

# Numerical approach to quantum cosmology using Bohmian trajectories

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# 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:

$$ds^2 = -N^2 d\tau^2 + a_i^2 dx_i^2, \quad i = 1, 2, 3.$$

The scale factors associated to each direction can be recast as

$$a_1 = V^{1/3} e^{\beta_+ + \sqrt{2}\beta_-},$$

$$a_2 = V^{1/3} e^{\beta_+ - \sqrt{2}\beta_-},$$

$$a_3 = V^{1/3} e^{-2\beta_+},$$

The action for this model (empty Bianchi I) reads

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

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:

$$\begin{aligned} p_+ &= k \cos \alpha, & p_- &= k \sin \alpha, \\ p_k &\equiv -(\cos \alpha \beta_+ + \sin \alpha \beta_-), & p_\alpha &\equiv (k \sin \alpha \beta_+ - k \cos \alpha \beta_-), \end{aligned}$$

where  $k > 0$ . This leads to:

$$\begin{aligned} d\theta &= p_V dV + p_k dk + \alpha dp_\alpha, \\ H &= \frac{3V}{8} \left( -p_V^2 + \frac{k^2}{9V^2} \right). \end{aligned}$$

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

# The time problem – solving the Hamiltonian constraint

The classical equations of motion are:

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

The solution must also satisfy

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

Note that:

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

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

# The time problem – solving the Hamiltonian constraint

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

$$d\theta = p_V dV + \frac{T}{2} dk^2$$

And then, solve the Hamiltonian constraint explicitly:

$$d\theta = p_V dV - \frac{V^2 p_V^2}{2} dT.$$

Now, with the constraint solved the action is simply:

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

and the unconstrained Hamiltonian is  $H_u = V^2 p_V^2 / 2$ .

- 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:

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

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.,

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

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:

$$i\dot{\psi} = \hat{H}_u \psi, \quad \hat{H}_u = \left( -\frac{d^2}{dV^2} + \frac{\lambda}{V^2} \right).$$

where we chose the representation

$$\hat{V}\psi = V\psi, \quad \hat{p}\psi = -i\frac{d\psi}{dV}.$$

The potential  $\lambda/V^2$  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

$$\dot{V}_B = \left. \frac{dS}{dV} \right|_{V=V_B}.$$

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

# Numerical approach

There are many numerical approaches to solve the Schrodinger equation

$$i\dot{\psi} = \hat{H}_u \psi, \quad \hat{H}_u = \left( -\frac{d^2}{dV^2} + \frac{\lambda}{V^2} \right),$$

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

$$\dot{V}_B = \left. \frac{dS}{dV} \right|_{V=V_B} = \frac{1}{2i|\psi|^2} \left( \psi^* \frac{d\psi}{dV} - \psi \frac{d\psi^*}{dV} \right) \Big|_{V=V_B}.$$

## 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  $\psi(V_B)$  since  $V_B$  will not coincide with the knots.
- ▶ The derivatives of  $\psi$  will also be computed from the interpolation.
- ▶ The interpolation of both  $\psi$  and  $d\psi/dV$  must have the correct behavior near the boundary.

For example, any polynomial interpolation will fail. Around the first knot  $V = 0$  the interpolating function  $\psi_{\text{poly}} = bV + cV^2 + dV^3$ , 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  $\psi_{\text{poly}}(0) = 0$ . However, we also have

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

## Numerical approach

More generally, expanding in  $\tau$ , we have

$$\psi(\tau, V) \approx \psi(0, V) - iH_c\psi(0, V)\tau + (-iH_c)^2\psi(0, V)\frac{\tau^2}{2!} + \dots$$

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

$$\lim_{V \rightarrow 0} (-iH_c)^n \psi(0, V) = 0,$$

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  $\psi$  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

$$\psi(V) = \sum_{n=1}^N K(V, W_n) \beta_n,$$

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

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

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

$$\lim_{V \rightarrow 0} (-iH_c)^n K(V, W) = 0,$$

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:

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

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

$$c_0 [\lambda - \alpha(\alpha-1)] = 0,$$

$$c_1 [\lambda - \alpha(\alpha+1)] = 0.$$

Since we cannot use  $\alpha$  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  $H_c K(V, W)$ , 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,  $K_g(V, W)$  and define:

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

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

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

Then, inverting  $K_{nm}$  we can obtain the initial conditions for  $\beta_n$ .

## Radial Basis Functions discretization

The Schrodinger equation calculated at the knots is

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

Diagonalizing the matrix  $M_{nl} \equiv \sum_{m=1}^N K_{nm}^{-1}(HK)_{ml}$  we can project  $\beta_n$  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:

$$\psi_0(V) \propto e^{-\frac{(V-\mu)^2}{4\sigma^2} + \frac{3iH_0 V^2}{2}}.$$

- 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!