eta^{AB}p_A p_B + \tilde{\Lambda}\right]. \qquad (4)$$

The configuration space, $\mathcal{C}$, is Rindler space defined as the set of points contained in (and including) the forward light-cone of Minkowski space centred on the origin.

Rindler space is geodesically incomplete because geodesics cannot be extended past its boundary, $\partial\mathcal{C}$, the *Rindler horizon* at $v = 0$. This boundary leads to the most physically important properties, both classical and quantum, of this cosmological model.

It is important to distinguish between the geodesic incompleteness of the *configuration space* and that of the *space-time* metric, which are logically distinct. In this model, $\partial\mathcal{C}$ corresponds to the region in *configuration* where we it was shown in [20] that: i) the expansion parameter of some congruence of geodesics in *space-time* becomes negative and unbounded, implying that the *space-time* geodesics terminate in finite proper time; and ii) there is a curvature pathology in *space-time* signaled by a divergence in all Kretschmann invariants. This implies a classical singularity in both relevant senses of the Penrose–Hawking singularity theorems.

The importance of the boundary in the quantum theory relates to the existence of self-adjoint representations of the operator algebra. Consider the Hilbert space, $\mathbb{H} = L^2(\mathcal{C}, \mathrm{d}\theta)$ of square integrable functions on $\mathcal{C}$ under the Borel measure $\mathrm{d}\theta = \mathrm{d}^2 q\sqrt{-\eta}$, where $\eta = \det \eta_{AB}$. This space is spanned by all functions $(\Phi, \Psi) \in \mathbb{C}$ satisfying

$$\langle \Phi, \Psi\rangle \equiv \int_{\mathcal{C}} \mathrm{d}^2 q\sqrt{-\eta}\,\Phi^\dagger\Psi < \infty. \qquad (5)$$

We can build an infinite family of generalized configuration representations of symmetric operators acting on $\mathbb{H}$ in terms of the operators

$$\hat{q}^A\Psi = q^A\Psi \quad \hat{p}_A\Psi = -i\hbar(-\eta)^{-1/4}\frac{\partial}{\partial q^A}\left[(-\eta)^{1/4}\Psi\right]. \qquad (6)$$

Given a global coordinate chart on $\mathcal{C}$, arbitrary diffeomorphisms on $\mathcal{C}$ bijectively induce symplectomorphisms on the classical phase space via the Legendre transform. One might, therefore, expect that these changes of chart should bijectively induce changes of basis in the representations (6) of $\mathbb{H}$. However, while the square integrability condition, (5), that defines $\mathbb{H}$ transforms like a scalar on $\mathcal{C}$, the condition for self-adjointness of the symmetric momentum operators, $\hat{p}_A$, is (see [20])

$$\oint_{\mathcal{C}} \mathrm{d}\ell_A\sqrt{\eta}\,\Phi^\dagger\Psi = 0, \qquad (7)$$

and transforms like a co-vector on $\mathcal{C}$. This condition can be obtained from the definition of the self-adjointness of $\hat{p}_A$ after an application of integration by parts, and ultimately results from the fact that the $\hat{p}_A$ are co-vectors on $\mathcal{C}$. The mismatch between the transformation properties of the square integrability condition and the self-adjointness condition for $\hat{p}_A$ implies that, when $\partial C \neq 0$, not all phase space charts have corresponding self-adjoint representations in $\mathbb{H}$.

This signals a potential breakdown of the correspondence principle for quantum mechanics. Fortunately, in the model considered here, this breakdown occurs precisely for the classically conserved quantities that are responsible for the classically singular behaviour. This avoids the potential for quantum singular behaviour resulting from a direct application of the Ehrenfest theorem (once a self-adjoint Hamiltonian is provided). Whether a breakdown of the correspondence principle due to this mechanism can be understood more generally as a way to avoid a classical pathology is an interesting question for further investigations.

To construct representations of a self-adjoint operator algebra and Hilbert space, it will be necessary to restrict to a specific coordinate chart. To motivate our choice, we consider the conformal completion $(\mathcal{C}_0, \eta_0)$ of Rindler space, where, in the (v, φ) chart,

$$\eta^0_{AB} = \frac{1}{v^2}\eta_{AB} \qquad (8)$$

and $\mathcal{C}_0$ is the full Minkowski plane. The *tortoise* coordinate,

$$\mu = \log v, \qquad (9)$$

then puts $\eta^0_{AB} = \mathrm{diag}(-1, 1)$ into Minkowskian form. Because the square integrability condition (5) for $\mathbb{H}$ is conformally invariant, square integrable functions on $(\mathcal{C}_0, \eta_0)$ are also square integrable on $(\mathcal{C}, \eta)$. We can, therefore, define representations of $\mathbb{H}$ using the standard eigenstates of $\hat{\mu} \equiv \mu$ and its momentum operator $\hat{\pi}_\mu \equiv -i\hbar(-\eta_0)^{-1/4}\frac{\partial}{\partial\mu}\left[(-\eta_0)^{1/4}\right]$, which is manifestly self-adjoint in the (μ, φ) chart where $\eta_0 = 1$. Similarly, $\hat{\varphi}$ and $\hat{\pi}_\varphi$ are manifestly self-adjoint, and their eigenstates complete the basis for $\mathbb{H}$. Undoing the conformal transformation (and suitably transforming Hilbert space states), we obtain the self-adjoint operators

$$\hat{\mu}\Psi = \mu\Psi \qquad \hat{\pi}_\mu = -i\hbar e^{-\mu}\frac{\partial}{\partial\mu}\left(e^{\mu}\Psi\right) \tag{10}$$

$$\hat{\varphi}\Psi = \mu\Psi \qquad \hat{\pi}_\varphi = -i\hbar\frac{\partial\Psi}{\partial\varphi}\,. \tag{11}$$

whose eigenstates

$$\psi_{\pi_\mu} = \frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{i}{\hbar}\mu\pi_\mu - \mu} \qquad \psi_k = \frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{i}{\hbar}\varphi k} \tag{12}$$

are orthonormal under the measure $\mathrm{d}\theta = \mathrm{d}\varphi\mathrm{d}\mu e^{2\mu}$ and span $\mathbb{H}$. It is straightforward to verify that the operators above satisfy the self-adjointness condition (7) while the momentum operator $\hat{\pi}_v$ in the $v\varphi$-chart defined by (6) does not. This recovers the well-known result, studied in detail by Isham [22], that the momentum operator is not well-defined on $\mathbb{R}^+$. We believe these geometric methods provide deeper insight into this problem and its conventional solution.

Unitary Quantum Cosmology Application of relational quantization [6–8] leads to a Schrödinger-type evolution equation for the system of the form

$$\hat{H}\Psi = i\hbar\partial_t\Psi\,, \tag{13}$$

where the eigenvalues of $\hat{H}$ are to be identified with the (dimensionless) cosmological constant $\tilde{\Lambda}$. The classical Hamiltonian (4) suggests the real and symmetric chart-independent Hamiltonian operator

$$\hat{H} \equiv \frac{1}{2}\Box\,, \tag{14}$$

where $\Box$ is the d'Alambertian operator on Rindler space. Unlike $\hat{p}_A$, $\hat{H}$ is a scalar on $\mathcal{C}$. Diffeomorphisms on $\mathcal{C}$ therefore bijectively induce changes of basis of self-adjoint representations of $\hat{H}$. Integration by parts can be used to show that $\hat{H}$ is equal to its dual provided

$$\oint_{\partial\mathcal{C}} \mathrm{d}l_{(A}\sqrt{\chi}\,\eta^{AB}\left(\Phi^\dagger\partial_{B)}\Psi - \Psi\partial_{B)}\Phi^\dagger\right) = 0 \tag{15}$$

for all states in $(\Phi,\Psi) \in \mathbb{H}$.

A theorem by Von-Neumann (see [23] theorem X.3) guarantees that self-adjoint extensions of the real, symmetric operator $\hat{H}$ exist. Given an explicit self-adjoint representation of $\hat{H}$, the time evolution is guaranteed to be unitary by Stone's theorem [24, p.264]. The deficiency subspaces of $\hat{H}$ can be calculated from the square integral solutions to (18) when $\tilde{\Lambda} \to \pm i$. These are easily seen to be one dimensional. We, therefore, expect a $U(1)$ family of self-adjoint extensions, which we parametrize by the log-periodic, positive reference scale Λ_{ref}. The coordinate invariance of $\hat{H}$ implies that it is sufficient to construct representations in a particular basis. To find these extensions explicitly and to construct the general solution to (13), we compute the eigenstates of $\hat{H}$ (with eigenvalues $\tilde{\Lambda}$) in the $v\varphi$-chart. Using the separation Ansatz

$$\Psi^{\pm}_{\Lambda}(v,\varphi) = \psi_{\Lambda,k}(v)\nu^{\pm}_k(k)\,, \tag{16}$$

we find

$$\nu^{\pm}_k(\varphi) = \frac{1}{\sqrt{2\pi\hbar}}e^{\pm\frac{i}{\hbar}k\varphi}\,, \tag{17}$$

and

$$v\frac{\mathrm{d}}{\mathrm{d}v}\left(v\frac{\mathrm{d}}{\mathrm{d}v}\psi_{\Lambda,k}\right) + \left(2\tilde{\Lambda}v^2 + \frac{k^2}{\hbar^2}\right)\psi_{\Lambda,k} = 0\,. \tag{18}$$

The latter equation is Bessel's differential equation for purely imaginary orders, $ik/\hbar$.

The solutions of Bessel's equation are qualitatively different depending on the sign of Λ. For $\Lambda < 0$, solutions are modified Bessel functions of the first (exponentially growing) and second kind (exponentially decaying) kind. The self-adjointness condition, (15), leads us to reject the growing solutions, leaving only the decaying 'bound' modes, $\mathcal{K}_{ik}$. The asymptotic expansion of the Bessel functions about $v = 0$ further implies (see [20]) that only discrete values of $\tilde{\Lambda}$ are allowed. These follow the geometric series

$$\tilde{\Lambda}_n = \tilde{\Lambda}_{\text{ref}}\,e^{2n\pi\hbar/k} \quad (\forall n \in \mathbb{N})\,, \tag{19}$$

which is seeded by the self-adjoint extension parameter $\tilde{\Lambda}_{\text{ref}}$. The general normalized 'bound' eigenstates are then

$$\psi^{\text{bound}}_{\Lambda,k} = \sqrt{\frac{4\hbar|\tilde{\Lambda}|\sinh\left(\pi k/\hbar\right)}{\pi k}}\,\mathcal{K}_{ik/\hbar}(\sqrt{2\tilde{\Lambda}}v)\,. \tag{20}$$

For $\Lambda > 0$, solutions are the oscillating Bessel functions of the first, $\mathcal{J}_{ik/\hbar}$, and second kind, $Y_{ik/\hbar}$. The condition (15) can be satisfied by analyzing the behaviour of the Bessel functions near $v = 0$ from the perspective of the conformal completion, $(\mathcal{C}_0, \eta_0)$. There, the Bessel functions behave as ordinary sines and cosines whose phase difference, $\theta = \frac{k}{2\hbar}\log\left(\frac{\tilde{\Lambda}}{\tilde{\Lambda}_{\text{ref}(k)}}\right)$, parametrizes the $U(1)$ space of self-adjoint extensions (see [20]).[1] The general normalized solutions are continuous in $\tilde{\Lambda}$ and are explicitly given by

$$\psi^{\text{undound}}_{\Lambda,k} = \frac{\text{Re}\left[e^{-i\theta}\mathcal{J}_{ik/\hbar}(\sqrt{2\tilde{\Lambda}}v)\right]}{\left|\cosh\left(\frac{\pi k}{2\hbar} + i\theta\right)\right|}\,. \tag{21}$$

The 2π periodicity in θ implies a $\pi k/\hbar$ log-periodicity in Λ_{ref} that is consistent with the bound spectrum (19).

[1] Note that, in general, different choices of θ can be made for different values of k.

The general solution to (13) is then,

$$\Psi(v,\varphi,t) = \frac{1}{\sqrt{2}}\sum_{\pm}\int_{-\infty}^{\infty}\mathrm{d}k\left[\sum_{n=-\infty}^{\infty} e^{i\tilde{\Lambda}_n t/\hbar}A_n^{\pm}(k)\Psi^{\pm,\mathrm{bound}}_{-\Lambda_n,k} + \int_0^{\infty}\mathrm{d}\Lambda\, e^{-i\tilde{\Lambda}t/\hbar}B^{\pm}(\tilde{\Lambda},k)\Psi^{\pm,\mathrm{unbound}}_{\Lambda,k}\right], \quad (22)$$

for the suitably normalized coefficients $A_n^{\pm}$ and $B^{\pm}(\tilde{\Lambda})$.

Singularity Resolution In our view, the basic condition for non-singular behaviour in a quantum theory is that the expectation value of all observable operators, as evaluated on all possible states in Hilbert space, remains finite. Given a classical theory in which some classical observable is pathological, it is a necessary and sufficient condition for singularity resolution, in our sense, that the expectation value of all elements of the quantum observable algebra be always finite. This definition is equivalent to the requirement, in the sense of [25, 26], that the evolution on the quantum phase space be everywhere finite. Thus, in requiring finiteness of expectation values, we are not implicitly relying upon extending the correspondence principle into the quantum bounce regime, but rather simply insisting that a physically reasonable quantum theory can be defined at all times.

It is straightforward to demonstrate that our model satisfies the finite-expectation-value condition for singularity avoidance. Given the self-adjointness of $\hat{H}$, the unitary evolution equation (13) implies the generalised Ehrenfest theorem:

$$\frac{\partial}{\partial t}\left\langle \hat{O}(t)\right\rangle = \frac{1}{i\hbar}\left\langle [\hat{O}(t),\hat{H}]\right\rangle + \left\langle \frac{\partial \hat{O}(t)}{\partial t}\right\rangle. \quad (23)$$

Provided that $\hat{O}$ is a bounded member of a well-defined quantum observable algebra, the commutator on the RHS is bounded and the evolution of the expectation value of all $\hat{O}$ will be well-behaved. Thus, for quantum cosmology with a unitary evolution equation, the condition for singularity avoidance ultimately amounts to the usual requirement for a well-defined quantum theory.

Modeling Constraints The choice of physically relevant particular solutions is under-constrained by observational data. Here we assume that constraints placed upon the model that are *not* based upon observational data should be minimally specific in the precise sense defined in [21]. Below, we will use this as a guiding principle to briefly justify the choices made for the free-parameters of the model. For much greater detail on the justification for these choices, see [21].

Observational data imply that the current universe is well-approximated by a semi-classical state with a definite positive Λ. If the bound negative Λ states had significant support at large v, then linearity would imply that these bound states would be currently observable. Since they are not, this restricts the bound part of the wavefunction to be confined to a region of configuration space where v is much smaller than it is currently. Since we wish to be minimally specific with regard non-observational constrains, we set the bound part of the wavefunction to vanish by setting $A_n^{\pm}(k) = 0$.

We can characterise the semi-classical regime in a minimally specific way by the vanishing of higher order generalized moments of the wavefunction [26]. This is equivalent to requiring that the non-Gaussianties of the wavefunction are very small in a particular basis. The minimally specific choice of basis is that which is maximally stable.[2] This is provided by considering the large-v asymptotic Killing vectors of the classical configuration space, which allow us to select a preferred basis given in terms of the eigenstates of $\hat{\pi}_\varphi$ and $\hat{\pi}_v$. Because, in this asymptotic limit, $H = \frac{1}{2\hbar^2}\pi_v^2$, we take the semi-classical state to be expressed in terms of Gaussians of k (the eigenvalues of $\hat{\pi}_\varphi$) and $\omega = \sqrt{2\tilde{\Lambda}}\hbar$ (the approximate eigenvalues of $\hat{\pi}_v$ in the large-v limit).

Requiring Λ and π_φ to be well-resolved implies that the absolute value of the means of the scalar densities $B^{\pm}(k,\tilde{\Lambda}) = \frac{\omega}{\hbar}B^{\pm}(k,\omega)$ must be much larger than the variances, otherwise the quantum mechanical uncertainty, given by σ_ω and σ_k respectively, would make them indistinguishable from zero. This leads to:

$$\frac{\omega}{\hbar}B^{\pm}(k,\omega) = \left(\frac{\hbar^2}{2\pi\sigma_\omega\sigma_k}\right)^{1/2}\exp\left\{-\frac{(\omega-\omega_0)^2}{4\sigma_\omega^2} - \frac{i}{\hbar}(\omega-\omega_0)v_0 - \frac{(k-k_0^{\pm})^2}{4(\sigma_k^{\pm})^2} - \frac{i}{\hbar}(k-k_0^{\pm})\varphi_\infty^{\pm}\right\}, \quad (24)$$

where $\omega_0 \gg \sigma_\omega > 0$ and $|k_0^{\pm}| \gg \sigma_k^{\pm} > 0$.

Two further minimally specific choices consistent with observation are: i) to select $t = 0$ as the time of minimal dispersion by appeal to time-translational invariance; and ii) to assume a semi-classical regime for $t \to \pm\infty$. Given current observational constraints, the quantum bounce wipes out the vast majority of the information about pre-bounce physics. The minimally specific assumption is, therefore, to impose the maximum amount of time-reflection symmetry around the bounce. This is achieved by: i) setting the phase shift between in- and out-going $\hat{\pi}_\varphi$-eigenstates to zero by setting $B^+ = B^-$ using a single mean, k_0, and variance; σ_k, and offset, φ_∞; ii) requiring the bounce time to occur at $t = 0$ by setting $v_0 = 0$; and iii) fixing the self-adjoint extensions to minimize the phase-shift between in- and out-going $\hat{H}$-eigenstates (the specific choice that accomplishes this is specified below).

[2] In fact, what is ultimately needed is a super-selection principle for such a basis, which would require a way to model an 'environment' for this system. Lacking this, we note that our stability criterion is at least consitent with definitions of environmentally induced super-selection arizing from decoherence.

We can use the global 'boost' isometry of $\mathcal{C}$ to restrict to $\varphi_\infty = 0$ without loss of generality. The parameter pairs (k_0, σ_k) and $(\omega_0, \sigma_\omega)$ can only be independently defined via reference to an external scale. We can avoid having to specify such a scale by noticing that the Gaussians of (24) depend only on the ratios k_0/σ_k and ω_0/σ_ω, which are well defined parameters of the model, when $v_0 = \varphi_\infty = 0$.

Fixing the self-adjoint extensions by specifying θ does require introduction of an external reference scale however. Inspection of (21) reveals a dependence on $k/\hbar$, which suggests $k_0/\hbar$ as the third parameter of the model. We will discuss the physical interpretation of this scale in relation to Planck-scale effects in the final section. For our present purpose, it suffices to note that the choice:

$$\Lambda_{\rm ref} = \frac{V_0^2}{\kappa^2\hbar^2}\frac{\omega_0^2}{2\hbar^2}\,, \tag{25}$$

is minimally specific since it does not involve introducing any new parameters. It is also the choice that allows θ to be as close to zero as possible and, therefore, maximizes time-reflection symmetry.

de Sitter and Rayleigh limits Let us designate the limit in which $\frac{\omega_0/\sigma_\omega}{|k_0|\sigma_k} \gg 1$ as the *de Sitter limit* and the limit in which $\omega_0/\sigma_\omega \gg 1$ as the *Rayleigh limit*. In the Rayleigh limit, Planck-scale effects will be found to be negligible in a manner analogous to the negligibility of molecular effects in Rayleigh scattering. In the de Sitter limit, the energy of the cosmological constant dominates over that of the scalar field when quantum effects due to Rayleigh scattering take over. The effective dynamics is, therefore, dominated by the quantization of a de Sitter geometry.[3] This can be modelled by taking $C(k) = \delta(k/\hbar)$. However, care must be taken because $\mathrm{Im}\{\mathcal{J}_0\} = 0$, so it can no longer be taken as a linearly independent solution. Fortunately, $\mathcal{Y}_0$ is integrable and provides an adequate second solutions. The self-adjoint extensions are arbitrary phases, α, between these, and the general wavefunction is

$$\Psi(v,t) = \int_0^\infty \frac{\mathrm{d}\omega\omega}{\hbar^2} e^{i\omega^2 t/\hbar^3} E(\omega/\hbar)\left(\cos\tfrac{\alpha}{2}\mathcal{J}_0\left(\tfrac{\omega v}{\hbar}\right) - \sin\tfrac{\alpha}{2}\mathcal{Y}_0\left(\tfrac{\omega v}{\hbar}\right)\right)\,. \tag{26}$$

In the combined Rayleigh and de Sitter limits, v and ω are approximately canonically conjugate. At the bounce when $\langle v\rangle$ is at a minimum, the wavefunction (26) will have most of its support in the region $v \sim \sigma_v \sim \hbar/\sigma_\omega$.[4]

[3] Because we have imposed spatial curvature equal to zero, the relevant geometry is the de Sitter half-plane, which has an initial singularity.

[4] The last approximation holds because, as we will see, the wavefunction remains reasonably close to Gaussian during the bounce in this limit.

Thus,

$$v\omega \sim \frac{\omega_0}{\sigma_\omega} \gg 1\,. \tag{27}$$

In this limit, the Bessel functions can be expanded to give

$$\cos\tfrac{\alpha}{2}\mathcal{J}_0(\omega v) + \sin\tfrac{\alpha}{2}\mathcal{Y}_0(\omega v) \approx \sqrt{\frac{2}{\pi\omega v}}\cos(\omega v - \Delta/2)\,, \tag{28}$$

where $\Delta = \frac{\pi}{2} - \alpha$. Inserting a Gaussian function for $E(\omega)$ leads to

$$\Psi(v,t) = \mathcal{N}\sum_\pm A^\pm e^{iS^\pm}\,, \tag{29}$$

where $\mathcal{N} = \left(\frac{2}{\pi}\right)^{1/4}\sqrt{\frac{\sigma_\omega}{1+2i\sigma_\omega^2 t}}$.

$$A^\pm = \exp\left\{-\frac{\sigma_\omega^2(v \mp \omega_0 t)^2}{1+4\sigma_\omega^4 t^2}\right\}$$
$$S^\pm = \frac{\pm\omega_0 v - \frac{\omega_0^2 t}{2} + 2\sigma_\omega^2 v^2 t}{1+4\sigma_\omega^4 t^2} \mp \Delta/2\,. \tag{30}$$

The amplitudes $A^\pm$ and phases $S^\pm$ are those of free in- and out-going Gaussian wavepackets phase shifted by Δ.

The total Born amplitude in the $v\varphi$-basis is the sum of the Born amplitudes of both in-, $(A^+)^2$, and out-, $(A^-)^2$, going envelopes plus an interference term of the form:

$$2A^+A^-\cos\left(\frac{2\omega_0 v - \Delta}{1+4\sigma_\omega^4 t^2}\right)\,. \tag{31}$$

The interference indicates that the beat frequency is proportional to ω_0 in v-space when A^+ and A^- overlap. This beat frequency implies that there are many beats in a single envelope of size $\sim \sigma_v$, and confirms that the beat effects should be attributed to the micro- (i.e., Planck-scale) physics of the system. It also follows that the interference term can be approximately ignored when computing expectation values, which are integrals over v. We can, therefore, use a variety of analytic techniques to compute the mean

$$\langle\hat{v}\rangle \approx \sqrt{\frac{2}{\pi}}e^{-\omega_0^2 t^2/2\sigma_v^2}\sigma_v + \omega_0 t\,\mathrm{erf}\left(\frac{\omega_0 t}{\sqrt{2}\sigma_v}\right)\,, \tag{32}$$

and variance

$$\mathrm{Var}(\hat{v})^2 = \sigma_v^2 + \omega_0^2 t^2 - \langle\hat{v}\rangle^2\,, \tag{33}$$

of $\hat{v}$, where $\sigma_v(t) \equiv \frac{\sqrt{1+4\sigma_\omega^4 t^2}}{2\sigma_\omega}$. This behaviour can be checked against numerically computed expectation values (see [20]), and shows excellent agreement. FIG. 1 illustrates the general behaviour.

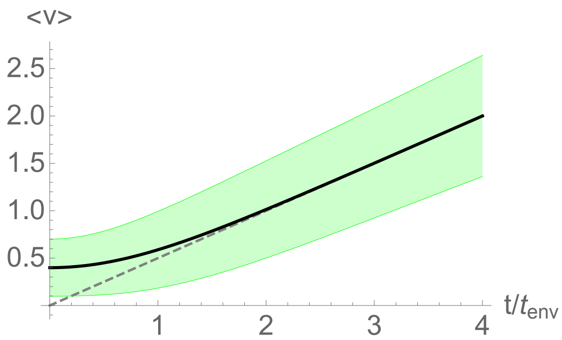

FIG. 1: $\langle \hat{v} \rangle (t)$ for $\omega_0/\sigma_\omega = 5$ with confidence interval computed from $\mathrm{Var}(\hat{v})$. The expectation value (solid), $\langle \hat{v} \rangle$, follows the classical curve (dashed) until $v \sim \hbar/\sigma_\omega$, when quantum effects due to Rayleigh scattering take over. The minimum, $v_{\min} = \frac{1}{\sqrt{2\pi}\sigma_\omega}$ of $\langle \hat{v} \rangle$ is reached at the bounce time, $t = 0$. (Note: $t_{\rm env} \equiv 1/2\sigma_\omega\omega_0$.)

Bouncing Cosmology Given the log-periodicity of $\Lambda_{\rm ref}$, the limit

$$e^{|k_0|/\hbar} \gg e^{\omega_0/\sigma_\omega} \tag{34}$$

implies that for any choice of $\Lambda_{\rm ref}$, there is an equivalent one imperceptibly close to Λ_0. The limit (34), therefore, implies that the self-adjoint extension behaviour becomes universal. Combined with the Rayleigh limit, (34) is such that the scalar field momentum is sufficiently large in units of $\hbar$ and is reasonably dominant, at early times, over the effects of the cosmological constant.

In this limit, the normalization of the unbound eigenstates, (21), simplifies to $\mathrm{sech}\left(\frac{\pi k}{2\hbar}\right)$, which is ω-independent. If we regularize the Gaussian of $E(\omega)$ in terms of the function

$$E(\omega) \approx \left(\frac{\hbar^2}{\sqrt{2\pi}\sigma_\omega \omega}\right)^{1/2} \left(\frac{\omega}{\omega_0}\right)^{\omega_0^2/4\sigma_\omega^2} \times \exp\left\{-\frac{2\omega_0^2}{\sigma_\omega^2}\left[\left(\frac{\omega}{\omega_0}\right)^2 - 1\right]\right\}, \tag{35}$$

which is a good approximation to a Gaussian in the Rayleigh limit, the ω_0-space integrals can be evaluated analytically in terms of confluent hypergeometric functions ${}_1F_1$. The explicit form of the result of this integration is unilluminating and can be found explicitly in [21]. The remaining integral reduces to a Fourier transform in k. The Fourier transform can be evaluated using the Fast Fourier Transform (FFT) algorithm after cutting off the k-integral at $\pm 6\sigma_k$ from k_0 and sampling at the Nyquist frequency, f_s. Modest oversampling (i.e., $2f_s$) allows for standard spline interpolations of the Fourier transformed function. Plotting and numerical integrations of various functions of Ψ can be performed using these interpolations in reasonable computation times.

To analyze the resulting solutions, we consider the effect of the three independent parameters $k_0/\hbar$, ω_0/σ_k, and k_0/σ_k separately. The choice of self-adjoint extension (25) minimizes the phase difference between in- and outgoing modes due to non-zero $k_0/\hbar$. We, therefore, expect this choice to lead to a negligible correction to the beat frequency as predicted by the interference term, (31), of the de Sitter model. Explicit comparison of the Born amplitudes of the wavefunction in the $v\varphi$-basis for modest parameter values[5] confirms this expectation. This provides numerical evidence that the Rayleigh limit, understood analytically in the de Sitter solution, persists when $\frac{k_0}{\hbar} \neq 0$.

The parameter ω_0/σ_ω should be expected to control the beat frequency according to (31), given that the overlap between in- and out-going envelopes occurs in the region $v \sim \hbar/\sigma_\omega$. To verify this, we can plot (see FIG 2) the Born amplitude of the wavefunction in the $v\varphi$-basis at $t = 0$, where the overlap is maximum. Comparison of the beat frequency for different values of ω_0/σ_ω is in excellent agreement with the de Sitter results.

The parameter k_0/σ_k controls how tightly the individual envelopes stay peaked on the classical solutions. This can be studied by varying the parameter $s = k_0/\omega_0$ for fixed ω_0/σ_ω and $k_0/\hbar$ and parametrically plotting $\langle \hat{v} \rangle / s$ and $\langle \hat{\varphi} \rangle$. The advantage of this choice of parameterization of the quantum solutions in terms of s is that the classical equations of motion can be written parametrically as

$$\frac{v}{s} = \left|\mathrm{cosech}\,(\varphi - \varphi_\infty)\right| . \tag{36}$$

Thus, the quantum curve for different choices of s can be compared with the same universal classical curve. FIG 3 illustrates the relevant features. The expectation values begin to diverge from their classical values in the region $v \sim 1/\sigma_\omega$ as expected. The expectation value of $\hat{\varphi}$ reaches a maximum value, which increases as s increases. The expectation value of $\hat{v}$ reaches a minimum at $t = 0$ as expected.

Prospectus Following [27, 28], we can connect the physics of our model to inflationary cosmology by considering an effective Hubble parameter, H_e, given by a function of the expectation value of $\hat{\phi}$. Because the Hubble parameter, as a phase space function, is proportional to π_v, this translates into computing the expectation value of $\hat{\pi}_v$ as a function of the expectation value of $\hat{\varphi}$. Effective slow-roll parameters, ϵ_{H_e} and η_{H_e}

$$\epsilon_{H_e}(\phi) = \frac{m_{\rm Pl}^2}{4\pi}\left(\frac{H_e'(\phi)}{H_e(\phi)}\right)^2 \quad \eta_{H_e}(\phi) = \frac{m_{\rm Pl}^2}{4\pi}\frac{H_e''(\phi)}{H_e(\phi)}, \tag{37}$$

can then be conveniently expressed in terms of the expectation values computed in our model.

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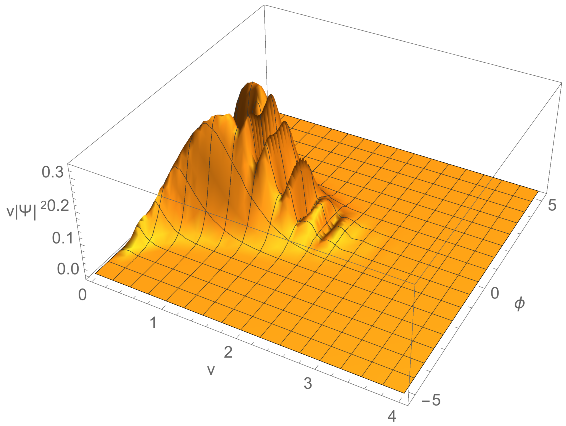
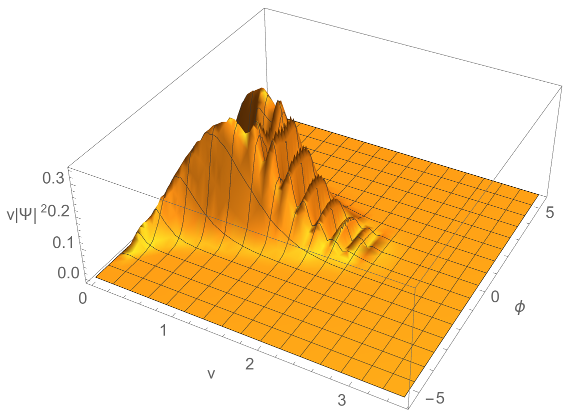
[5] E.g., $\omega_0/\sigma_\omega = 10$, $k_0/\sigma_k = 10$, $\hbar = 1, 2$



(a) $v|\Psi|^2$ for $\omega_0/\sigma_\omega = 10$, $s = 1$



(b) $v|\Psi|^2$ for $\omega_0/\sigma_\omega = 15$, $s = 1$

FIG. 2: Comparison of Born amplitude at bounce time for different choices of ω_0 and s (for $\sigma_\omega = \sigma_k = \hbar = 1$). The beat physics is affected in the same way by ω_0 as it was in the de Sitter limit.

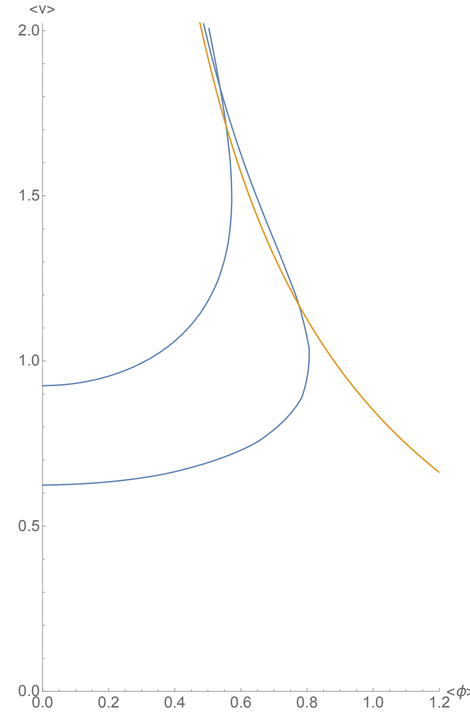


FIG. 3: Plot of $\langle \hat{v} \rangle / s$ versus $\langle \hat{\varphi} \rangle$ for different values of s. The top blue line represents $s = 1$, the bottom blue line $s = 2$, and the yellow line is the classical curve with $\omega_0 = 10$. Increasing s can be seen to decrease v_{min} and increase φ_{max}. Changing ω_0 has negligible effect. The figure is symmetric upon the reflection $\varphi \to -\varphi$, which represents $t \to -t$.

The curve of FIG. 3 shows a reasonably flat region near the maximum of $\langle \hat{\varphi} \rangle$ indicating a modestly stable de Sitter-like epoch of super-inflation. The existence of the Rayleigh limit suggests that this super-inflation epoch could be found to take place far below the Planck energy. This leaves open the possibility that the super-inflation of our model could be connected to power-spectrum data of the CMB. Because analytic methods break down in precisely the super-inflation regime, numerical techniques are required for such an identification. It is hoped that the existence of the Rayleigh limit, which is an exclusive feature of our model, may avoid instabilities and other issues found in existing models with super-inflation. These computations will be the subject of future investigations.

The general features of our quantization can be applied to the unitary quantization of anisotropic Bianchi models [29]. While the extension to Bianchi I is almost trivial, Bianchi IX models will lead to modified Bessel equations. However, the asymptotic behaviour of the wavefunction near the singularity and near the late-time attractors (i.e., the large v limit) will be identical to the model treated here. Since the construction of the self-adjoint extensions depends on the behaviour of the wavefunction near $v = 0$ and since the existence of the semi-classical approximation depends on the Gaussianity of the wavefunction near the late-time attractors, one may expect that many of the qualitative features of the present model will carry forward to unitary solutions of the Bianchi IX model that persist semi-classically to the late-time attractors. The Bianchi IX model may be particularly valuable for studying general singularity resolution in quantized GR in light of the BKL conjecture [30]. Such a framework may be useful for studying singularity resolution of time-like singularities via, for example, black-to-white hole transitions.

Inclusion of a non-trivial potential for ϕ will have a similar effect on the Bessel equation as the Bianchi IX model, and can be handled similarly.

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[1] S. W. Hawking and G. F. R. Ellis, *The large scale structure of space-time*, vol. 1. Cambridge university press, 1973.

[2] R. Brandenberger and P. Peter, "Bouncing cosmologies: progress and problems," *Foundations of Physics* **47** no. 6, (2017) 797–850.

[3] C. Isham, "Canonical quantum gravity and the problem of time," *Arxiv preprint gr-qc* (1992) . `http://arxiv.org/abs/grqc/9210011`.

[4] K. Kuchař, "The problem of time in canonical quantization of relativistic systems," in *Conceptual Problems of Quantum Gravity*, A. Ashtekar and J. Stachel, eds., p. 141. Boston University Press, 1991.

[5] E. Anderson, "Relationalism," 05, 2012. `http://arxiv.org/abs/1205.1256`.

[6] S. Gryb and K. P. Y. Thébault, "The role of time in relational quantum theories," *Foundations of Physics* (2011) 1–29.

[7] S. Gryb and K. P. Y. Thébault, "Symmetry and evolution in quantum gravity," *Foundations of Physics* **44** no. 3, (2014) 305–348.

[8] S. Gryb and K. P. Y. Thébault, "Schrödinger Evolution for the Universe: Reparametrization," *Classical and Quantum Gravity* **33** no. 6, (2016) 065004.

[9] W. G. Unruh and R. M. Wald, "Time And The Interpretation Of Canonical Quantum Gravity," *Phys. Rev.* **D40** (1989) 2598.

[10] W. G. Unruh, "A Unimodular Theory Of Canonical Quantum Gravity," *Phys. Rev.* **D40** (1989) 1048.

[11] D. Page and W. Wootters, "Evolution without evolution: Dynamics described by stationary observables," *Physical Review D* **27** no. 12, (1983) 2885–2892.

[12] C. Rovelli, "Quantum mechanics without time: A model," *Phys. Rev. D* **42** (Oct., 1990) 2638–2646.

[13] C. Rovelli, "Time in quantum gravity: An hypothesis," *Phys. Rev. D* **43** (1991) 442.

[14] C. Rovelli, "Partial observables," *Phys. Rev. D* **65** (2002) 124013.

[15] R. Gambini and R. A. Porto, "Relational time in generally covariant quantum systems: four models," *Physical Review D* **63** no. 10, (2001) 105014.

[16] B. Dittrich, "Partial and complete observables for hamiltonian constrained systems," *General Relativity and Gravitation* **39** (2007) 1891.

[17] B. Dittrich, "Partial and complete observables for canonical general relativity," *Classical and Quantum Gravity* **23** (2006) 6155.

[18] R. Gambini, R. A. Porto, J. Pullin, and S. Torterolo, "Conditional probabilities with dirac observables and the problem of time in quantum gravity," *Physical Review D* **79** no. 4, (2009) 041501.

[19] A. Ashtekar, A. Corichi, and P. Singh, "Robustness of key features of loop quantum cosmology," *Physical Review D* **77** no. 2, (2008) 024046.

[20] S. Gryb and K. P. Y. Thébault, "Bouncing unitary cosmology i. mini-superspace general solution,". Preprint.

[21] S. Gryb and K. P. Y. Thébault, "Bouncing unitary cosmology ii. mini-superspace phenomenology,". Preprint.

[22] C. J. Isham, "Topological and global aspects of quantum theory," in *Relativity, groups and topology. 2.* 1984.

[23] M. Reed and B. Simon, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness*, vol. 2. Elsevier, 1975.

[24] M. Reed and B. Simon, *Methods of modern mathematical physics. vol. 1. Functional analysis.* Academic, 1980.

[25] M. Bojowald and A. Skirzewski, "Effective equations of motion for quantum systems," *Reviews in Mathematical Physics* **18** no. 07, (2006) 713–745.

[26] D. Brizuela, "Statistical moments for classical and quantum dynamics: formalism and generalized uncertainty relations," *Physical Review D* **90** no. 8, (2014) 085027.

[27] D. S. Salopek and J. R. Bond, "Nonlinear evolution of long-wavelength metric fluctuations in inflationary models," *Phys. Rev. D* **42** (Dec, 1990) 3936–3962.

[28] A. R. Liddle, P. Parsons, and J. D. Barrow, "Formalizing the slow roll approximation in inflation," *Phys. Rev.* **D50** (1994) 7222–7232, `arXiv:astro-ph/9408015 [astro-ph]`.

[29] J. Wainwright and G. Ellis, eds., *Dynamical Systems in Cosmology*. Cambridge University Press, 1997.

[30] V. A. Belinsky, I. M. Khalatnikov, and E. M. Lifshitz, "Oscillatory approach to a singular point in the relativistic cosmology," *Adv. Phys.* **19** (1970) 525–573.