Numerical approach to quantum cosmology using Bohmian trajectories

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Verão Quântico

Motivations: Why quantum cosmology?

- Quantum cosmology removes most of the complexity (going from quantum field theory to quantum mechanics) but includes some of the hard questions present in full quantum gravity, e.g.:
  - Interpretation problem;
  - Time problem;
- May be the only way to measure a quantum gravity effect, i.e., through the primordial cosmology.
- When combined with quantum field theory for perturbations around a quantum background, it may give us hints about the full quantum gravity.

Quantum cosmology action

Lets consider a Bianchi I mini-superspace with a metric:

$$\mathrm{d}s^2 = -N^2 \mathrm{d}\tau^2 + a_i^2 \mathrm{d}x_i^2, \qquad i = 1, 2, 3.$$

The scale factors associated to each direction can be recast as

$$\begin{aligned} a_1 &= V^{1/3} e^{\beta_+ + \sqrt{2}\beta_-}, \\ a_2 &= V^{1/3} e^{\beta_+ - \sqrt{2}\beta_-}, \\ a_3 &= V^{1/3} e^{-2\beta_+}, \end{aligned}$$

The action for this model (empty Bianchi I) reads

$$S = \int \mathrm{d}\tau \left(\frac{\mathrm{d}\theta}{\mathrm{d}\tau} - NH \right), \quad \dot{} \equiv \frac{\mathrm{d}}{\mathrm{d}\tau}, \quad \mathrm{d}\theta \equiv p_V \mathrm{d}V + p_+ \mathrm{d}\beta_+ + p_- \mathrm{d}\beta_-$$

where the Hamiltonian H is

$$H = \frac{3V}{8} \left(-p_V^2 + \frac{p_+^2 + p_-^2}{9V^2} \right).$$

The time problem

If we quantize the theory as it is, we have (modulo operator ordering ambiguities):

$$H|\Psi\rangle = \frac{3\hat{V}}{8}\left(-\hat{p}_V^2 + \frac{\hat{p}_+^2 + \hat{p}_-^2}{9\hat{V}^2}\right)|\Psi\rangle = 0.$$

- There is no clear time definition;
- The model is (time) reparametrization invariant;
- All operators are considered observables;

The time problem – solving the Hamiltonian constraint

Instead of quantizing the model using H, we can solve the constraint already in the Hamiltonian formalism.
First, classically we have: $\dot{p}_\pm = 0$. Thus, we can change variables to combine both variables in a single constant:

$$p_+ = k\cos\alpha, \qquad p_- = k\sin\alpha,$$
$$p_k \equiv -\left(\cos\alpha\beta_+ + \sin\alpha\beta_-\right), \quad p_\alpha \equiv \left(k\sin\alpha\beta_+ - k\cos\alpha\beta_-\right),$$

where $k > 0$. This leads to:

$$\mathrm{d}\theta = p_V \mathrm{d}V + p_k \mathrm{d}k + \alpha \mathrm{d}p_\alpha,$$
$$H = \frac{3V}{8}\left(-p_V^2 + \frac{k^2}{9V^2}\right).$$

From here on we ignore $(\alpha,\ p_\alpha)$.

The time problem – solving the Hamiltonian constraint

The classical equations of motion are:

$$\dot{k} = 0, \qquad \dot{V} = -N\frac{3Vp_V}{4},$$
$$\dot{p}_k = -N\frac{k}{12V}, \qquad \dot{p}_V = -N\left[\frac{3}{8}\left(-p_V^2 + \frac{k^2}{9V^2}\right) - \frac{k^2}{12V^2}\right].$$

The solution must also satisfy

$$\frac{3V}{8}\left(-p_V^2 + \frac{k^2}{9V^2}\right) = 0.$$

Note that:

$$\frac{\mathrm{d}T}{\mathrm{d}\tau} = -\frac{3}{4}\frac{N}{V} < 0, \quad T \equiv 9\frac{p_k}{k}.$$

in other words, T is monotonically decreasing function of τ and consequently has a one-to-one relation with τ.

The time problem – solving the Hamiltonian constraint

Going back to the action, we can write the canonical one-form as:

$$\mathrm{d}\theta = p_V \mathrm{d}V + \frac{T}{2}\mathrm{d}k^2$$

And then, solve the Hamiltonian constraint explicitly:

$$\mathrm{d}\theta = p_V \mathrm{d}V - \frac{V^2 p_V^2}{2}\mathrm{d}T.$$

Now, with the constraint solved the action is simply:

$$S = \int \mathrm{d}\theta = \int \mathrm{d}T \left(p_V \frac{\mathrm{d}V}{\mathrm{d}T} - \frac{V^2 p_V^2}{2} \right),$$

and the unconstrained Hamiltonian is $H_\mathrm{u} = V^2 p_V^2/2$.

- It is easy to check that this Hamiltonian plus the constraint gives the same dynamics as the constrained version.

The time problem – solving the Hamiltonian constraint

In this approach we solved the time problem by choosing a function of the dynamical variables to describe a time variable.

- This function when quantized will have status of time, the wave-function will not be normalized with respect to it.
- There are many choices of time variable. A convenient choice leads us to:

$$S = \int \mathrm{d}\theta = \int \mathrm{d}\tau \left(p\dot{V} - H_{\mathrm{u}} \right), \qquad H_{\mathrm{u}} \equiv \frac{p^2}{2}.$$

  The problem reduces to a free particle in a half-line $V \in \mathbb{R}^+$.
- A similar calculation in a Friedmann universe filled with a single barotropic fluid leads to the same action as above.

Boundary conditions

Our quantum cosmology problem is then reduced to a simple one-dimensional particle in a half-line, a well known problem. To make the Hamiltonian H_{u} self-adjoint we need to impose boundary conditions on the wave-function $\psi(V)$, i.e.,

$$\psi(0) = b_0 \left.\frac{\mathrm{d}\psi}{\mathrm{d}V}\right|_{V=0} .$$

For any choice of boundary conditions we have a different physical scenario, different values of b_0 result in different reflections of the wave-function at the $V = 0$ boundary.

- Here we work with $b_0 = 0$, but the numerical methods we will discuss can be adapted to any choice of b_0.

Equation of motion

The Schrodinger equation we need to solve is:

$$i\dot{\psi} = \hat{H}_{\mathrm{u}}\psi, \qquad \hat{H}_{\mathrm{u}} = \left(-\frac{\mathrm{d}^2}{\mathrm{d}V^2} + \frac{\lambda}{V^2}\right).$$

where we chose the representation

$$\hat{V}\psi = V\psi, \qquad \hat{p}\psi = -i\frac{\mathrm{d}\psi}{\mathrm{d}V}.$$

The potential λ/V^2 may appear as the result of the coherent state quantization which we are also interested in comparing with the canonical quantization ($\lambda = 0$).

Physical interpretation: Bohmian trajectories

Another problem in quantum cosmology is of the interpretation of the wave-function. Using the Bohmian trajectories the problem is completely resolved, at least for the mini-superspace.
Given the polar parametrization of the wave-function

$$\psi = Re^{iS},$$

the trajectories are given by

$$\dot{V}_{\mathrm{B}} = \left.\frac{\mathrm{d}S}{\mathrm{d}V}\right|_{V=V_{\mathrm{B}}}.$$

- This provides a well defined value of $V_{\mathrm{B}}(t)$ given an initial condition $V_{\mathrm{B}}(t_0)$.
- When dealing with perturbations the conditional wave-function for the perturbations $\Psi\left[\delta g_{\mu\nu}|V_{\mathrm{B}}(t)\right]$, gives a better approximation than the semi-classical approach.

Numerical approach

There are many numerical approaches to solve the Schrodinger equation

$$i\dot{\psi} = \hat{H}_{\mathrm{u}}\psi, \qquad \hat{H}_{\mathrm{u}} = \left(-\frac{\mathrm{d}^2}{\mathrm{d}V^2} + \frac{\lambda}{V^2}\right),$$

with the boundary condition $\psi(\tau, V = 0) = 0$. However, here we need to solve both this equation and the Bohmian trajectory:

$$\dot{V}_{\mathrm{B}} = \left.\frac{\mathrm{d}S}{\mathrm{d}V}\right|_{V=V_{\mathrm{B}}} = \left.\frac{1}{2i|\psi|^2}\left(\psi^*\frac{\mathrm{d}\psi}{\mathrm{d}V} - \psi\frac{\mathrm{d}\psi^*}{\mathrm{d}V}\right)\right|_{V=V_{\mathrm{B}}}.$$

Numerical approach

This imposes a set of numerical difficulties:

- Any discretization of the function $\psi(V_i)$ at $\{V_i\}_{i=1,N}$ will need to be interpolated to compute $\psi(V_{\mathrm{B}})$ since V_{B} will not coincide with the knots.
- The derivatives of ψ will also be computed from the interpolation.
- The interpolation of both ψ and $\mathrm{d}\psi/\mathrm{d}V$ must have the correct behavior near the boundary.

For example, any polynomial interpolation will fail. Around the first knot $V = 0$ the interpolating function $\psi_{\mathrm{poly}} = bV + cV^2 + dV^3$, the coefficients b, c, d are obtained from a local polynomial or spline interpolation, the constant part is set to zero to satisfy the boundary condition $\psi_{\mathrm{poly}}(0) = 0$. However, we also have

$$i\dot{\psi}_{\mathrm{poly}}(0) = 0 \neq \lim_{V\to 0} H_{\mathrm{c}}\psi_{\mathrm{poly}} \to 2c + \frac{b\lambda}{V}.$$

Numerical approach

More generally, expanding in τ, we have

$$\psi(\tau, V) \approx \psi(0, V) - iH_{\mathrm{c}}\psi(0, V)\tau + (-iH_{\mathrm{c}})^2\psi(0, V)\frac{\tau^2}{2!} + \dots.$$

Thus, to satisfy $\psi(\tau, 0) = 0$ for any time τ, we need to satisfy

$$\lim_{V \to 0}(-iH_{\mathrm{c}})^n\psi(0, V) = 0,$$

for any positive integer n. For this reason a simple polynomial interpolation does not have the correct asymptotic behavior near the boundary.

- In the usual spectral approach ψ is decomposed in the eigenfunctions of H_{c}, which naturally satisfy the condition above.
- Even if the initial condition does not satisfy the condition above, we first project it on the eigenfunctions.

Radial Basis Functions discretization

We can circumvent this problem using Radial Basis Functions (RBF). In this approach, we write the wave-function as

$$\psi(V) = \sum_{n=i}^{N} K(V, W_n)\beta_n,$$

where $K(V, W)$ are the RBF functions. Some common choices for K are:

- Gaussian $K_{\mathrm{g}}(V, W) = e^{-h^2(V-W)^2}$,
- Inverse quadratic: $K_{\mathrm{ic}}(V, W) = \frac{1}{1+h^2(V-W)^2}$.

Note that these functions, differently from a local polynomial interpolation, have support in the whole domain $\mathbb{R}^+$. For this reason, we can adapt this basis in order to satisfy

$$\lim_{V\to 0}(-iH_{\mathrm{c}})^n K(V, W) = 0,$$

for any value of n.

Radial Basis Functions discretization

Using the ansatz $K(V,W) = V^{\alpha}\left(\sum_{n=0}^{\infty} c_n \frac{V^n}{n!}\right)$, we obtain:

$$H_{\mathrm{c}}K(V,W) = V^{\alpha}\left\{\sum_{n=0}^{\infty} c_n \frac{V^{n-2}}{n!}\left[-\alpha(\alpha-1) - 2n\alpha - n(n-1) + \lambda\right]\right\}.$$

To obtain the same behavior as $K(V,W)$, we need to satisfy

$$\begin{aligned} c_0\left[\lambda - \alpha(\alpha-1)\right] &= 0, \\ c_1\left[\lambda - \alpha(\alpha+1)\right] &= 0. \end{aligned}$$

Since we cannot use α to satisfy both equations, we choose $\alpha(\alpha+1) = \lambda$ and $c_0 = 0$. Finally, since $c_0 = 0$, we need to impose $c_2 = 0$ to have the same behavior for $H_{\mathrm{c}}K(V,W)$, consequently, for any power of the Hamiltonian we need to impose that $c_{2n} = 0$ for any integer n.

Radial Basis Functions discretization

In order to satisfy the conditions above, we start with a standard RBF, e.g, $K_{\mathrm{g}}(V, W)$ and define:

$$\begin{aligned} K(V, W) &= (VW)^{\alpha} \left[K_{\mathrm{g}}(V, W) - K_{\mathrm{g}}(-V, W) \right], \\ &= (VW)^{\alpha} \left[e^{-h^2 (V-W)^2} - e^{-h^2 (V+W)^2} \right]. \end{aligned}$$

It is easy to see that this RBF satisfy all the conditions above. Now, given a set of N knots $\{V_n\}_{n=1,N}$, we have

$$\psi_n = \sum_{m=1}^{N} K_{nm} \beta_m, \qquad K_{nm} \equiv K(V_n, V_m), \qquad \psi_n \equiv \psi(V_n).$$

Then, inverting K_{nm} we can obtain the initial conditions for β_n.

Radial Basis Functions discretization

The Schrodinger equation calculated at the knots is

$$i\dot{\beta}_n = \sum_{m=1,l=1}^{N,N} K^{-1}_{nm}(HK)_{ml}\beta_l, \qquad (HK)_{ml} \equiv H_{\mathrm{u}}K(V_m, V_l).$$

Diagonalizing the matrix $M_{nl} \equiv \sum_{m=1}^{N} K^{-1}_{nm}(HK)_{ml}$ we can project β_n in the basis of eigenvectors of M_{nl} and solve the evolution analytically. Then, once we have $\psi(\tau, V)$ we compute the evolution of the Bohmian trajectories.
We used two classes of initial conditions:

- Gaussian:

$$\psi_0(V) \propto e^{-\frac{(V-\mu)^2}{4\sigma^2} + \frac{3iH_0V^2}{2}}.$$

- Exponential:

$$\psi_0(V) \propto \left(\frac{V}{V_i}\right)^{\frac{\alpha-1}{2}} e^{\frac{\alpha-1}{2}\frac{V}{V_i} + iVp_0}.$$

Solutions: Classical, Expected values, Bohmian trajectories

Initial condition (Semi-classical = Classical solutions!):

- Gaussian $\lambda = 0$, $\mu = 0$, $H_0 = -0.5$, $\sigma = 1$;
- Gaussian $\lambda = 0$, $\mu = 2.5$, $H_0 = -0.5$, $\sigma = 1$;
- Gaussian $\lambda = 2$, $\mu = 0$, $H_0 = -0.5$, $\sigma = 1$;
- Exponential $\lambda = 0$, $V_i = 2$, $\alpha = 3$, $p_0 = -1.5$;
- Exponential $\lambda = 1$, $V_i = 2$, $\alpha = 3$, $p_0 = -1.5$;

Concluding remarks

- General method for solving Schrodinger equation in the presence of boundaries.
- Scalable method for higher dimensions (does not scale exponentially as grid methods N^d).
- Have asymptotic behavior compatible with the boundary condition, allows a well defined computation of the phase gradient.
- Simple Gaussian initial conditions can be misleading.
- Gaussian initial conditions seems to lead to Bohmian trajectories that oscillates around the expected value.
- Exponential initial conditions seems to lead to Bohmian trajectories that oscillates around the classical trajectories.

Concluding remarks

Thank you!