Quantum empty Bianchi I spacetime with internal time

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We discuss the question of time in a Bianchi I quantum cosmology in the framework of singularity avoidance. We show that time parameters fall into two distinct classes, that are such that the time development of the wave function either always leads to the appearance of a singularity (fast-gauge time) or that always prevents it from occurring (slow-gauge time). Furthermore, we find that, in the latter case, there exists an asymptotic regime, independent of the clock choice. This may point to a possible solution of the clock issue in quantum cosmology if there exists a suitable class of clocks all yielding identical relevant physical consequences.

I. INTRODUCTION

The problem of time [1–4] in quantum gravity [5,6] is a longstanding one [7] that stems from the fact that the underlying notions in general relativity (GR) and quantum theory are incompatible. Among the numerous proposals that have been suggested is that of using a perfect fluid [8] whose Hamiltonian, being linear in a momentum, naturally transforms the Wheeler-De Witt equation in the Schrödinger form upon quantization of this momentum. Such a solution also permits, in the trajectory approach of quantum mechanics, one to naturally avoid cosmological singularities [9–11]. Note that using an internal degree of freedom (d.o.f.) to define time was also used in completely different contexts; see, e.g., Ref. [12].

It is well known that the canonical formulation of general relativity is given by a totally constrained Hamiltonian system. In these systems the dynamics takes place inside the first-class constraints hypersurface and as a consequence the symplectic structure projected on this hypersurface is no longer symplectic (it is actually a presymplectic form). The hypersurface orbits generated by the vector constraint representing infinitesimal spatial diffeomorphisms are removed by imposing appropriate gauge-fixing conditions, whereas the hypersurface orbits generated by the

Hamiltonian constraint representing the physical motion of the gravitational system require another treatment.

For this physical motion, one can choose a foliation for the constrained manifold such that in each sheet the restriction of the 2-form yields again a symplectic structure, which consequently defines a Hamiltonian system (where the Hamiltonian generates the motion across sheets). In this language, the example of the perfect fluid cited above (with spatial diffeomorphisms being absent), where the Hamiltonian depends linearly on a momentum variable p_T and is independent of its conjugate variable T, defines a natural foliation: the constraint is solved in terms of p_T and $T = $ const. gives the desired foliation; and consequently p_T generates "time" translations. Thus, as discussed in [13], even at the classical level, if the constraints hypersurface $\mathcal{M}$ does not admit a global foliation of the form $\mathcal{M} = \mathbb{R} \times \mathcal{N}$, it seems that even classically one cannot define time globally in these cases.

When a time variable is well defined (and consequently a foliation on the constraints hypersurface), it is usually not unique. Classically, this is not a problem: it just corresponds to different ways to parametrize time with respect to some internal d.o.f., using a combination of the canonical variables. On the other hand, it is not clear if this choice of time variable affects the quantized system, i.e., if the choice of time variable implies any physical consequence for the quantized system. Arguably, one can demand, as a desired property of a reasonable quantum gravity theory, that changing the time variable should not modify the physical

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content of the theory. However, within the reduced phase space approach, where we use a particular foliation for $\mathcal{M}$, considered in the present paper we explicitly show that this seemingly reasonable property does not necessarily hold once the system is quantized. Let us briefly overview the reason why this happens, postponing a more detailed description to the later sections.

The key observation to make here is that the gauge-invariant content of a constrained theory, such as canonical general relativity, comprises expressions solely in terms of gauge-invariant variables, defined as quantities that commute with the constraints; they are called Dirac observables. Since the Hamiltonian in canonical relativity is a constraint itself, no dynamical variable can be gauge invariant as none can commute with the Hamiltonian constraint. As a result, dynamical variables are not equipped with a well-defined Poisson structure, and this forbids straightforward quantization. As discussed above, one way to circumvent this difficulty is to introduce a foliation with an internal time variable which, by assumption, commutes with all the Dirac observables. This way, the internal time and all the dynamical quantities, which are functions of Dirac observables, can be included in the reduced phase space formalism. An immediate consequence of this prescription is that the commutation relations involving dynamical variables depend on the choice of internal time.

Another idea to circumvent the conceptual difficulty discussed above is expressed in the idea of evolving constants [13–15]. This approach relies on the observation that Dirac observables, though nondynamical themselves, could in fact be seen as particular functions of dynamical variables and therefore encoding the dynamics as relations between these variables. For instance, the value of a dynamical quantity X when another dynamical quantity Y takes the value $y = y_0$ is constant along any dynamical trajectory and is thus a Dirac observable. In this way, the entire dynamical trajectory of X is given by a y-parametrized family of Dirac observables. As far as we can tell, such an approach does not contradict that presented below. We note that the values of a dynamical quantity X when another dynamical quantity Z takes the values $z = z_0$ form a different, now z-parametrized, family of Dirac observables. Hence, for a fixed quantization of Dirac observables, the y and z families may exhibit different quantum properties though they describe the dynamics of the same dynamical observable, X. Therefore, it is meaningful to speak about dynamical observables at the quantum level only with respect to specific internal time variables.

In this paper, we discuss the quantization of the vacuum Bianchi I case, showing how it generates a time whose arbitrariness in the definition produces a clock-choice issue. We discuss some choices (fast and slow gauge times), and this leads to a possible criterion: some clocks, upon quantization of the system, are singularity free, while others do exhibit a singularity. By imposing a specific

ordering of the operators in the Hamiltonian, we can put the latter in a canonical form and obtain exact singularity-free solutions for the average trajectories. We provide a clear illustration of the dependence of quantum dynamics on the choice of internal time. Surprisingly, we identify a certain property of quantum gravitational dynamics which does not depend on the choice of internal time and points to a possible solution of the time problem.

II. EMPTY BIANCHI I

Our starting point is the vacuum GR gravitation theory, whose classical Einstein-Hilbert action $\mathcal{S}$ reads, in units with $8\pi G_N = 1$,

$$\mathcal{S} = \frac{1}{2} \int R\sqrt{-g}\,\mathrm{d}^4 x. \tag{1}$$

This theory admits the Bianchi I metric, given in terms of the lapse function N by

$$\mathrm{d}s^2 = -N^2\mathrm{d}\tau^2 + \sum_{i=1}^{3} a_i^2(\mathrm{d}x^i)^2, \tag{2}$$

as a solution of the corresponding vacuum Einstein equations for a flat homogeneous but anisotropic spacetime.

The scale factors associated to each direction can be recast as [16]

$$a_1 = e^{\beta_0 + \beta_+ + \sqrt{3}\beta_-}, \tag{3}$$

$$a_2 = e^{\beta_0 + \beta_+ - \sqrt{3}\beta_-}, \tag{4}$$

$$a_3 = e^{\beta_0 - 2\beta_+}, \tag{5}$$

where we introduced the anisotropy variables $\beta_\pm$ and β_0, the latter providing the volume V of the manifold, assumed compact, through

$$V \equiv a_1 a_2 a_3 = e^{3\beta_0}. \tag{6}$$

The action $\mathcal{S}$ for the metric (2) reads

$$\mathcal{S} = \int \mathrm{d}\tau(p_0\dot\beta_0 + p_+\dot\beta_+ + p_-\dot\beta_- - NC), \tag{7}$$

where the Hamiltonian $H = NC$ is such that the constraint C satisfies

$$C = \frac{e^{-3\beta_0}}{24}(-p_0^2 + p_+^2 + p_-^2). \tag{8}$$

The canonical one-form can be read directly from Eq. (7) as

$$\mathrm{d}\theta = p_0\mathrm{d}\beta_0 + p_+\mathrm{d}\beta_+ + p_-\mathrm{d}\beta_-. \tag{9}$$

In terms of this one form the action is

$$S = \int d\tau \left(\frac{d\theta}{d\tau} - NC \right). \tag{10}$$

The volume variable V turns out to be more convenient than β_0. One has

$$d\beta_0 = \frac{e^{-3\beta_0}}{3} dV, \tag{11}$$

and the new momentum associated to it has to be

$$p_V \equiv \frac{e^{-3\beta_0}}{3} p_0, \tag{12}$$

in order to keep the one-form canonical, i.e.,

$$d\theta = p_V dV + p_+ d\beta_+ + p_- d\beta_-. \tag{13}$$

Using this new variable the constraint (8) is written as

$$C = \frac{3V}{8} \left(-p_V^2 + \frac{p_+^2 + p_-^2}{9V^2} \right). \tag{14}$$

This constrained system must classically satisfy

$$C = 0, \tag{15}$$

the quantization of which we turn to below.

Let us first parametrize the above problem explicitly, and to achieve that goal first rewrite the problem using variables that evince the system symmetries. The variables $\beta_\pm$ are clearly cyclic, and therefore their momenta are conserved, i.e.,

$$\dot{p}_\pm = 0. \tag{16}$$

To avoid carrying these two constants around we perform the transformation

$$p_+ = k \cos \alpha, \qquad p_- = k \sin \alpha, \tag{17}$$

where we can choose $k > 0$ without loss of generality. Ensuring the one-form remains canonical, we obtain

$$d\theta = p_V dV + p_k dk + p_\alpha d\alpha + \text{S.T.}, \tag{18}$$

where we defined the new two momentum variables

$$p_k \equiv -(\cos \alpha \beta_+ + \sin \alpha \beta_-), \tag{19}$$

$$p_\alpha \equiv (k \sin \alpha \beta_+ - k \cos \alpha \beta_-), \tag{20}$$

and the surface term S.T. $= d(k \cos \alpha \beta_+ + k \sin \alpha \beta_-)$ in Eq. (18) is an exact form, which we can and thus do ignore

from here on. Note also that neither p_α nor α appears in the Hamiltonian and consequently both are constant. We thus also ignore them.

In terms of the above variables, our system is described by the action (10), where the canonical one-form and the constraint are

$$d\theta = p_V dV + p_k dk, \tag{21}$$

$$C = \frac{3V}{8} \left(-p_V^2 + \frac{k^2}{9V^2} \right). \tag{22}$$

III. PARAMETRIZING THE PROBLEM

The system action (10) is constrained. The lapse function N acts as a Lagrange multiplier and imposes that $C = 0$. It turns out that one can solve this constraint explicitly and then obtain a parametrized Hamiltonian. While this is a trivial recasting of the classical problem, when we move to quantization this has a nontrivial effect. The parametrization of the problem involves turning one of its d.o.f. in a monotonically evolving variable which, upon quantization, acts as a time in the corresponding Schrödinger equation. It therefore acquires a different status than the other variables: with a physical clock (which in our case is internal to the system) thus defined, this entails the existence of a time parameter related to that particular clock, in terms of which one derives the evolution of the dynamical variables.

Before starting with the parametrization, it is useful to study the Hamilton equations of motion of our problem. They read

$$\dot{k} = 0,$$

$$\dot{p}_k = -\frac{k}{12V} N,$$

$$\dot{V} = -\frac{3V p_V}{4} N,$$

$$\dot{p}_V = -\left[\frac{3}{8} \left(-p_V^2 + \frac{k^2}{9V^2} \right) - \frac{k^2}{12V^2} \right] N, \tag{23}$$

together with the constraint

$$\frac{3V}{8} \left(-p_V^2 + \frac{k^2}{9V^2} \right) = 0. \tag{24}$$

Since $V \neq 0$, Eqs. (23) reduce to

$$\dot{k} = 0 \quad \text{and} \quad \dot{V} = -\frac{3V p_V}{4} N, \tag{25}$$

for the variables, and

$$\dot{p}_k = -\frac{k}{12V} N \quad \text{and} \quad \dot{p}_V = \frac{3 p_V^2}{4} N \tag{26}$$

for the associated momenta.

The system above is closed for p_V and V and therefore can be solved first for these two variables and then for k and p_k (when one has to impose the constraint above when choosing the initial conditions for k and p_k).

A. Reduced phase space and choice of time

Thus far, we have not chosen the time variable τ appearing in the line element (2), and indeed the above problem can be solved for any choice of this time, and hence of the lapse function N. Indeed, in the previous section, we wrote the equations of motion as derived from the Hamiltonian as first order in time, which we called "τ" but otherwise left undefined, merely assuming there exists such an ordering of events labeling. In order to move forward, we need to be more specific in the choice of this time variable.

Classically, one can define/choose a time parametrization by solving the constraint directly in the one-form $d\theta$: using $k^2 = 9p_V^2 V^2$ (note that we do not have an ambiguity in choosing the sign of k since we have assumed $k > 0$), we obtain

$$d\theta = p_V dV + \frac{p_k}{2k} dk^2 = p_V dV + \frac{9p_k}{2k} d(V^2 p_V^2). \quad (27)$$

Now, one can easily reduce the one-form above to a single term,

$$d\theta = \left(\frac{9p_k}{k} - \frac{\ln V}{V p_V} \right) d\left(\frac{V^2 p_V^2}{2} \right) + \text{S.T.}, \quad (28)$$

and ignoring the surface term S.T. $= d(V p_V \ln V)$ since it does not contribute to the action, we get

$$d\theta = -\frac{V^2 p_V^2}{2} d\Upsilon, \quad (29)$$

where we removed another surface term $d(\Upsilon V^2 p_V^2 / 2)$, and set

$$\Upsilon \equiv \frac{9p_k}{k} - \frac{\ln V}{V p_V}; \quad (30)$$

both Υ and $(V p_V)$ are constants of the motion.

Let us introduce an arbitrary function of the dynamical variables $T(V, p_V, p_k)$, through which we define a time t

$$t = \Upsilon + T(V, p_V, p_k), \quad (31)$$

which also thus depends on the dynamical variables. Setting

$$Q \equiv V p_V T, \quad (32)$$

$$p_Q \equiv V p_V, \quad (33)$$

and plugging (32) and (33) into (29), we get

$$d\theta = P_Q dQ - \frac{p_Q^2}{2} dt, \quad (34)$$

where we again removed a surface term $-\frac{1}{2} d(p_Q Q)$. We note that the role of the phase space function T is twofold: it defines both the time parameter t and the position variable Q.

A given choice of T therefore implies, once the equations of motion are solved, a classical solution $Q(t)$. Assuming one can invert this relation, one can thus find the interval over which the corresponding time parameter varies. As the dynamics of the system is that of a freely moving particle independently of the choice of T, the ranges of Q and t must be related. Many cases are then possible, depending on whether Q and t are bounded or unbounded. If the range of Q is real ($Q \in \mathbb{R}$), then the motion is unbounded and the singularity is never reached. If, on the other hand, the range of Q contains a finite limit, say $Q \in [Q_0, \infty]$ for instance, then the motion originates/terminates at $Q = Q_0$ in a finite time and the dynamics is singular. Indeed, from (32) and (33) we obtain the singularity time as $t_0 = \Upsilon + Q_0/p_Q$. The former case is dubbed the fast-gauge time because the relevant clock ticks an infinite number of times before reaching the singularity, whereas the latter is known as the slow-gauge time. We see below examples of both situations. In both cases the time variable t is globally well defined in the sense that it is always growing as the particle approaches or recedes from the boundary (or, minus infinity). We notice that any given value of the fast-gauge clock is taken twice: once for the expanding and once for the contracting universe, whereas any given value of the slow-gauge clock is taken only once: either in the expanding or contracting universe, depending on whether $t > t_0$ or $t < t_0$. As we see, this property of slow-gauge clocks enables one to remove the singularity by quantization while extending the time variable across t_0. In order to have a single point t_0 of the time axis correspond to the singularity, we choose T such that $Q_0 = 0$.[1]

B. Fast-gauge time τ

Let us first consider a fast-gauge time example and assume that

$$T_{\text{fast}} = \frac{\ln V}{V p_V}, \quad (35)$$

which diverges for $V \to 0$. From (32), we see that the relevant canonical variable is $Q_{\text{fast}} = \ln V$ for a time defined through (31), namely, $t_{\text{fast}} = 9p_k/k$, which is

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[1] Otherwise we would have a whole interval of values of t for which the system is singular.

indeed monotonically related to the original time. We expand below on the properties of this choice.

1. Classical time choice

We begin by noting that it is possible to rewrite the equation for p_k as

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\left(9\frac{p_k}{k}\right) = -\frac{3}{4}\frac{N}{V}, \tag{36}$$

implying, as stated above, that the quantity $9p_k/k$ is a monotonic function of the arbitrary time τ appearing in the metric (2), as V is positive definite and N is non-vanishing, and hence either always positive or always negative. As a result, the quantity $9p_k/k$ can itself be used as a time parameter. Assuming this is the case, we choose $\tau = t_{\mathrm{fast}} = 9p_k/k$, which agrees with our general framework (31) with the fast-gauge time function T_{fast} from (35), leading to the following lapse function:

$$N = -\frac{4}{3}V < 0. \tag{37}$$

This clearly shows that this choice of time parameter is globally well defined.

For the sake of clarity, we repeat below the steps of Sec. III A, starting directly with the action. As we have seen above, solving the constraint directly in the one-form $\mathrm{d}\theta$ using $k^2 = 9p_V^2 V^2$ leads to (27), and therefore to

$$\mathrm{d}\theta = p_V \mathrm{d}V + \mathrm{d}\left(\frac{9p_k}{2k}V^2 p_V^2\right) - \frac{V^2 p_V^2}{2}\mathrm{d}\left(\frac{9p_k}{k}\right). \tag{38}$$

We can again safely ignore the exact form above since it will not contribute to the equations of motion. Since we solved the constraint the action is now merely given by

$$\mathcal{S} = \int \mathrm{d}\theta = \int \mathrm{d}\tau\left(p_V \dot{V} - \frac{V^2 p_V^2}{2}\right), \tag{39}$$

where we simply relabeled $\tau \equiv 9p_k/k$. This is an unconstrained one-dimensional system whose dynamics stems from the Hamiltonian $H = V^2 p_V^2/2$.

It is now a simple matter to check that the Hamilton equations are indeed those obtained earlier. Indeed, they read

$$\dot{V} = V^2 p_V, \qquad \dot{p}_V = -V p_V^2, \tag{40}$$

which are the correct equations of motion after substitution of the lapse (37) in Eqs. (25) and (26). Once the equations for V and p_V are solved, we can use the constraint (24) to obtain k^2. Finally, since $\tau = 9p_k/k$, we can determine both quantities

$$k = 3V|p_V|, \qquad \text{and} \qquad p_k = \frac{k\tau}{9}. \tag{41}$$

We note that in the proposed internal time $\tau = 9p_k/k$, the classical dynamics is completely determined as the solution to Eq. (40) reads

$$\frac{\mathrm{d}}{\mathrm{d}\tau}(Vp_V) = 0 \Rightarrow Vp_V = V_0 p_{V0}, \tag{42}$$

and

$$V = V_0 e^{(Vp_V)\tau} \qquad \text{and} \qquad p_V = p_{V0}e^{-(Vp_V)\cdot\tau}. \tag{43}$$

The singularity is pushed to $\tau \to \pm\infty$ for expanding and contracting universes, respectively. These sorts of internal times are sometimes called fast-gauge times, while the slow-gauge times are those in which the dynamics terminates at finite values. It has been conjectured [17] that the canonical quantization cannot resolve the singularity problem in fast-gauge times since the Hamiltonian flow is complete in this case. Although the relation between the singularity resolution and the choice of time might be a more subtle issue [18], it seems to us that using the fast-gauge internal time chosen above can indeed not prevent the appearance of a singularity even in the quantum case. Let us illustrate this point.

2. Quantum dynamics

The Hamiltonian derived from the action (39) and acting on the half-plane phase space $(V, p_V) \in \mathbb{R}_+ \times \mathbb{R}$ can be promoted to a symmetric operator on a suitable dense subspace of the Hilbert space of square-integrable functions on the half-line, $L^2(\mathbb{R}_+, \mathrm{d}V)$.[2] One can choose the symmetric ordering

$$H = \frac{1}{2}V^2 p_V^2 \mapsto \hat{H} = \frac{1}{2}\sqrt{V}\frac{1}{i}\partial_V\sqrt{V} \cdot \sqrt{V}\frac{1}{i}\partial_V\sqrt{V}. \tag{44}$$

In order to understand the quantum dynamics generated by the above Hamiltonian, we make a coordinate transformation from the half-line to the real line, $V \mapsto Q_{\mathrm{fast}} = \ln V \equiv Z$. The corresponding unitary map between the respective Hilbert spaces, $U\colon L^2(\mathbb{R}_+, \mathrm{d}V) \mapsto L^2(\mathbb{R}, \mathrm{d}Z)$, reads

$$\int_{\mathbb{R}_+} |\psi(V)|^2 \mathrm{d}V = \int_{\mathbb{R}} |(U\psi)(Z)|^2 \mathrm{d}Z \Rightarrow \psi(V) \mapsto (U\psi)(Z)$$
$$= e^{\frac{Z}{2}}\psi(e^Z). \tag{45}$$

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[2]The measure $\mathrm{d}V$ is chosen so that $\hat{V} = V$ and $\hat{p}_V = -i\partial_V$ are symmetric operators provided the wave functions vanish both at $V = 0$ and at $V \to \infty$. One could include an arbitrary function of the volume in the definition of the measure such as, e.g., the scale factor $a = V^{1/3}$ and correspondingly modify the definition of the relevant operators; such a choice would however merely complicate matters with no physically meaningful difference.
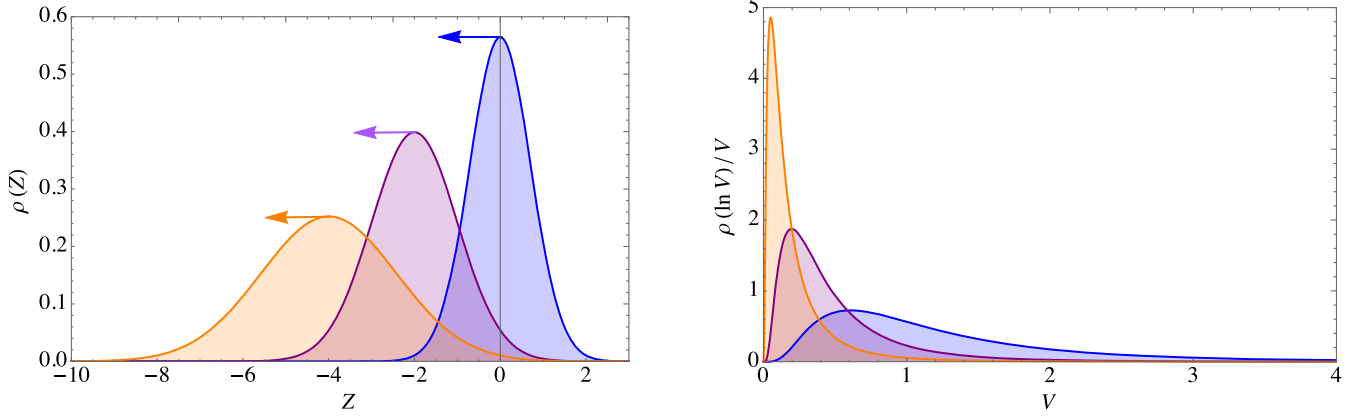
FIG. 1. The fast-gauge evolution of the probability distribution for a Gaussian packet on the real line Z (left panel) for $k = -1$, $\tau = 0$, 2, 4 and the respective packet to the half-line V (right panel) for $k = -1$ and $\tau = 0$, 1, 2. Because of the packet spreading, the probability density can initially grow with time for any sufficiently large V. Nevertheless, the probability of finding the system on the interval $[0, \epsilon]$ for any $\epsilon > 0$ tends to 1 as $\tau \to \infty$ and thus, the distribution converges to $\delta(0)$. Notice that for every value of τ the probability vanishes at $V = 0$.

It is straightforward to find that

$$\left(\sqrt{V} \frac{1}{i} \partial_V \sqrt{V} \right) \psi(V) = e^{-\frac{Z}{2}} \frac{1}{i} \partial_Z e^{\frac{Z}{2}} \psi(e^Z), \quad (46)$$

leading to

$$U \left(\sqrt{V} \frac{1}{i} \partial_V \sqrt{V} \right) U^{-1} = \frac{1}{i} \partial_Z, \quad (47)$$

and hence

$$\int_{\mathbb{R}_+} \psi^*(V) H(V) \psi(V) dV$$
$$= \int_{\mathbb{R}} |(U\psi)(Z)|^* (UHU^\dagger)(U\psi)(Z) dZ \Rightarrow U\hat{H}U^{-1}$$
$$= -\frac{1}{2} \partial_Z^2, \quad \text{and} \quad Z \in \mathbb{R}. \quad (48)$$

It is now clear that the Hamiltonian (44) must be essentially self-adjoint and the unique dynamics it generates is unbounded with wave packets approaching the singularity $Z \to -\infty$ (i.e., $V \to 0$) as $\tau \to \pm\infty$, depending on the initial condition. Figure 1 illustrates the fast-gauge evolution of the probability distribution $\rho(Z, \tau) \equiv |\psi(Z, \tau)|^2$ carried by a Gaussian wave packet as it approaches the singularity, $Z \to -\infty$,

$$\rho(Z, \tau) = \frac{1}{\sqrt{\pi(1 + \tau^2/4)}} \exp\left[-\frac{(Z - k\tau)^2}{1 + \tau^2/4} \right], \quad (49)$$

which when mapped onto the half-line reads $\rho(\ln V, \tau)/V$ and approaches the Dirac delta picked at $V = 0$. As the

singularity does not seem to be avoided in the present case let us now turn to considering a slow-gauge internal time.

C. Slow-gauge time η

Let us now consider another transformation, using the function

$$T_{\text{slow}} = \frac{1}{p_V}, \quad (50)$$

whose limit is well defined when $V \to 0$: since $V p_V = p_Q$ is a constant, we must have $p_V \to \pm\infty$, and thus $T_{\text{slow}} \to 0^\pm$. The choice (50) translates into $t_{\text{slow}} = \Upsilon + 1/p_V$ and $Q_{\text{slow}} = V$, again monotonically related to the original time. Now t_{slow} is not defined in the full real line, but only in two separate branches, namely, $t_{\text{slow}} \in [\Upsilon, \infty[$ if $p_V > 0$ or $t_{\text{slow}} \in] -\infty, \Upsilon]$ for $p_V < 0$. This entails a contracting universe ending at a singularity, or an expanding one originating from a singularity. The complete solution is then given by

$$V = p_Q(t_{\text{slow}} - \Upsilon). \quad (51)$$

Let us develop these points.

As before, we solve the constraint directly in the one-form $d\theta$, now using a different parametrization, namely

$$d\theta = (V p_V) dV - \left(\frac{V^2 p_V^2}{2} \right) d\left(\frac{9 p_k}{k} + \frac{V - \ln V}{V p_V} \right)$$
$$+ d\left(\frac{9 p_k}{2k} V^2 p_V^2 + \frac{1}{2} V \ln V p_V - \frac{1}{2} V^2 p_V \right). \quad (52)$$

We can again safely ignore the exact form above since it does not contribute to the equations of motion. Then, since we solved the constraint the action is given by

$$S = \int d\theta = \int d\eta \left(V p_V \acute{V} - \frac{1}{2} V^2 p_V^2 \right), \qquad (53)$$

where we introduced the notation $\acute{V} \equiv dV/d\eta$ and simply relabeled the new time variable η through

$$\eta \equiv \frac{9 p_k}{k} + \frac{V - \ln V}{V p_V} = t_{\text{slow}}, \qquad (54)$$

which one can directly check indeed satisfies the requirements for being a time, in the sense that it is a monotonic function: using the equations of motion (25) and (26), one readily obtains

$$\frac{d}{d\tau} \left(\frac{9 p_k}{k} + \frac{V - \ln V}{V p_V} \right) = -\frac{3}{4} N. \qquad (55)$$

Note that the unconstrained Hamiltonian again is just $H = \frac{1}{2} V^2 p_V^2$. However, unlike in the previous case, Eq. (53) shows that it is now $p_V V$ and not p_V anymore that plays the role of the canonically conjugate momentum to the volume V. This seemingly innocuous fact actually drastically transforms the problem as upon introducing a new canonical variable, $\pi_V = p_Q = p_V V$, the Hamiltonian H again becomes that of a freely moving particle, but in this case the dynamics is limited to the half-line,

$$H = \frac{1}{2} \pi_V^2, \qquad \{V, \pi_V\} = 1, \quad \text{where } (V, \pi_V) \in \mathbb{R}_+ \times \mathbb{R}. \qquad (56)$$

The dynamics therefore terminates at a finite value of η, forwards/backwards in time for contracting/expanding universes, respectively. As we show in the next section, in this case the singularity can be resolved by quantization of the Hamiltonian formalism.

D. Other time variables η'

It is worth noting that there are many more allowed choices of time variable when we parametrize the system. Let us consider a new internal time,

$$\eta' = \eta'(\eta, V, \pi_V), \qquad (57)$$

and redefine the dynamical variables,

$$\pi_V' = \pi_V, \qquad V' = V + \pi_V(\eta' - \eta). \qquad (58)$$

Then Eq. (52) without the exact form is

$$d\theta = \pi_V dV - \frac{\pi_V^2}{2} d\eta = \pi_V' dV' - \frac{\pi_V'^2}{2} d\eta' + d\left[(\eta - \eta') \frac{\pi_V'^2}{2} \right]. \qquad (59)$$

Since the exact form can be again ignored, the last expression above shows that the formulation of the dynamics in a new internal time (57) is *formally* identical to the initial formulation provided that Eq. (58) holds. This property has significant practical value as now it suffices to quantize *one* formalism in order to obtain quantum formulation in *any* internal time remembering that the basic variables may have different physical meaning for different choices of time.

Note that the general transformation (57) and (58) includes transformations to fast-gauge clocks, the situation that we want to avoid. Indeed, writing the difference between the new and old time variables, thereby defining the delay function $\Delta = \eta' - \eta$ from now on, we find that one goes from the slow to the fast-gauge times through

$$\Delta_{\text{slow}\to\text{fast}} = \frac{V - \ln V}{V p_V}, \qquad (60)$$

whose limit diverges when $V \to 0$. In order to ensure that such a situation never occurs, we assume the transformation does not alter the ranges of basic variables; i.e., we demand that

$$0 < V' = V + \pi_V \Delta < \infty. \qquad (61)$$

If we furthermore assume that the delay function depends on the phase space only, i.e.,

$$\Delta = \Delta(V, \pi_V), \qquad (62)$$

the transformation (58) does not involve time variables. This largely simplifies comparison between different time variables dynamics. Note that the new time variable is monotonic if and only if

$$\frac{d\eta'}{d\eta} = \frac{\partial \eta'}{\partial \eta} + \{\Delta, H\} = \frac{\partial \eta'}{\partial \eta} + \left\{ \Delta, \frac{1}{2} \pi_V^2 \right\} \neq 0, \qquad (63)$$

i.e.,

$$\frac{\partial \Delta}{\partial \eta} + 1 + \pi_V \frac{\partial \Delta}{\partial V} \neq 0, \qquad (64)$$

which in the simpler case $\partial\Delta/\partial\eta = 0$ yields

$$\frac{\partial V'}{\partial V} \neq 0. \qquad (65)$$

Observe that this condition is equivalent to simply assuming that the time transformation (57) and (58) is C^1-invertible, ensuring that the canonical one-form $d\theta$ in both parametrizations is identical (up to a total derivative).

IV. QUANTIZATION IN THE SLOW-TIME GAUGE

Quantization of the half-plane phase space $(V, \pi_V) \in \mathbb{R}_+ \times \mathbb{R}$ is not an obvious task.[3] The problem occurs because π_V does not generate a global translation on that phase space and the respective operator, $-i\partial_V$ on the half-line $V > 0$, admits no self-adjoint extension. Nevertheless, the square of this operator, i.e., the (minus) Laplacian, can be given a self-adjoint extension (in fact, it admits uncountably infinite many such extensions).

There are many ways to obtain a unitary evolution with the Laplacian, and Sec. IV B emphasizes one involving reordering of the basic operators, making use of the commutation relations to produce a "naturally" self-adjoint Hamiltonian. Another, perhaps more straightforward, method, which we discuss below, consists in restricting the action of the Laplacian to functions that satisfy the Dirichlet condition at the boundary $V = 0$,

$$-\triangle_D \psi(V) = -\triangle \psi(V) \quad \text{for } \psi(0) = 0, \qquad (66)$$

and then to close the operator $-\triangle_D$ in $L^2(\mathbb{R}_+, dV)$. It can be shown that the generalized eigenfunctions are

$$\psi_\lambda(V) = e^{i\sqrt{\lambda}V} - e^{-i\sqrt{\lambda}V}, \qquad \lambda \in \mathrm{Sp}(-\triangle_D) = \mathbb{R}_+, \qquad (67)$$

and the propagator reads

$$G_D(\eta, V, V') = \frac{\exp\left[-\frac{(V-V')^2}{4i\eta}\right]}{\sqrt{4\pi i\eta}} - \frac{\exp\left[-\frac{(V+V')^2}{4i\eta}\right]}{\sqrt{4\pi i\eta}}, \qquad (68)$$

taking the original wave function from 0 to η.

A. Comparison with fast-time gauge

Let us consider an initial wave function given by a Gaussian wave packet centered at V_0 with standard deviation σ and initial phase ikV, namely

$$u_0(V) = \frac{1}{\sqrt{\sqrt{2\pi}\sigma}} \exp\left[-\frac{(V-V_0)^2}{4\sigma^2} + ikV\right]. \qquad (69)$$

In order for this waveform to satisfy the Dirichlet boundary condition at $V = 0$ and thus be an acceptable initial wave function, we consider its odd part, i.e.,

$$\psi_0(V) = \frac{u_0(V) - u_0(-V)}{\mathcal{N}}, \qquad (70)$$

where the normalization is given by

$$\mathcal{N} = \sqrt{1 - \exp\left(-\frac{V_0^2 + 4k^2\sigma^4}{2\sigma^2}\right)}. \qquad (71)$$

Applying the propagator to this wave function gives us

$$\psi(V, \eta) = -\frac{2\exp\left(-ik^2\eta - \frac{V^2 + V_\eta^2}{4\sigma\sigma_\eta}\right)}{\mathcal{N}(2\pi)^{1/4}\sqrt{\sigma_\eta}} \sinh\left(\frac{VV_\eta}{2\sigma\sigma_\eta} + ikV\right), \qquad (72)$$

where $V_\eta = V_0 + 2k\eta$ and $\sigma_\eta = \sigma + i\eta/\sigma$. Rewriting the sinh above in terms of exponentials, it is easy to see that we can complete the square in each exponent resulting in the following expression:

$$\psi(V, \eta) = \frac{\exp\left[+ik(V - k\eta) - \frac{(V - V_\eta)^2}{4\sigma\sigma_\eta}\right]}{\mathcal{N}(2\pi)^{1/4}\sqrt{\sigma_\eta}}$$
$$- \frac{\exp\left[-ik(V + k\eta) - \frac{(V + V_\eta)^2}{4\sigma\sigma_\eta}\right]}{\mathcal{N}(2\pi)^{1/4}\sqrt{\sigma_\eta}}. \qquad (73)$$

The above wave function (73) solves the Schrödinger equation corresponding to a freely moving particle on the half-line with the Hamiltonian $-\triangle_D$ with respect to our time variable η, namely

$$i\frac{\partial}{\partial\eta}\psi = -\triangle_D\psi. \qquad (74)$$

Disregarding the different phases, we end up with a linear combination of two Gaussian wave packets centered on
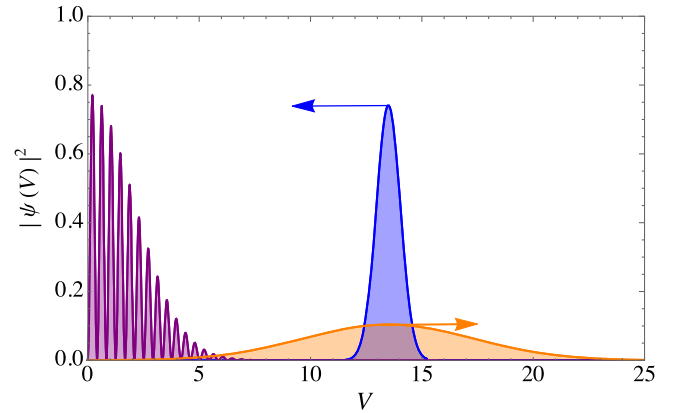

FIG. 2. The bouncing of a Gaussian wave packet against the end point $V = 0$ assuming the Dirichlet boundary condition. The wave packet momentum is $k = 7.5$ and times are as Fig. 1. The packet starts centered around $V_0 = 15$ and variance $\sigma = 1/2$ (arrow to the left); after one unit of time it reaches the boundary where it interferes with itself and after two units of time it returns to its initial position, though with larger spreading (arrow to the right).

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[3]Here and in what follows, we made a further canonical transformation, namely $\pi_V \to \sqrt{2}\pi_V$ and $V \to V/\sqrt{2}$, thus, removing the factor of one half from the Hamiltonian.

$V_\pm(\eta) = \pm(V_0 + 2k\eta)$ with spreading variance $\sigma(\eta) = \sqrt{\sigma^2 + \eta^2/\sigma^2}$. Its evolution is shown in Fig. 2. Contrary to the fast-gauge time, the boundary is now reached by the wave packet within a finite time interval, which must bounce in order to preserve the unitarity.

The quantum model presented here with $\hat{H} = -\Delta$ is based on an implementation of canonical quantization rules in the case of the half-line. This approach, however, is not fully satisfactory as it assumes the momentum on the half-line, $(-i\partial_V)$, to be one of the basic operators despite the fact that it is not a self-adjoint operator. As a related problem, the quantum Hamiltonian, $-\Delta$, is not an essentially self-adjoint operator either; therefore its domain is confined to a certain dense subspace of the full Hilbert space of the model and its action beyond this restricted domain is redefined in order to make it self-adjoint. This procedure is highly ambiguous and produces a significant technical inconvenience: once the action of $\hat{H}$ is redefined, its commutation with other operators can no longer be determined from its representation as a differential operator, i.e., as $-\Delta$. This is a drawback because, as we show below, by making use of commutation rules, one is able to prove the existence of a symmetry in the quantum dynamics of the Bianchi I model, which enables one to immediately obtain the evolution of some operators.

Therefore, in what follows, we implement *affine quantization* in which the nonself-adjoint momentum operator is replaced with the self-adjoint dilation operator,[4] $D \equiv \frac{1}{2}(V\frac{1}{i}\partial_V + \frac{1}{i}\partial_V V)$. The dilation and position operators provide two basic operators from which any compound operator such as the Hamiltonian can be obtained. In this case one is faced with the ordering issue. Nevertheless, all the orderings are shown to produce the same form of the quantum Hamiltonian and a wide class of them are self-adjoint operators which produce a unique dynamics and can be represented as differential operators.

B. Affine quantization

Our Hamiltonian thus reduces to π_V^2, which can be classically expressed in terms of the symmetric combination $D \equiv \frac{1}{2}(V\pi_V + \pi_V V)$ as $\pi_V^2 \sim D^2/V^2$. Upon quantization, it is well known that this leads to an ambiguity as the order of the corresponding operators becomes relevant.

Indeed, with the canonical commutation relation $[\hat{V}, \hat{\pi}_V] = i$, one finds $[\hat{V}, \hat{D}] = i\hat{V}$, so that one can express the Hamiltonian in the symmetric form

$$\hat{H} = \hat{V}^\alpha \hat{D}\hat{V}^\beta D\hat{V}^\alpha \quad \text{with} \quad 2\alpha + \beta = -2, \quad (75)$$

for generic values of α. Using the commutation relation

$$[\hat{V}^\alpha, \hat{D}] = i\alpha\hat{V}^\alpha$$

to move all the $\hat{V}$ factors to the left, and going back to $\hat{\pi}_V$ in the final result, leads to

$$\hat{H} = \hat{\pi}_V^2 + \frac{\mathcal{K}(\alpha)}{\hat{V}^2} \quad \text{with} \quad \mathcal{K}(\alpha) \equiv \alpha^2 + 2\alpha + \frac{3}{4}. \quad (76)$$

It turns out this new Hamiltonian is essentially self-adjoint if $\mathcal{K}(\alpha) > \frac{3}{4}$ (see Ref. [19], page 161), i.e., for $\alpha > 0$ or $\alpha < -2$. We assume in what follows that α is chosen to ensure the required self-adjointness of the Hamiltonian.[5] The appendix shows that the wave packet behavior in this case is essentially the same as that illustrated on Fig. 2, Eq. (A9) showing the generalization for $K(\alpha) \neq 0$ of Eq. (73).

Let us note at this point that one could expect self-adjointness to be naturally derived from some other physically justified assumptions and not, as we are here proposing, imposed as a mathematical input. One could however argue in the opposite direction: consider for instance the simple case of the Hydrogen atom. Applying the correspondence principle to the classical Hamiltonian already yields a self-adjoint operator whose quantization permits one to calculate the energy levels and compare those with data. Expanding the electron momentum operator into radial and angular components, one could apply our ordering procedure to find an extra potential of the form C/r^2, the arbitrary constant C being then fixed by comparison of the resulting (different) energy levels with the data. One could then argue that the operator ordering choice can be determined experimentally, even in situations where the original Hamiltonian is already self-adjoint.

C. General time evolution

Let us begin by working in the Heisenberg representation and discuss time evolution of the relevant operators. Using the usual relation $[\hat{\pi}_V, f(\hat{V})] = -i\frac{\mathrm{d}f(\hat{V})}{\mathrm{d}\hat{V}}$ together with the commutation relations $[\hat{\pi}_V, \hat{H}] = 2iK\hat{V}^{-3}$ and $[\hat{V}, \hat{H}] = 2i\hat{\pi}_V$, one readily finds that the algebra made with $\hat{V}^2$, $\hat{D}$ and $\hat{H}$ is closed, namely

$$\begin{cases} [\hat{V}^2, \hat{H}] = 4i\hat{D}, \\ [\hat{D}, \hat{H}] = 2i\hat{H}, \\ [\hat{V}^2, \hat{D}] = 2i\hat{V}^2, \end{cases} \quad (77)$$

leading to the Heisenberg equations of motion for the time development of the operators, namely

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[4]The name affine is due to the fact that the dilation and position operators generate the unitary irreducible representation of the affine group of the real line.

[5]One recovers exactly the same result by assuming the correspondence $\pi_V^2 \mapsto \hat{V}^s \hat{\pi}_V \hat{V}^{-2s} \hat{\pi}_V \hat{V}^s$, leading to a similar potential term: $\pi_V^2 \mapsto \hat{\pi}_V^2 + s\hat{V}^{-2}$, and a self-adjoint Hamiltonian provided $s > 3/4$.
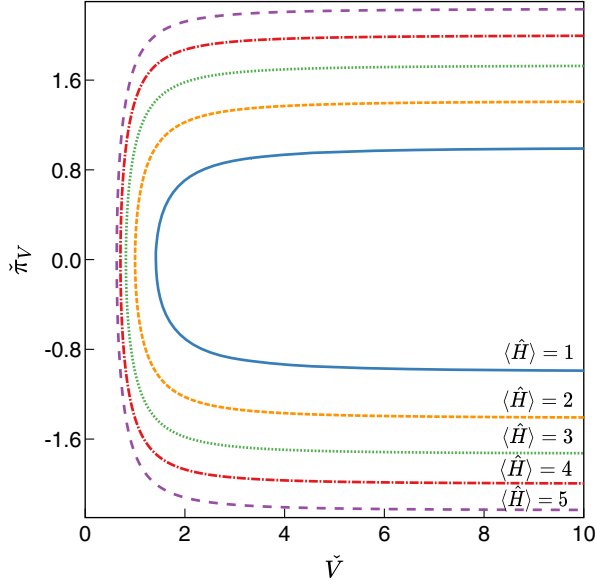
FIG. 3. Effective phase space trajectories (85) for the effective Hamiltonian (86), taking $\langle \hat{H} \rangle \in [1, 5]$ from the inside to the outside of the graph, as indicated, full ($\langle \hat{H} \rangle = 1$), dashed ($\langle \hat{H} \rangle = 2$), dotted ($\langle \hat{H} \rangle = 3$), dot-dashed ($\langle \hat{H} \rangle = 4$) and long-dashed ($\langle \hat{H} \rangle = 5$). We use $\mathcal{K}(\alpha) = 2$ for the plot.

$$\frac{\mathrm{d}}{\mathrm{d}\eta} \hat{V}^2 = -i[\hat{V}^2, \hat{H}] = 4\hat{D}, \tag{78}$$

for the squared volume operator, and

$$\frac{\mathrm{d}}{\mathrm{d}\eta} \hat{D} = -i[\hat{D}, \hat{H}] = 2\hat{H}, \tag{79}$$

with $\hat{H}$ being a constant operator.

Because of the constancy of $\hat{H}$ in time, one can explicitly integrate (79), namely

$$\hat{D}(\eta) = 2\hat{H}\eta + \hat{D}(0), \tag{80}$$

which, once plugged into (78), leads to

$$\hat{V}^2 = 4\hat{H}\eta^2 + 4\hat{D}(0)\eta + \hat{V}^2(0). \tag{81}$$

The expectation values of these operators follow simple trajectories, whatever the state one integrates over. They read

$$\langle \hat{D}(\eta) \rangle = 2\langle \hat{H} \rangle \eta + d_0 \tag{82}$$

where we have set $d_0 \equiv \langle \hat{D}(0) \rangle$, and

$$\langle \hat{V}^2(\eta) \rangle = 4\langle \hat{H} \rangle \eta^2 + 4d_0 + v_0^2, \tag{83}$$

with $v_0^2 \equiv \langle \hat{V}^2(0) \rangle$.

Shifting the time variable to $t = \eta + d_0/(2\langle \hat{H} \rangle)$ and setting $V_0^2 = v_0^2 - d_0^2/\langle \hat{H} \rangle$ (assuming $v_0^2 \langle \hat{H} \rangle \geq d_0^2$), one can now define semiclassical variables $\check{V}(t)$ and $\check{\pi}_V(t)$ through
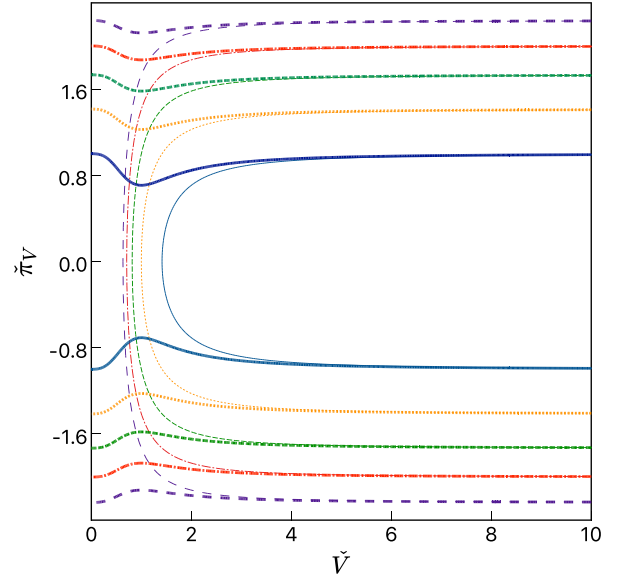

FIG. 4. Same as Fig. 3 after application of the delay function (60). The originally regular trajectories (thin lines) are now all singular (thick lines).

$$\check{V}(t) = \sqrt{\langle \hat{V}^2(t) \rangle} \qquad \text{and} \qquad \check{\pi}_V(t) = \frac{\langle \hat{D}(t) \rangle}{\check{V}(t)}, \tag{84}$$

and finally obtain a set of trajectories in phase space labeled by the arbitrary time t, namely

$$\check{V}(t) = \sqrt{4\langle \hat{H} \rangle t^2 + V_0^2},$$
$$\check{\pi}_V(t) = \frac{2\langle \hat{H} \rangle t}{\sqrt{4\langle \hat{H} \rangle t^2 + V_0^2}}. \tag{85}$$

Each trajectory is thus labeled by two parameters, namely the average value of the Hamiltonian $\langle \hat{H} \rangle$ and the minimum volume V_0, and indeed, we have

$$\langle \hat{H} \rangle = \frac{\check{V}^2(t)\check{\pi}_V^2(t)}{\check{V}^2(t) - V_0^2} = \check{\pi}_V^2(t) + \frac{\mathcal{K}}{\check{V}^2(t)}, \tag{86}$$

provided one sets $\mathcal{K} = \langle \hat{H} \rangle V_0^2$.

It is interesting to realize that the phase portrait for the regular case of the slow-gauge time is transformed, using the delay function (60), into singular solutions: as shown on Fig. 4, all solutions now either terminate in or originate from a singularity $V \to 0$.

D. Comparison of different slow-gauge dynamics

So far we have shown quantization of the model in a single internal time, η. As we have shown in Sec. III D, all other choices of internal time, denoted by η', can lead to formally the same Hamiltonian framework provided that a suitable choice of the new canonical pair, V' and π_V',

defined in Eq. (58), is made. In this case, the quantization introduced in Sec. IV B and the subsequent integration of the quantum motion given in Sec. IV C can be repeated simply by replacing the labels of the canonical variables, $V \rightarrow V'$ and $\pi_V \rightarrow \pi'_V$. Actually, there is a much better reason than mere technical convenience for repeating the quantization in this particular manner: since the Hamiltonian frameworks are formally identical, the constants of motion derived within them must be formally identical functions of the respective basic variables and internal time. Hence, repeating the quantization in all internal times promotes the constants of motion to the

same operators irrespectively of the choice of internal time. On the other hand, the constants of motion enjoy a physical interpretation that must not depend on the particular choice of time. Therefore, the quantization of the system is in this sense unique for all internal frames. One also notices that since the number of elementary constants of motion is equal to the dimensionality of the phase space, the quantization cannot be *more* unique, i.e., it is completely determined by the quantization of the constants.

We expect that, contrary to the case of constants of motion, quantization of dynamical observables in general leads to different operators for different internal times.
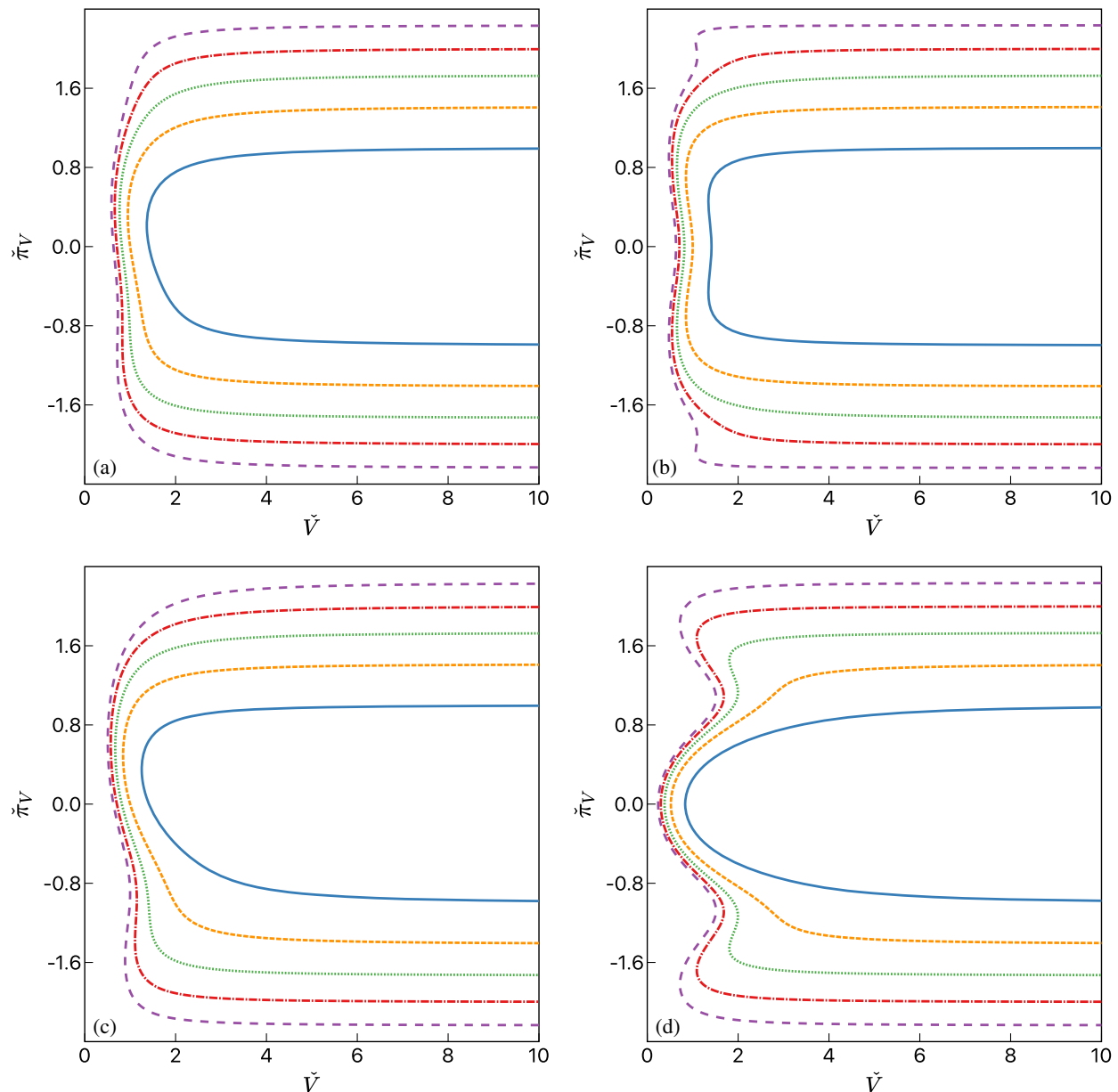

FIG. 5.   Same as Fig. 3 after application of the delay functions $\Delta = V e^{-2|\pi_V|/3} \sin(3V\pi_V)/(10\pi_V)$ (a), $\Delta = V(\pi_V - 10^{-0.2}\pi_V^3 + \pi_V^5/10)$ (b), $\Delta = 10^{-0.5} V \sin(2\pi_V)/\pi_V$ (c) and $\Delta = 10^{-0.5}(V+1)\cos(3\pi_V)/\pi_V$ (d). It can be checked that these delay functions satisfy the requirement (64). The new trajectories happen to be not necessarily symmetric like their counterpart of Fig. 3.

This is the reflection of the fact already mentioned in the introduction that dynamical observables are not gauge invariant in Hamiltonian constraint systems. For a more detailed discussion of these and related issues, we refer the reader to [20].

Let us explain our approach to making the comparison between quantum dynamics in different internal times. First, we note that all quantum dynamics are placed in a single Hilbert space that carries a unique quantum representation of constants of motion. Second, the quantum dynamics viewed as a curve in the Hilbert space is actually unique because the quantum Hamiltonian generating the dynamics is a quantum constant of motion that is unique in all internal times. Third, to describe the quantum dynamics, one needs operators that do not commute with the Hamiltonian and are not quantum constants of motion. However, such operators are exactly the operators which correspond to different physical observables in different internal clocks. Therefore, using the same operator(s) for the purpose of describing the time evolution of the quantum system must be complemented by a physical interpretation of the operator(s), which must depend on the choice of internal time. Hence, formally the same dynamics in the Hilbert space will render different physical portraits for different internal times. The extent to which the physical portraits differ is the result of the choice of internal time and we refer to it as "time effect."

Finally, let us notice that one could instead choose the same physical observable and determine the respective operators in each internal time and then compare the dynamics of these operators. Such an approach, in principle valid, is technically much more involved or even impossible to apply if a given physical observable does not enjoy a self-adjoint representation in a given internal time.

Let us now establish a concrete computational scheme for the comparison method outlined above. Equation (85) defines the semiclassical portrait of the dynamics of the model in terms of $\check{V}$ and $\check{\pi}_V$ in one internal time. As discussed above, the quantization of the same model in another internal time yields the same form of the semiclassical portrait except for that now the coordinates are $\check{V}'$ and $\check{\pi}'_V$ rather than $\check{V}$ and $\check{\pi}_V$. In order to compare the two portraits we use the relation between the basic observables given in Eq. (58), i.e.,

$$\check{\pi}_V = \check{\pi}'_V, \qquad \check{V} = \check{V}' + \check{\pi}'_V \Delta(\check{V}', \check{\pi}'_V). \qquad (87)$$

By choosing various delay functions $\Delta(\check{V}', \check{\pi}'_V)$ we are able to generate infinitely many new semiclassical portraits, all of which describe the quantum dynamics of the Bianchi I model in terms of the same observables $\check{V}$ and $\check{\pi}_V$ but produced with different internal times.

Figure 5 shows various cases for which we have picked arbitrary but acceptable delay functions $\Delta_i(\check{V}', \check{\pi}'_V)$. It is clear from these graphs that the "actual" motion in phase
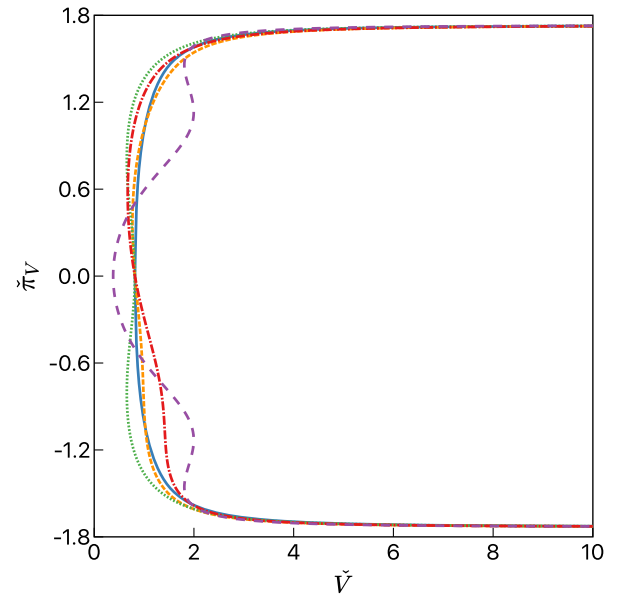

FIG. 6. Comparison between five delay functions Δ (shown on Fig. 5) and the original time phase space trajectories from Fig. 3, illustrated here on the case $\langle \hat{H} \rangle = 3$. The asymptotic behaviors being identical, the classical limit appears to be well defined whatever the delay function used, which is significant only around the bouncing epoch.

space can be for the most part arbitrary. In particular, it is neither necessarily symmetric in the $(\check{V}', \check{\pi}'_V)$ plane. Moreover, one can even find a minimum volume at points for which the momentum is nonvanishing, thereby ruining the usual interpretation of the latter as the Hubble factor.

V. CONCLUSIONS

We studied the empty Bianchi I universe to exemplify the use of a clock in quantum cosmology. Solving the classical Hamilton equations, we find two different categories of clocks, dubbed fast and slow-gauge times. The fast-gauge time appears in a more natural way in the canonical one-form, and yields a singular classical motion, although it requires an infinite amount of fast-gauge time to reach it (hence the gauge name). It has been conjectured, and we provide an explicit example that canonical quantization cannot remove the singularity, the wave function eventually evolving toward a Dirac distribution at vanishing volume.

Solving the constraint using a more sophisticated solution provides another category of clocks, dubbed slow-gauge times. Classically, such clocks are slow in the sense that the singularity is now reached in a finite amount of time. The question of time is now manifested by the fact that there exist many choices, all involving a delay function thanks to which new sets of canonical variables may be defined.

The main difference between fast and slow-gauge times, in the Bianchi I case, resides in the domain of definition of

the variables. In the fast case, the evolution is naturally unbounded, the Hamiltonian being that of a free particle on the full real line, whereas the slow-gauge time yields a similar evolution but only on the half-line. Up to some technical points regarding the self-adjointness of operators, this permits one to resolve the classical singularity through quantum mechanical effects.

We show that in the Heisenberg picture, it is possible to explicitly solve the relevant operators (Hamiltonian, dilation and square of the volume) as functions of time, allowing to draw phase portraits. We then find that, in a way mostly independent of the explicit choice of state itself (which is an advantage of the Heisenberg picture over Schrödinger's), the phase space trajectories are always similar, depending on the eigenvalue of the Hamiltonian. A Gaussian wave packet evolution shows exactly the same behavior, as expected.

Shifting to different times by picking arbitrary delay functions, one finds that the phase space trajectories depend strongly on the time choice only when quantum effects are relevant, i.e., close to the bouncing point (minimum of the volume). However, we also show that there exists an asymptotic regime in which the semiclassical motion is a good approximation and which does not depend on the choice of time (Fig. 6). These results are in agreement with earlier results on the time issue for the Friedmann model filled with radiation [21]. It could thus be conjectured that the question of time in a quantum cosmological setting is naturally resolved in the classical domain provided such a regime exists. In other words, time would cease to be a relevant physical object in the quantum gravitational realm, recovering its meaning only for configurations for which the use of general relativity is appropriate. At the moment, one needs to implement a time parameter to order events, but it may not be necessary in a more complete theory.

Since the empty Bianchi I model with internal time effectively becomes one dimensional, it is fully justified to ask whether the results obtained in this paper are restricted to one-dimensional models and no longer hold when an additional d.o.f. is present and the space of solutions has more structure. This question was in fact to some extent already investigated for the case of the Bianchi I with a fluid playing the role of the internal time variable [22], and the results obtained there appear to be in full agreement with the ones presented herein. Nevertheless, it seems to us that more such studies are desirable.

The next and related question that needs be asked concerns perturbations, and in particular whether they also enjoy a unique classical limit independent of the choice of time. If true, such a statement would permit deriving "matching conditions" (as discussed, e.g., in Ref. [23]); we postpone a discussion of perturbations in a vacuum Bianchi I universe for future work.

APPENDIX: WAVE PACKET FOR THE AFFINE CASE

In Sec. IV A, we presented the evolution of a Gaussian wave packet for the simple case where the Hamiltonian is given by $\hat{H} = -\triangle_D$. In this appendix, we discuss the equivalent situation for the affine case (75) for which we obtained the Hamiltonian (76). Still using the representation for which $\hat{V}$ is multiplicative, i.e.,

$$\hat{V}\psi(V) = V\psi(V), \qquad \hat{\pi}_V\psi(V) = -i\partial_V\psi(V),$$

the Hamiltonian operator reads

$$\hat{H} = -\partial_V^2 + \frac{\mathcal{K}(\alpha)}{V^2}. \tag{A1}$$

All the eigenfunctions of this operator satisfy the Dirichlet conditions $\psi_\ell(0) = 0$, and they read

$$\psi_\ell = \sqrt{\ell V}J_\nu(\ell V), \qquad \ell \in \mathrm{Sp}(\hat{H}) = \mathbb{R}_+,$$
$$\nu = \frac{\sqrt{1 + 4K(\alpha)}}{2}, \qquad \hat{H}\psi_\ell = \ell^2\psi_\ell, \tag{A2}$$

where $J_\nu(x)$ is the Bessel function of the first kind.

The propagator G is given by the integral of the eigenfunctions over the spectrum, namely

$$G(\eta, V, V') = \sqrt{VV'} \int_0^\infty d\ell\, \ell e^{-i\ell^2\tilde{\eta}} J_\nu(\ell V)J_\nu(\ell V'), \tag{A3}$$

where $\tilde{\eta} = \eta(1 \mp i\epsilon)$ for $\epsilon > 0$ gives the correct propagator prescription after taking $\epsilon \to 0$ for $\eta > 0$ and $\eta < 0$ respectively. This integral can be done analytically using Weber second integrals (see [24], Sec. 10.22.67),

$$G(\eta, V, V') = \frac{\sqrt{VV'}}{2i\tilde{\eta}} \exp\left(-\frac{V^2 + V'^2}{4i\tilde{\eta}}\right) I_\nu\left(\frac{VV'}{2i\tilde{\eta}}\right), \tag{A4}$$

where $I_\nu(x)$ is the modified Bessel function of the first kind. Note that $\mathcal{K}(\alpha) \to 0 \Rightarrow \nu \to 1/2$, and the Bessel function reduces to the sinh : $I_{1/2}(x) = \sinh(x)/\sqrt{\pi x/2}$. Substituting this expression in the propagator above then reproduces, up to an irrelevant phase, Eq. (68).

One useful property of the propagator (68) is that its integral over a Gaussian distribution generates another Gaussian distribution, as we have seen in Sec. IV A. Although the integral of the propagator (A4) does not have the same property when integrated over Gaussian distribution, it is still possible to choose a different initial wave packet that reduces to our earlier choice (74) when $\nu \to 1/2$ and retains the same functional form when propagated through time. By analogy with the Gaussian case, we consider an initial wave function having the same functional form as the propagator, namely

$$\psi_0(V) = \frac{\sqrt{VV_0}}{\mathcal{N}_\nu} \exp\left(-\frac{V^2 + V_0^2}{4\sigma^2}\right) I_\nu\left(\frac{VV_0}{2\sigma^2} + ikV\right),$$

$$(A5)$$

whose normalization is found, still using Weber second integral, to be given by

$$\mathcal{N}_\nu^2 = \sigma^2 V_0 \exp\left(-\frac{V_0^2}{4\sigma^2} - \sigma^2 k^2\right) I_\nu\left(\frac{V_0^2}{4\sigma^2} + \sigma^2 k^2\right); \quad (A6)$$

this choice reduces to Eq. (74) for $\nu \to 1/2$.

In the large volume limit $V, V_0 \gg 1$, we can use the asymptotic expansion of $I_\nu(x)$,

$$I_\nu(x) \sim \frac{e^x}{\sqrt{2\pi x}} - \frac{e^{-x+i\pi(\nu-\frac{1}{2})}}{\sqrt{2\pi x}}, \quad (A7)$$

(with corrections of order x^{-1} for each term) to obtain

$$\psi(V) \underset{V\to\infty}{\approx} \frac{e^{i\mu}}{\sqrt{\sqrt{2\pi}\sigma}} \left\{\exp\left[-\frac{(V+V_0)^2}{4\sigma^2} - ikV\right]\right.$$
$$\left. - \exp\left[-\frac{(V-V_0)^2}{4\sigma^2} + ikV + i\pi\left(\nu - \frac{1}{2}\right)\right]\right\},$$

$$(A8)$$

where μ is a constant phase given by

$$\frac{V_0}{2\sigma^2} + ik = \sqrt{\frac{V_0^2}{4\sigma^4} + k^2} e^{i\mu}.$$

The asymptotic expansion above shows that our choice of wave packet reduces to a Gaussian when computed far from the boundary. In addition, we can again use Weber second integral to calculate explicitly the solution by applying the propagator to the initial wave function, namely

$$\psi(V, \eta) = \int_0^\infty dV' G(\eta, V, V') \psi_0(V').$$

This yields

$$\psi(V, \eta) = \frac{\sqrt{VV_0}}{\mathcal{N}_\nu(\sigma_\eta/\sigma)} \exp\left(-ik^2\eta - \frac{V^2 + V_\eta^2}{4\sigma\sigma_\eta}\right)$$
$$\times I_\nu\left(\frac{VV_\eta}{2\sigma\sigma_\eta} + ikV\right), \quad (A9)$$

where $V_\eta = V_0 + 2k\eta$ and $\sigma_\eta = \sigma + i\eta/\sigma$ are the same parameters used in the free particle case. As below Eq. (A4), the limit $\mathcal{K} \to 0$ reproduces the solution (72), up to an irrelevant phase.

Far from the boundary, this solution reduces to a simple Gaussian packet traveling with speed $2k$. On the other hand, if the packet travels towards the boundary, V_η eventually vanishes and consequently the modified Bessel function argument, whose real part reads

$$\Re\left(\frac{VV_\eta}{2\sigma\sigma_\eta} + ikV\right) = \frac{VV_\eta}{2|\sigma_\eta|^2},$$

also vanishes. At this stage, the asymptotic expansion is clearly not valid so the wave function cannot be approximated by a Gaussian packet. Nonetheless, $-V_\eta$ subsequently again increases monotonically, so that, given enough time, the wave function again behaves as a Gaussian wave packet traveling away from the boundary. This happens because as the sign of the real part of the
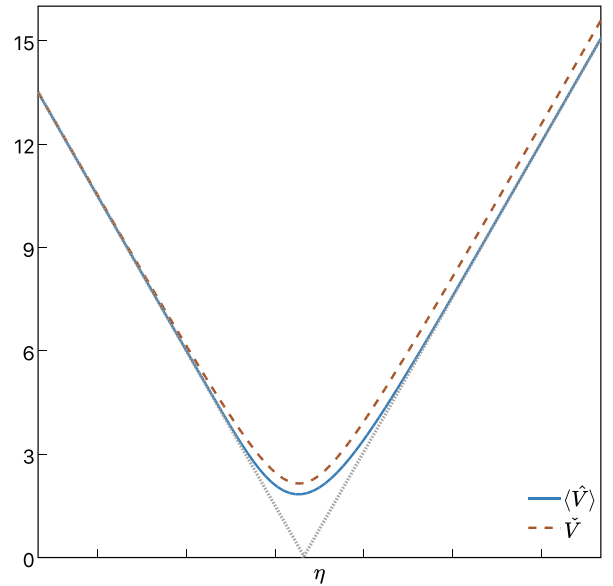

FIG. 7. Variation of the mean value $\langle \hat{V} \rangle$ with the conformal time η using the solution (A9) (full line), compared with the semiclassical approximation given by the $\check{V}$ (85) (dashed line). Also shown is the classically singular trajectory (dotted line).
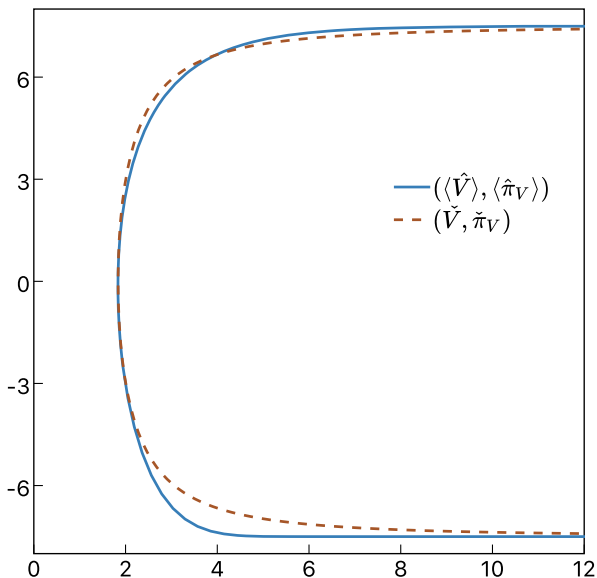
FIG. 8. Phase space evolution comparing the $(\langle\hat{V}\rangle, \langle\hat{\pi}_V\rangle)$ trajectory using (A9) (full line), with the symmetric semiclassical approximation given by the $(\check{V}, \check{\pi}_V)$ (85) (dashed line). The asymptotic behavior is identical.
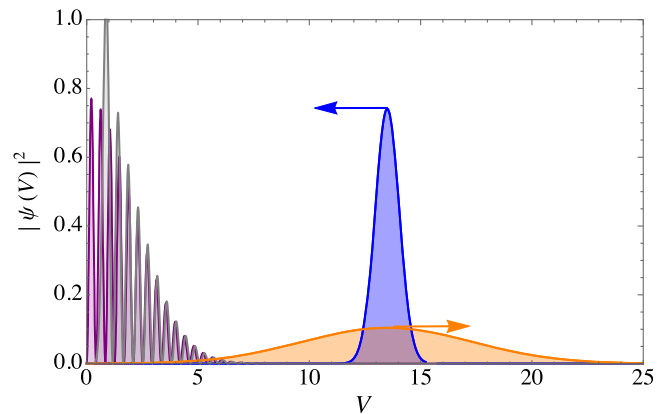

FIG. 9. Same as Fig. 2 for the affine case with $\mathcal{K} = 7/4$, i.e., the solution (A9). Two sets of oscillations are shown, namely those stemming from the free case $\nu = \frac{1}{2}$ discussed in Sec. IV A, and the new situation with $\nu = 2$. Although there are important differences near the bounce, the asymptotic behavior does not depend on the operator ordering choice, as expected for a meaningful semiclassical approximation; this comes from the fact that the potential becomes negligibly small far from the bounce.

argument changes to negative, the asymptotic expansion of the modified Bessel function (A7) becomes dominated by the second term.

With the help of the actual wave function solution (A9), it is possible to estimate the average value of the relevant variable $\hat{V}$, namely

$$\langle\hat{V}\rangle = \int_0^\infty |\psi(V,\eta)|^2 dV$$

and $\hat{\pi}_V$,

$$\langle\hat{\pi}_V\rangle = -i \int_0^\infty \psi^*(V,\eta)\partial_V\psi(V,\eta)dV.$$

Figure 7 shows $\langle\hat{V}\rangle$ as a function of the conformal time and compares with the semiclassical trajectory. It is clear from

this figure that although using $\sqrt{\langle\hat{V}^2\rangle}$ may be questionable, it provides a reasonable approximation to $\langle\hat{V}\rangle$ almost at all times. This is due to the fact that we considered a very peaked Gaussian state for large negative times, and although the variance increases with time after the bounce, the difference remains small because the growing variance is just compensated by the simultaneous shift of the wave packet to larger and larger values of V: for large values of η, we have $\langle\hat{V}\rangle \propto \sigma_\eta \propto \eta$.

The relevant phase space trajectory is illustrated on Fig. 8, showing again that the semiclassical approximation is a valid one, especially if one is interested in the asymptotic (large time) behaviors. The solution (85) is symmetric, contrary to the mean value case. This stems from the fact that the variance of the wave packet has a nonsymmetric evolution in time (Fig. 9).

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