Unitarity and clock dependence in quantum cosmology

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Relational clocks in classical GR

"What is observable in classical and quantum gravity?" [Rovelli 1991]

Due to diffeomorphism symmetry, there is no meaningful way to identify spacetime points by coordinates: the Ricci scalar $R(x_0)$ at a point identified by coordinates x_0 is **not** an observable quantity.

Similarly, in cosmology cannot ask "what was the spatial curvature of the Universe at $t = 0$?"

The (ADM) Hamiltonian in GR generates gauge transformations $\Rightarrow$ observable (gauge-invariant) quantities must be constants of motion (e.g., [Unruh & Wald 1989])

Way out: **material reference systems** which label spacetime points not by arbitrary coordinates but by the values taken by reference matter fields:
"Matter energy density when $\varphi = \varphi_0$" *is* observable (and a constant of motion!)

Problem of time in canonical quantum gravity

In classical cosmology we can <u>choose</u> a time coordinate. Consider, e.g., a cosmological model of a flat FLRW universe with a free massless scalar field ϕ, with Hamiltonian

$$H = N\left(-\frac{2\pi G}{3}\frac{p_a^2}{a} + \frac{p_\phi^2}{2a^3}\right)$$

where N is the lapse. We can set $N = 1$ (for example) and compute time evolution

$$\frac{\mathrm{d}a}{\mathrm{d}t} = \{a, H\}, \quad \text{etc.},$$

and we obtain the full solution (starting from initial data that satisfies $H = 0$) expressed in a specific gauge.

However, the quantum theory does <u>not</u> contain this gauge-dependent information: since H needs to vanish quantum states are <u>frozen</u>.

$$\hat{H}|\psi\rangle = 0 \quad \Rightarrow \quad e^{\mathrm{i}\hat{H}t}|\psi\rangle = |\psi\rangle$$

Problem of time in canonical quantum gravity

We can pick an **internal** time, specified by a suitable degree of freedom (e.g., a reference scalar field). This is in general not possible globally, as the clock might not be monotonic everywhere. Even if it is, there are basic questions:

- How to specify an inner product for the quantum theory? Should we require a probability interpretation and unitarity of the theory?
- If there are multiple candidate clocks, are theories defined with respect to different clocks equivalent?

One approach to these issues is *Dirac quantisation* where we first specify a kinematical inner product and construct the physical inner product through group averaging. Here one can show equivalence of theories defined for different clocks in a wide class of systems [Höhn, Smith & Lock 2021]. We will see an example where this equivalence does not hold, so that the above questions seem to remain open.

Outline

1. Relational clocks and problem of time
2. The cosmological model
3. Three different quantum theories
4. Numerical analysis
5. Discussion

The cosmological model

We consider a homogeneous, isotropic, spatially flat universe with metric

$$\mathrm{d}s^2 = -N(\tau)^2\mathrm{d}\tau^2 + a(\tau)^2 h_{ij}\mathrm{d}x^i\mathrm{d}x^j$$

where h is a flat metric, $a(\tau)$ is the scale factor and $N(\tau)$ is the lapse function.

Matter: a free massless scalar $\phi(\tau)$ and perfect fluid with energy density $\rho(\tau)$ and equation of state parameter $w < 1$ (e.g., $w = 0$ for dust, $w = -1$ for dark energy) so that

$$m := \rho(\tau)a(\tau)^{3(w+1)} = \mathrm{const.}$$

Minisuperspace action for this model given by (setting $8\pi G = 1$)

$$S[a,\phi,m,\chi,N] = V_0 \int_{\mathbb{R}} \mathrm{d}\tau \left(-\frac{3\dot{a}^2 a}{N} + \frac{a^3}{2N}\dot{\phi}^2 - N\frac{m}{a^{3w}} + m\dot{\chi}\right)$$

where χ and N are treated as Lagrange multipliers, and $V_0 := \int \mathrm{d}^3x\,\sqrt{h}$.

Hamiltonian analysis

After going to the Hamiltonian formulation, we can change variables to

$$v = 4\sqrt{\frac{V_0}{3}}\,\frac{a^{\frac{3(1-w)}{2}}}{1-w}\,, \quad \pi_v = \sqrt{\frac{1}{12V_0}}\pi_a\, a^{\frac{3w-1}{2}}$$

(we always assume $a > 0, v > 0$) and rescale the scalar field variables as $\varphi = \sqrt{\frac{3}{8}}(1-w)\phi$, $\pi_\varphi = \sqrt{\frac{8}{3}}\frac{\pi_\phi}{1-w}$ to obtain a canonical form

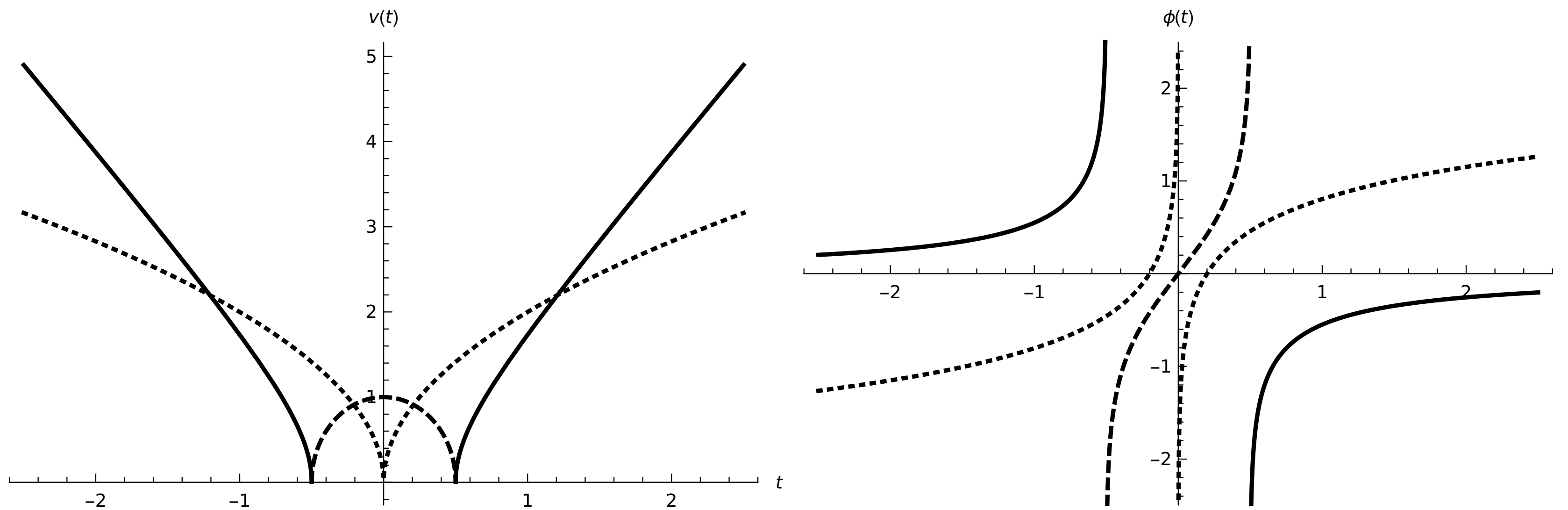
$$\mathcal{H} = \tilde{N}\left[-\pi_v^2 + \frac{\pi_\varphi^2}{v^2} + \lambda\right], \quad \{v,\pi_v\} = \{\varphi,\pi_\varphi\} = \{t,\lambda\} = 1$$

where also $\lambda = V_0 m$ and $\tilde{N} = N a^{-3w}$.

There is a preferred gauge: $\tilde{N} = 1$ leads to **simplest** dynamics with $\mathrm{d}t/\mathrm{d}\tau = 1$. **In this gauge** t becomes "time". This is unimodular time for $w = -1$, conformal time for $w = \frac{1}{3}$; . . . Each fluid has its own time (multi-fluids [Magueijo 2021–])

Solutions in t time

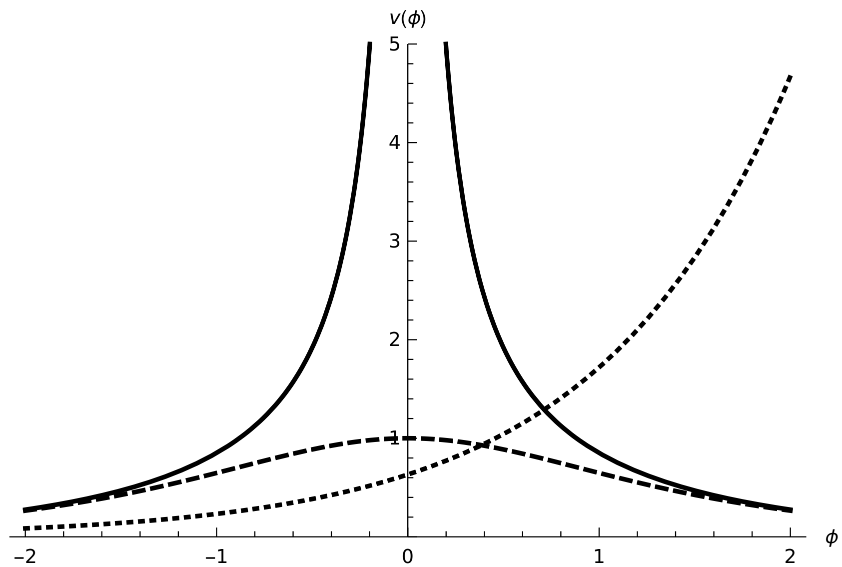
Classically, the variables t and φ evolve monotonically (if we exclude $\pi_\varphi = 0$) so are always good relational clocks. For v this is true if $\lambda \not< 0$; for $\lambda < 0$ there is a turning point (recollapse of the Universe).

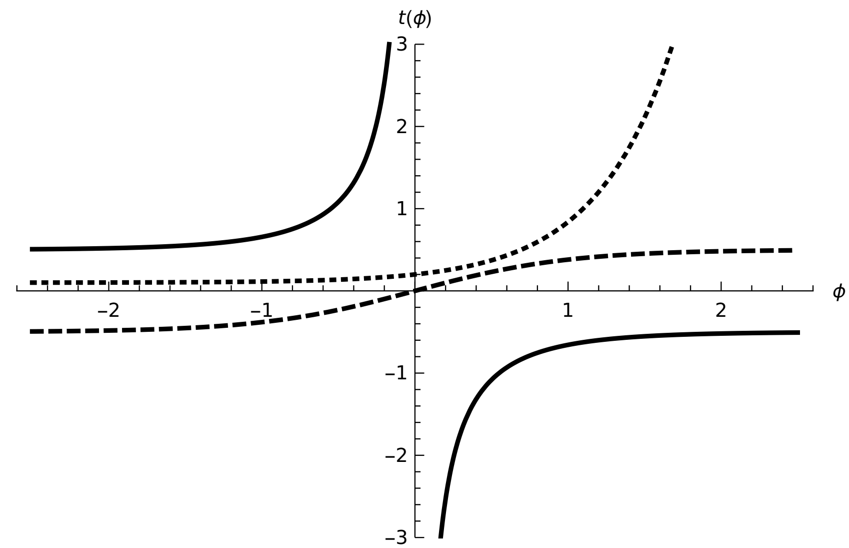


Classical solutions $v(t)$ and $\varphi(t)$ as functions of the clock t, with $\pi_\varphi = 1$ and $\lambda = 1$ (solid), $\lambda = -1$ (dashed) and $\lambda = 0$ (dotted).

All solutions have a (Big Bang/Big Crunch) singularity with $v \to 0$ and $\varphi \to \infty$.

Solutions in φ time





Parameters: $\pi_\varphi = 1$, $\lambda = 1$ (solid), $\lambda = -1$ (dashed) and $\lambda = 0$ (dotted).

When φ is used as a clock, the Big Bang/Big Crunch singularity is pushed to $\varphi \to \pm\infty$. For $\lambda > 0$ there is a finite value of φ where v and t diverge.

The explicit form of cosmological solutions highly depends on the clock.

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Defining the Wheeler–DeWitt equation

Our Hamiltonian constraint is

$$g^{AB}\pi_A\pi_B + \lambda := -\pi_v^2 + \frac{\pi_\varphi^2}{v^2} + \lambda \approx 0$$

where g^{AB} is a two-dimensional flat metric on the Rindler wedge, a portion of Minkowski spacetime bounded by $v = 0$. We quantise this as

$$\left(-\hbar^2\Box_g - \mathrm{i}\hbar\frac{\partial}{\partial t}\right)\Psi(v,\varphi,t) = \left(\hbar^2\frac{\partial^2}{\partial v^2} + \frac{\hbar^2}{v}\frac{\partial}{\partial v} - \frac{\hbar^2}{v^2}\frac{\partial^2}{\partial\varphi^2} - \mathrm{i}\hbar\frac{\partial}{\partial t}\right)\Psi(v,\varphi,t) = 0\,.$$

General solution to the Wheeler–DeWitt equation ($k \in \mathbb{R} \cup \mathrm{i}\mathbb{R}$, $\lambda \in \mathbb{R}$):

$$\Psi(v,\varphi,t) = \sum_{k,\lambda} e^{\mathrm{i}k\varphi} e^{\mathrm{i}\lambda\frac{t}{\hbar}} \left(\alpha(k,\lambda) J_{\mathrm{i}|k|}\left(\frac{\sqrt{\lambda}}{\hbar}v\right) + \beta(k,\lambda) J_{-\mathrm{i}|k|}\left(\frac{\sqrt{\lambda}}{\hbar}v\right)\right)\,.$$

We now need to define a Hilbert space for these, with appropriate inner product.

Schrödinger-like quantum theory (first discussed in [Gryb & Thébault 2018/19])

We can see the Wheeler–DeWitt equation as a Schrödinger equation in t,

$$\left(\hbar^2\frac{\partial^2}{\partial v^2}+\frac{\hbar^2}{v}\frac{\partial}{\partial v}-\frac{\hbar^2}{v^2}\frac{\partial^2}{\partial\varphi^2}\right)\Psi(v,\varphi,t)=\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(v,\varphi,t)\,. \tag{1}$$

This suggests defining the inner product ($\mathcal{R}$ is the Rindler wedge)

$$\langle\Psi|\Phi\rangle_t:=\int_{\mathcal{R}}\mathrm{d}v\,\mathrm{d}\varphi\sqrt{g}\,\bar{\Psi}\Phi=\int_0^\infty\mathrm{d}v\int_{\mathbb{R}}\mathrm{d}\varphi\;v\,\bar{\Psi}(v,\varphi,t)\Phi(v,\varphi,t)$$

which is **not** automatically conserved under evolution in t: the operator appearing on the left-hand side of (1) is not essentially self-adjoint. Needs reflecting boundary condition at $v=0$! Analogous to self-adjointness problem for

$$\hat{\mathfrak{H}}=\hbar^2\left(-\frac{\partial^2}{\partial v^2}-\frac{k^2+\frac{1}{4}}{v^2}\right)\qquad(k\in\mathbb{R})\ \text{ on }\ L^2(\mathbb{R}_+,\mathrm{d}v)\,.$$

General normalisable solution

We can derive the general solution to the boundary condition needed for unitarity and determine the most general normalisable state which is

$$\Psi(v,\varphi,t) = \int_{\mathbb{R}} \frac{\mathrm{d}k}{2\pi} e^{\mathrm{i}k\varphi} \left\{ \sum_{n=-\infty}^{\infty} e^{\mathrm{i}\frac{\lambda_n^k}{\hbar}t} B(k,\lambda_n^k) \frac{1}{\hbar} \sqrt{\frac{-2\lambda_n^k \sinh(k\pi)}{k\pi}} K_{\mathrm{i}k}\left(\frac{\sqrt{-\lambda_n^k}}{\hbar} v\right) \right.$$
$$\left. + \int_0^\infty \frac{\mathrm{d}\lambda}{2\pi\hbar} e^{\mathrm{i}\frac{\lambda}{\hbar}t} A(k,\lambda) \frac{\sqrt{2\pi}\,\mathrm{Re}\left[e^{\mathrm{i}\vartheta(k)-\mathrm{i}\log\sqrt{\frac{\lambda}{\lambda_0}}} J_{\mathrm{i}k}\left(\frac{\sqrt{\lambda}}{\hbar}v\right)\right]}{\sqrt{\hbar\cos\left(-2\vartheta(k)+k\log\frac{\lambda}{\lambda_0}\right)+\hbar\cosh(k\pi)}} \right\}$$

where $\vartheta(k)$ is a free function, λ_0 is an arbitrary reference scale and

$$\lambda_n^k = -\lambda_0 e^{-\frac{(2n+1)\pi}{k}+\frac{2\vartheta(k)}{k}}\,.$$

($\vartheta(k)$ generalises the usual one-parameter family of self-adjoint extensions.)

Using the scalar field or volume as a clock

We now write the Wheeler–DeWitt equation as

$$-\hbar^2\frac{\partial^2}{\partial\varphi^2}\Psi(v,\varphi,t) = \left(-\hbar^2\left(v\frac{\partial}{\partial v}\right)^2 + \mathrm{i}\hbar v^2\frac{\partial}{\partial t}\right)\Psi(v,\varphi,t)$$

and see it as a Klein–Gordon-like equation on the Rindler wedge with an extra "potential" term. This motivates defining the inner product

$$\langle\Psi|\Phi\rangle_\varphi = \mathrm{i}\int_{\mathbb{R}}\mathrm{d}t\int_0^\infty\frac{\mathrm{d}v}{v}\left(\bar{\Psi}\frac{\partial\Phi}{\partial\varphi} - \Phi\frac{\partial\bar{\Psi}}{\partial\varphi}\right).$$

Again, **not** automatically conserved under evolution in φ: this time some solutions need boundary condition at $v = \infty$! Analogous to self-adjointness problem for

$$\hat{\mathfrak{O}} = -\hbar^2(\partial^2/\partial u^2) - \lambda e^{2u} \qquad (\lambda\in\mathbb{R}) \text{ on } L^2(\mathbb{R},\mathrm{d}u).$$

However, the third theory defined using v as clock **is** automatically unitary.

The role of unitarity

Classical solutions, when expressed in terms of one of the "natural" clock variables, can terminate at a finite time as measured by the clock.

In t time this reflects the Big Bang/Big Crunch singularity of classical GR.

In φ time and with $\lambda > 0$ it reflects the fact that $\varphi \to \varphi_0$ as the Universe expands and φ becomes an "infinitely slow" clock asymptotically.

Classically, clocks are not defined beyond the point where the solution terminates. But what happens quantum mechanically? If we require quantum theory to be **unitary** any state must have a globally well-defined time evolutuion.
$\Rightarrow$ Evolution must extend beyond points where classical solution terminates!

Conjecture [Gotay & Demaret 1983]: *unitary slow-time quantum dynamics is always nonsingular, while unitary fast-time quantum dynamics inevitably leads to collapse*. We extend this conjecture to clocks reaching infinity in finite "time".

Relation to previous work

- The model was analysed by Gryb and Thébault in a series of papers (2018/19) using t as clock; generic resolution of the singularity was found in the sense that $\langle v(t)\rangle \geq C_\psi > 0$ where C_ψ is some state-dependent constant. We confirm and extend these results.

- Bojowald and Halnon (2018) studied the model using deparametrisation and an effective (semiclassical) approach, finding inequivalent results for different clocks since different factor orderings are needed.

- GR with a massless scalar field and fixed cosmological constant is similar to our model (for us, since Λ is a conserved momentum, superpositions in Λ are possible). This model was quantised by Pawłowski and Ashtekar (2012) using φ as a clock. The authors found recollapse of the Universe at large volume, but no singularity resolution, consistent with our general framework.

Connection to Dirac quantisation

In our constructions we made a choice of inner product which might seem *ad hoc*. Results can be seen from the more systematic perspective of group averaging/Dirac quantisation, where one defines a physical inner product through

$$|\psi_{\rm ph}\rangle = \delta(\hat{\mathcal{C}})|\psi\rangle \quad \Rightarrow \quad \langle\phi_{\rm ph}|\psi_{\rm ph}\rangle := \langle\phi|\delta(\hat{\mathcal{C}})|\psi\rangle$$

where $\mathcal{C}$ is our Hamiltonian constraint. In practice, one needs to write the Hamiltonian constraint as *system + clock*, following [Höhn, Smith & Lock 2021]. So if

$$\hat{\mathcal{C}}\Psi(v,\varphi,t) := \left(\hbar^2\frac{\partial^2}{\partial v^2} + \frac{\hbar^2}{v}\frac{\partial}{\partial v} - \frac{\hbar^2}{v^2}\frac{\partial^2}{\partial\varphi^2} - \mathrm{i}\hbar\frac{\partial}{\partial t}\right)\Psi(v,\varphi,t)\,,$$

the theory using t as a clock is based on group averaging with respect to $\hat{\mathcal{C}}$ which is in this form. However, to use φ as a clock we would have to redefine $\hat{\mathcal{C}}' := v^2\hat{\mathcal{C}}$, and we end up with the same inequivalent theories.

Can be understood classically as different choice of lapse in $\mathcal{H} = N\mathcal{C}$.

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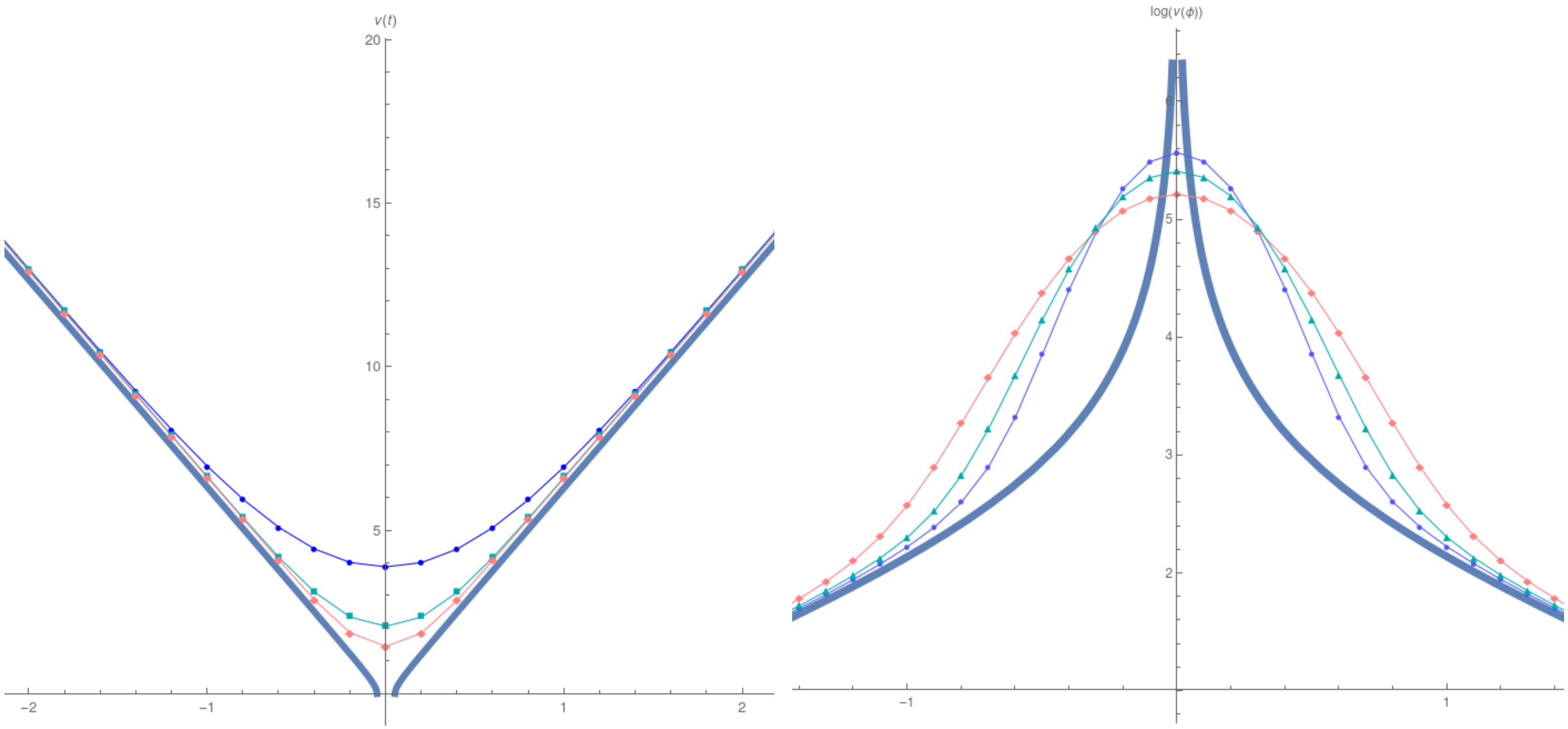
Numerical analysis

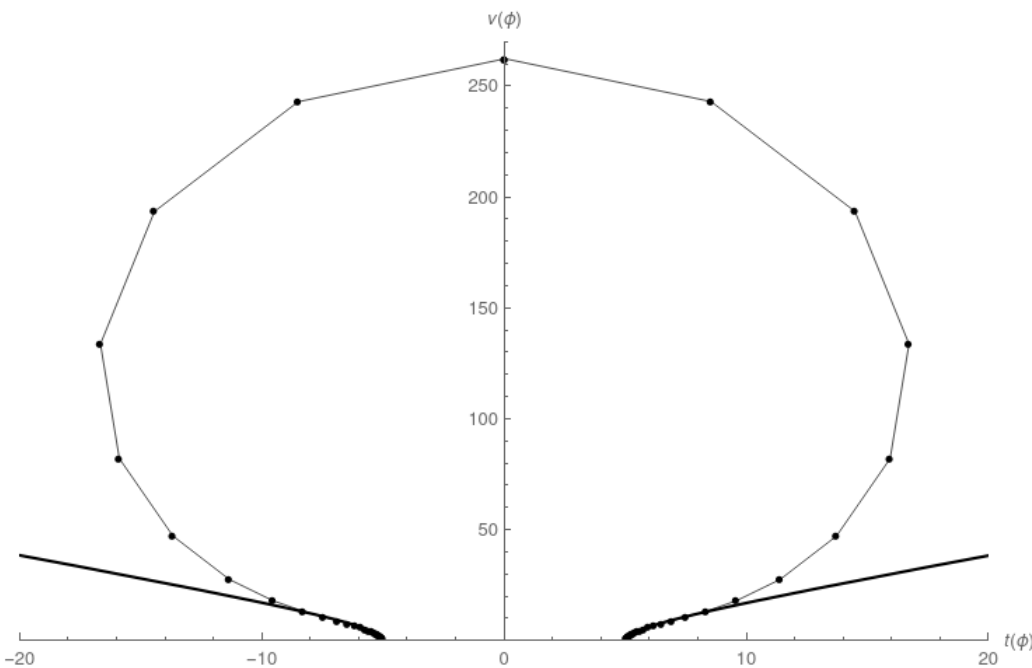
To illustrate the differences between the theories further, we numerically study the evolution of expectation values in semiclassical (Gaussian) states. Reflection at $v = 0$ (when t is the clock) and $v = \infty$ (when φ is the clock) can be seen.



Colours represent different values of the standard deviation in Gaussian states.

Time is running backwards

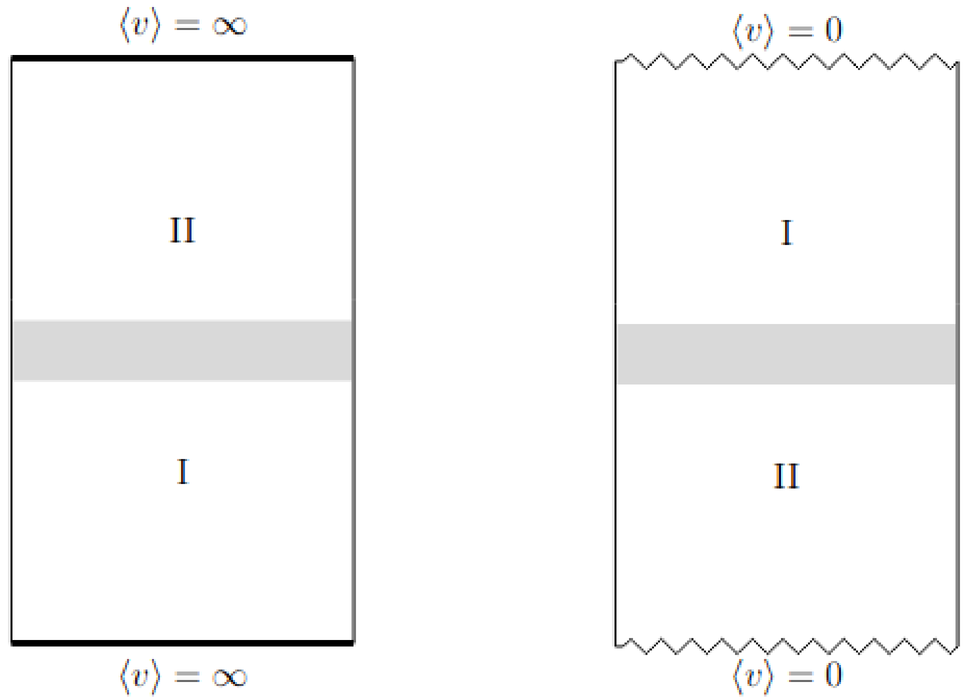
Recall that in the classical theory, $v(t)$ is a monotonic function in each branch of the classical solutions for $\lambda > 0$. However, this is very different if we now plot the quantum expectation values $\langle t(\varphi) \rangle$ and $\langle v(\varphi) \rangle$ against each other:



The clock variable t starts to run backwards shortly before the quantum recollapse. Very non-classical behaviour at what would be seen as low energies!

Penrose–Carter diagrams

We can visualise the singularity-resolving solution obtained by using t as a clock and the recollapsing solution obtained by using φ as a clock.



In both cases there is a region of large quantum fluctuations (shaded in grey) which connects the contracting and expanding branches of the classical solution.

Discussion

- Quantum theories defined with respect to different clocks inequivalent if we require unitarity. Non-classical behaviour triggered when classical solutions terminate in finite "time", leading to reflecting boundary conditions.

- Canonical quantisation does not appear covariant with respect to reparametrisations of time; these involve changing the lapse, and so change the Hamiltonian $\mathcal{H} = N\mathcal{C}$ which influences the choice of inner product.

- Should we see one choice of clock as more fundamental and only demand unitarity for that clock? (e.g., the clock measuring proper time $N = 1$)

- Is there a remedy in the path integral approach? (e.g., BFV formalism to implement formal gauge invariance with respect to time reparametrisations)

- Implications for claims of singularity resolution or other quantum corrections to classical cosmology?

Thank you!