Singularity avoidance in a quantum model of the Mixmaster universe

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We present a quantum model of the vacuum Bianchi-IX dynamics. It is based on four main elements. First, we use a compound quantization procedure: an affine coherent state quantization for isotropic variables and a Weyl quantization for anisotropic ones. Second, inspired by standard approaches in molecular physics, we make an adiabatic approximation (Born-Oppenheimer-like approximation). Third, we expand the anisotropy potential about its minimum in order to deal with its harmonic approximation. Fourth, we develop an analytical treatment on the semiclassical level. The resolution of the classical singularity occurs due to a repulsive potential generated by the affine quantization. This procedure shows that during contraction the quantum energy of anisotropic degrees of freedom grows much slower than the classical one. Furthermore, far from the quantum bounce, the classical recollapse is reproduced. Our treatment is put in the general context of methods of molecular physics, which can include both adiabatic and nonadiabatic approximations.

I. INTRODUCTION

The Belinskii, Khalatnikov and Lifshitz (BKL) scenario [1,2] (see [3] for numerical support for BKL) addresses the generic solution to the Einstein equations near the cosmological singularity. The purpose of our paper is to quantize the dynamics of the vacuum Bianchi-IX model that underlies the BKL scenario.

The BKL predicts that on approach to a spacelike singularity the dynamics of gravitational field may be significantly simplified as time derivatives in Einstein's equations dominate over spatial derivatives. The latter means that the evolution of the gravitational field in this regime is ultralocal and space splits into a collection of small patches whose dynamics is approximately given by spatially homogenous spaces, the Bianchi models (see, e.g., [4]).

Approaching the singularity the spatial curvature grows and the space further subdivides into homogenous slices. The size of each patch, modeled by one of the Bianchi spacetimes, corresponds to the magnitude of the spatial derivatives in the Einstein equations. As homogeneity of spatial fragments holds only at some level of approximation, dynamical evolution of the newly formed patches starts off with slightly different initial conditions. This almost negligible difference grows rapidly in subsequent evolution as geometries of new patches evolve almost independently of each other approaching the state of the so-called asymptotic silence [5]. The chaotic subdivisions result in the growth of fragmentation of spacetime suggesting that it may possess fractal structure close to the singularity [6,7].

Among the possible homogeneous models, the Bianchi-IX model has sufficient generality to describe the evolution of a small patch of space towards the singularity. The dynamics of the vacuum Bianchi-IX model (i.e., the mixmaster universe) is nonintegrable. However, close enough to the singularity, each solution can be qualitatively understood as a sequence of Kasner epochs, which correspond to the Kasner universe. The transitions between the epochs are

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described by the vacuum Bianchi-II-type evolution [8]. The Universe undergoes an infinite number of chaoticlike transitions and eventually collapses into the singularity in a finite proper time [1].

The imposition of quantum rules into the chaotic dynamics of the Bianchi-IX model has already been studied. The program initiated by Misner [9–11] led to the pessimistic result that quantum mechanics does not remove the singularity of the Bianchi-IX model. Nevertheless, the exploration of solutions to the corresponding Wheeler-DeWitt equation continues [12–15]. Recently, some effort has been made towards quantization of the Bianchi-type models within the loop quantum cosmology. The authors make use of the Dirac quantization method and combine it with the introduction of holonomies in place of the curvature of connection. The results obtained for the Bianchi-IX model at semiclassical level by Bojowald [4,16] suggest that the chaotic behavior stops once quantum effects become important. Another formulation taking into account holonomies has been proposed in [17], but it has not been applied to the examination of the dynamics. Still another proposal was given in [18], giving support to [16]. An effective dynamics considered recently [19] suggests a resolution of the cosmic singularity problem as well, but within an approach quite different from ours. In the above formulations, the search for solutions is quite challenging leaving the near big bang dynamics largely unexplored.

In this paper we formulate and make a quantum study of the Bianchi-IX model by combining canonical and affine coherent state (ACS) quantizations with a semiclassical approach. The cosmological system consists of isotropic variables (expansion and volume) and anisotropic ones (distortion and shear). They are treated in a separate manner. The canonical pair expansion volume is a half plane. Since the symmetry of the latter is the affine group "$AX + B$" and not the Abelian $\mathbb{R}^2$, they are consistently quantized by resorting to one of the two unitary irreducible representations (UIRs) of the affine group. Within this approach, we have found in [20] that for the Friedmann-Robertson-Walker (FRW) models the cosmological expansion squared, which plays the role of kinetic energy of the universe, is always accompanied at the quantum level by an extra term inversely proportional to the volume squared. As the Universe approaches the singularity, this term grows in dynamical significance, efficiently counterbalances the attraction of any matter and eventually halts the cosmological contraction. Afterwards, the Universe rebounds and reexpands. In the present work (see also [21]) we confirm that the same mechanism prevents the collapse of the Bianchi-IX universe, suggesting its universality. Making further use of the ACS we construct a semiclassical description of the isotropic part of the metric, with semiclassical observables replacing the classical ones in the phase space. In particular, the semiclassical Hamiltonian possesses the correction term, which regularizes the singularity.

Inspired by standard approaches in molecular physics, we make an assumption about the quantum evolution of the anisotropic variables based on the adiabatic approximation. In molecules, the motion of heavy nuclei is so slow in comparison with rapidly moving light electrons that it is legitimate to approximate the dynamics with electronic configurations being instantaneously and continuously adjusted to the position of nuclei. Analogously, we consider in our model, in its harmonic approximation, the anisotropic oscillations rapid in comparison with the contraction rate of the Universe. Within this approach, the oscillations of the classical scenario are suppressed and the development of chaos is blocked. Moreover, we find that while the classical energy of the oscillations behaves in terms of the scale factor a more or less as $\propto a^{-6}$, the respective quantum energy behaves as $\propto a^{-4}$, i.e. it contributes on a much softer level. Therefore, fluids with pressure equal to or higher than that of radiation, which are likely to be present in the early universe, will have their grasp on the cosmological collapse.

The paper is organized as follows: Sec. II concerns the definition of the classical model, some description of its dynamics and the choice of phase space variables convenient for our quantization. Section III is devoted to the quantization of the Hamiltonian constraint and its subsequent semiclassical approximation. Section III B explains the semiclassical Lagrangian approach. The resulting semiclassical dynamics is developed in Sec. IV. In Sec. V, we go beyond the adiabatic approximation to confirm the validity of our method. We discuss our results and conclude in Sec. VI. In Appendix A we give an introduction to the affine coherent states quantization together with its semiclassical aspects. Derivations of the quantum version of the anisotropic Hamiltonian both in harmonic and triangular box approximations are given in Appendix B.

II. BIANCHI-TYPE MODELS

We consider a spacetime admitting a foliation $\mathcal{M} \mapsto \Sigma \times \mathbb{R}$, where Σ is spacelike. Furthermore, we assume Σ to be identified with a simply transitive three-parameter group of motions. Such models are called Bianchi-type models. The left-invariant vector fields are associated with the Killing vectors and the right-invariant ones with the basis vectors with respect to which the metric components on Σ take constant values in space. We assume the following line element,

$$ds^2 = -\mathcal{N}^2(t)dt^2 + \sum_i q_i(t)\omega^i \otimes \omega^i, \qquad (1)$$

where the ω^is are right-invariant dual vectors. They satisfy

$$d\omega^i = \frac{1}{2}C^i{}_{jk}\omega^j \wedge \omega^k, \qquad (2)$$

where $C^i{}_{jk}$ are structure constants. We consider the so-called class A models with $C^i{}_{ik} = 0$ (summation is implied). The further simplification is gained for the diagonal ones, $C^i{}_{jk} = \mathfrak{n}^{(i)}\epsilon_{(i)jk}$, where ϵ_{ijk} is a totally skew-symmetric symbol. For such models, the computation of the Ricci curvature is straightforward:

$$R = \frac{\mathfrak{n}^1\mathfrak{n}^2}{q_3} + \frac{\mathfrak{n}^1\mathfrak{n}^3}{q_2} + \frac{\mathfrak{n}^2\mathfrak{n}^3}{q_1} - \frac{(\mathfrak{n}^1)^2}{2}\frac{q_1}{q_2q_3}$$
$$- \frac{(\mathfrak{n}^2)^2}{2}\frac{q_2}{q_1q_3} - \frac{(\mathfrak{n}^3)^2}{2}\frac{q_3}{q_1q_2}. \tag{3}$$

The vector $(\mathfrak{n}_1, \mathfrak{n}_2, \mathfrak{n}_3) \in \mathbb{R}^3$ specifies the Bianchi-type model (I, II, VI$_0$, VII$_0$, VIII, IX). Conventionally, the $\mathfrak{n}_i$s are chosen as $\mathfrak{n}_i \in \{0, \pm 1\}$ [22]. Special cases are $\mathfrak{n}_i = 0$ (type I) and $\mathfrak{n}_i > 0$ (type IX). From now on, we fix $\mathfrak{n}_i = \mathfrak{n}$ for the Bianchi-IX case examined in this work. We assume that the topology of the spatial leaf is S^3 and we find its coordinate volume as

$$\mathcal{V}_0 = \int_{S^3} \omega^1 \wedge \omega^2 \wedge \omega^3 = \frac{16\pi^2}{\mathfrak{n}^3}. \tag{4}$$

Two convenient choices are either $\mathfrak{n} = 1$ or $\mathfrak{n} = \sqrt[3]{16\pi^2}$. We make use of the latter option.

A. Canonical formulation

Following the work of Arnowitt, Deser and Misner [23], the convenient formulation of Bianchi models was derived by Misner [9–11]. With Misner's variables the dynamics assumes a convenient form: motion of a particle in three-dimensional Minkowskian spacetime and in a space-and-time-dependent confining potential. The spatial coordinates describe the anisotropic distortion of the shape of the Universe and the time coordinate describes the size of the Universe. The particle motion is ruled by a potential arising from the Ricci curvature of spatial leaf. Let us recall that the Hamiltonian constraint reads

$$\mathsf{H} = \frac{\mathcal{N}\mathcal{V}_0 e^{-3\beta_0}}{48\kappa}(-\tilde{p}_0^2 + \tilde{p}_+^2 + \tilde{p}_-^2 - 24e^{6\beta_0}R(\beta_0, \beta_\pm)), \tag{5}$$

where the Misner configuration variables are related to the metric components as follows,

$$\begin{pmatrix} \ln q_1 \\ \ln q_2 \\ \ln q_3 \end{pmatrix} = \begin{pmatrix} 2 & 2 & 2\sqrt{3} \\ 2 & 2 & -2\sqrt{3} \\ 2 & -4 & 0 \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_+ \\ \beta_- \end{pmatrix}, \tag{6}$$

and where $\tilde{p}_0$, $\tilde{p}_+$ and $\tilde{p}_-$ are the respective momenta, defined from the Poisson brackets in Eq. (7). $\mathcal{V}_0$ is the coordinate volume and $\kappa = 8\pi Gc^{-4}$. The momenta $\tilde{p}_i$ carry

the dimension L^{-1} while the positions β_i are dimensionless. Because we reduce a field theory to a mechanical system all the canonical variables are in fact averaged over the sphere and the Poisson brackets read as

$$\{\beta_0, \tilde{p}_0\} = \{\beta_\pm, \tilde{p}_\pm\} = \frac{2\kappa c}{\mathcal{V}_0}. \tag{7}$$

In order to work within the standard quantum mechanical framework, we introduce variables that are conjugated in the usual sense, i.e. $\{\beta_i, p_j\} = \delta_{ij}$, and so define the new momenta $p_i = (2\kappa c)^{-1}\mathcal{V}_0\tilde{p}_i$. The Hamiltonian of Eq. (5) now reads

$$\mathsf{H} = -\frac{\mathcal{N}\mathcal{V}_0 e^{-3\beta_0}}{48\kappa}\left(\left(\frac{2\kappa c}{\mathcal{V}_0}\right)^2(p_0^2 - p_+^2 - p_-^2)\right.$$
$$\left. + 24e^{6\beta_0}R(\beta_0, \beta_\pm)\right). \tag{8}$$

In what follows we put $\mathcal{V}_0 = 2\kappa = c = 1$ (in [21] we chose $\kappa = 1$). The physical constants $\mathcal{V}_0$, κ and c will be eventually restored in the presentation of the final results. Note that the averaged (isotropic) scale factor "a" is defined as $a = e^{\beta_0} = (q_1q_2q_3)^{1/6}$. Observe also that the usual diffeomorphism constraints vanish identically.

In the case of Bianchi-IX geometry we find

$$R(\beta_0, \beta_\pm) = -\frac{\mathfrak{n}^2}{2}e^{-2\beta_0 + 4\beta_+}$$
$$\times ([2\cosh(2\sqrt{3}\beta_-) - e^{-6\beta_+}]^2 - 4) \tag{9}$$

$$= -\frac{3}{2}e^{-2\beta_0}W_{\mathfrak{n}}(\beta), \tag{10}$$

with

$$W_n(\beta) = \mathfrak{n}^2\frac{e^{4\beta_+}}{3}([2\cosh(2\sqrt{3}\beta_-) - e^{-6\beta_+}]^2 - 4), \tag{11}$$

where the potential $W_{\mathfrak{n}}$ does not depend on the averaged scale factor a. By putting $p_\pm = 0 = \beta_\pm$ we retrieve the closed Friedmann-Robertson-Walker model, with $W_{\mathfrak{n}}(0) = -\mathfrak{n}^2$ giving rise to the isotropic and positive intrinsic curvature. For $\mathfrak{n} = 0$, we get the Bianchi-I model with $W_0 = 0$ and vanishing intrinsic curvature.

The potential $W_{\mathfrak{n}}$ is *bounded* from below and reaches its minimum value, $W_{\mathfrak{n}} = -\mathfrak{n}^2$, at $\beta_\pm = 0$. The potential $W_{\mathfrak{n}}$ is expanded around its minimum as follows:

$$W_{\mathfrak{n}}(\beta) = -\mathfrak{n}^2 + 8\mathfrak{n}^2(\beta_+^2 + \beta_-^2) + o(\beta_\pm^2), \tag{12}$$

which clearly shows its two-dimensional harmonic approximation. The $W_{\mathfrak{n}}$ is asymptotically *confining* except for the following three directions (shown in Fig. 1), in which $W_{\mathfrak{n}} \to 0$:
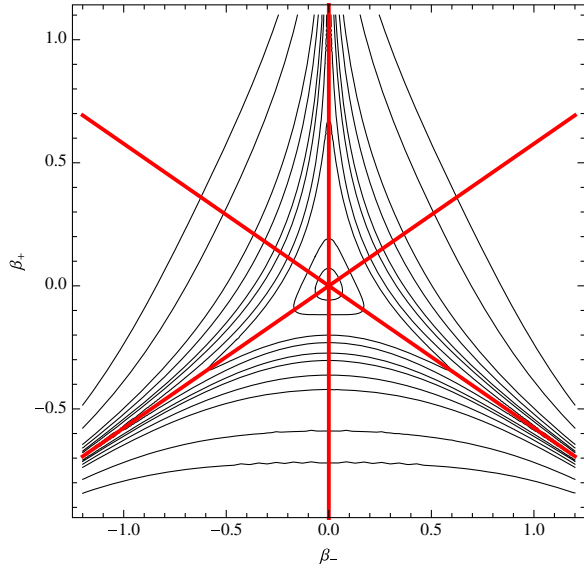
FIG. 1 (color online). Contour plot of $W_{\mathfrak{n}}(\beta)$ near its minimum. Red lines: the three C_{3v} symmetry axes $\beta_- = 0$, $\beta_+ = \beta_-/\sqrt{3}$, $\beta_+ = -\beta_-/\sqrt{3}$.

FIG. 2 (color online). The plot of $V_{\mathfrak{n}}$ for $\mathfrak{n} = 1$ near its minimum. Boundedness from below, confining aspects, and C_{3v} symmetry are illustrated.

$(i)\ \beta_- = 0, \beta_+ \to +\infty,$ $\qquad (ii)\ \beta_+ = -\dfrac{\beta_-}{\sqrt{3}}, \beta_- \to +\infty,$

$(iii)\ \beta_+ = \dfrac{\beta_-}{\sqrt{3}}, \beta_- \to -\infty.$

The form of the Bianchi-IX potential deserves particular attention due to its three "open" C_{3v} symmetry directions (see Figs. 1–2). One can view them as three deep "canyons," increasingly narrow until their respective wall edges close up at the infinity whereas their respective bottoms tend to zero. The motion of the Misner particle in this potential is chaotic [24]. Though the curvature, which is proportional to the potential, flattens with time, the confined particle undergoes infinitely many oscillations. In the so-called steep wall approximation, the particle is locked in the triangular potential with its infinitely steep walls moving apart in time. At the quantum level, the confining shape originates a discrete spectrum. On the other hand, it is unclear on a mathematical level whether or not the Bianchi-IX potential also originates a continuum spectrum. Nevertheless the following physical reasoning leads to the conclusion that a continuous spectrum probably does not exist. Indeed a continuous spectrum should be associated with the eigensystem $\{(\psi_k(\beta_-, \beta_+), \epsilon_k)\}_{k \in \mathcal{D} \subset \mathbb{R}^2}$ where (i) the scattering eigenstates (not $\mathbb{R}^2$-Lebesgue square integrable) $\psi_k(\beta)$ represent the possibility for the system to go from infinity to infinity in the (β_-, β_+)-plane; (ii) $k \in \mathcal{D} \subset \mathbb{R}^2$ represents the 2D-momentum of the incoming "particles"; (iii) k belongs to some 2D-domain $\mathcal{D}$ of $\mathbb{R}^2$ ($\mathcal{D}$ is not restricted to a subset of measure 0 for the $\mathbb{R}^2$-Lebesgue measure); and (iv) $k \in \mathcal{D}$ leads to an interval (generally unbounded) of eigenvalues ϵ_k (the continuous spectrum). In
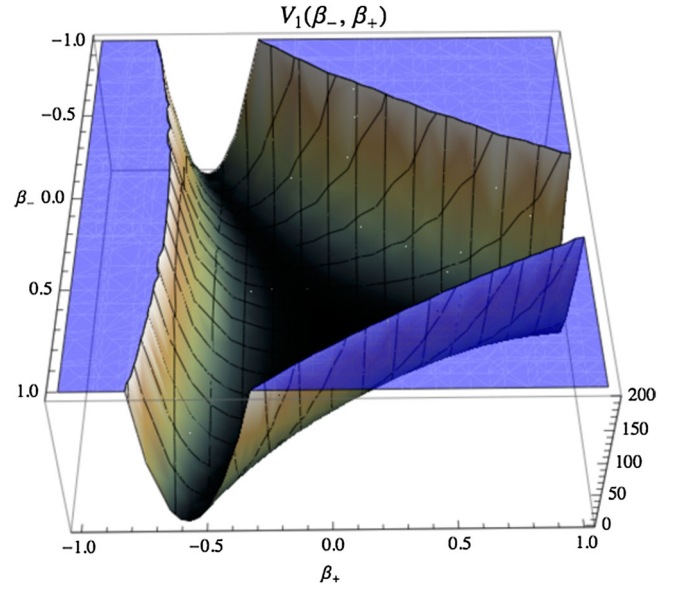
our case the potential only possesses three discrete open directions at infinity; therefore the incoming momentum k cannot belong to a 2D-domain $\mathcal{D}$ (a subset with a non-vanishing $\mathbb{R}^2$-Lebesgue measure). Then it is reasonable to think that a continuous spectrum does not exist.

The evolution of Bianchi IX can be viewed as a nonlinear model of a gravitational wave in dynamical isotropic geometry (see e.g. [10,25] and references therein). The wave, which consists of two nonlinearly coupled components $\beta_\pm$, is homogenous, that is, it is a pure time oscillation. Its wavelength is thought to be much larger than the extension of the considered patch of the Universe with its spatial derivatives neglected. The energy of the wave sources the gravitational contraction. As we later show, the quantization of the wave introduces important modifications to the dynamics of the whole Universe. The qualitative study of spatially homogeneous models was pioneered by Bogoyavlensky (see [26] and references therein).

B. Redefinition of basic variables

For the purpose of ACS quantization, we redefine the isotropic phase space variables as the canonical pair:

$$q := e^{3\beta_0/2}, \qquad p := \frac{2}{3} e^{-3\beta_0/2} p_0. \qquad (13)$$

Note that (q, p) lives in the half plane. The Hamiltonian (8) now assumes the form

$$\mathsf{H} = -\frac{\mathcal{N}}{24}\left(\frac{9}{4}p^2 - \frac{p_+^2 + p_-^2}{q^2} - 36q^{2/3} W_{\mathfrak{n}}(\beta)\right). \qquad (14)$$

Let us split the potential $W_{\mathfrak{n}}$ into its isotropic and anisotropic components. The isotropic part corresponds to that part of curvature which is independent of $\beta_\pm$, whereas the anisotropic part vanishes for $\beta_\pm = 0$:

$$W_{\mathfrak{n}}(\beta) = -\mathfrak{n}^2 + V_{\mathfrak{n}}(\beta). \tag{15}$$

The lapse function is not dynamical and its choice is irrelevant for the classical dynamics as it only fixes the magnitude and direction of the Hamiltonian flow in the constraint surface. From now on we put the lapse $\mathcal{N} = -24$. The Hamiltonian (14) now reads

$$\mathsf{H} = \frac{9}{4}p^2 + 36\mathfrak{n}^2 q^{2/3} - \mathsf{H}_q, \tag{16}$$

where H_q is the q-dependent Hamiltonian for the anisotropic variables,

$$\mathsf{H}_q := \frac{p_+^2 + p_-^2}{q^2} + 36q^{2/3}V_{\mathfrak{n}}(\beta). \tag{17}$$

C. Discussion of the constraint

The analytical expressions (16)–(17) for H remind us of the molecular system's Hamiltonian. The pair (q, p) plays the role of the nucleuslike dynamical variables and $(\beta_\pm, p_\pm)$ are electronlike dynamical variables. Quantum molecular systems are usually considered by making use of the Born-Oppenheimer approximation (BO) or its "diagonal correction" named Born-Huang (BH) [27,28]. In molecular physics, the validity of these approximations depends crucially on the ratio between nuclei and electron masses. Namely, a nucleus mass is very large when compared to the electron mass. In our case, Eq. (17) indicates that q^2 plays a role of mass for the anisotropic variables, whereas Eq. (16) shows that the mass of the isotropic variable is constant. Therefore, near the singularity $q = 0$, $\beta_\pm$s become *light* degrees of freedom and q with its constant mass may be treated as a *heavy* degree of freedom. Hence, we may follow either the BO or the BH approximation scheme in quantizing our system. This issue is considered in more detail in the next section.

For Eqs. (16)–(17), one checks that $\beta_\pm = 0 = p_\pm$ is a solution to the Hamilton equations of motion. In this case, the constraint $\mathsf{H} = 0$ reduces to

$$\frac{9}{4}p^2 + 36\mathfrak{n}^2 q^{2/3} = 0, \tag{18}$$

and we recover the closed vacuum FRW constraint, which possesses the unique singular and uninteresting solution $p = 0 = q$. Nevertheless, it makes sense to consider a small perturbation $\delta\beta_\pm$ from $\beta_\pm = 0$. The dynamical equation for $\delta\beta_\pm$ based on the harmonic approximation of Eq. (12) is

$$\delta\ddot{\beta}_\pm = -2\frac{\dot{q}}{q}\delta\dot{\beta}_\pm - 2\frac{\mathfrak{n}^2}{q^{4/3}}\delta\beta_\pm. \tag{19}$$

It can be demonstrated that the Friedmann model evolving towards the singularity is not stable in the phase space of the Bianchi-IX model. More precisely, any perturbation of isotropy will grow and develop into an oscillatory and chaotic behavior. The growth of isotropy is apparent from Eq. (19) for $\dot{q}/q < 0$. As the shear grows, the harmonic approximation breaks down and fully nonlinear dynamics develops. As we show, this behavior is suppressed on the quantum level and allows the harmonic approximation to remain valid all the way towards the big bounce. Moreover, we show in Sec. V that the BO approximation also survives the bounce phase. As the shear is known to dominate over any type of familiar matter close enough to the singularity, we consider only the vacuum case. Then the lack of solutions for the vacuum isotropic universe as concluded from (18) leads to the prediction that one should take into account the effect of the "quantum zero point energy" generated by the quantized anisotropy degrees of freedom of the Bianchi-IX model.

III. QUANTIZATION

In what follows we apply a quantization based on the Dirac method and inspired by Klauder's approach [29]: (i) quantizing H in kinematical phase space, (ii) finding the semiclassical expression $\check{\mathsf{H}}$ of the quantum Hamiltonian $\hat{\mathsf{H}}$ using Klauder's approach and our adiabatic approximation, and (iii) implementing the Hamiltonian constraint on the semiclassical level $\check{\mathsf{H}} = 0$.

A. Quantum constraint

Since in Eqs. (16)–(17) we have $(q, p) \in \mathbb{R}_*^+ \times \mathbb{R}$ and $(\beta_\pm, p_\pm) \in \mathbb{R}^4$, we can follow the idea of our previous paper [20] in the realization of the step (i):

(i) for the quantization of functions (or distributions) of the pair (q, p) living in the open half plane, we apply ACS quantization, whose principles and methods, as part of integral quantizations (see [30] and references therein), are explained in [20] and summarized in Appendix A. This procedure yields $\hat{p} = -i\hbar\partial_x$ and $\hat{q}$ defined as the multiplication by x, both acting in the Hilbert space $L^2(\mathbb{R}^+, dx)$,

(ii) for quantizing functions of the pairs $(\beta_\pm, p_\pm)$ we can choose either the Weyl-Heisenberg coherent state (CS) quantization [30], which has a regularizing role, or, directly, the canonical quantization. Due to the simplicity of the model we follow the latter option. Actually both yield $\hat{p}_\pm = -i\hbar\partial_{\beta_\pm}$ and the multiplication operator $\hat{\beta}_\pm$, both acting in $L^2(\mathbb{R}^2, d\beta_+ d\beta_-)$.

Thus, for the quantum Hamiltonian $\hat{\mathsf{H}}$ corresponding to Eqs. (16)–(17) we get

$$\hat{H} = \frac{9}{4}\left(\hat{p}^2 + \frac{\hbar^2 \mathfrak{K}_1}{\hat{q}^2}\right) + 36\mathfrak{n}^2 \mathfrak{K}_3 \hat{q}^{2/3} - \hat{H}_{\hat{q}}, \qquad (20)$$

$$\hat{H}_q := \mathfrak{K}_2 \frac{\hat{p}_+^2 + \hat{p}_-^2}{q^2} + 36\mathfrak{K}_3 q^{2/3} V_{\mathfrak{n}}(\beta), \qquad (21)$$

where the $\mathfrak{K}_i$ are positive and nonvanishing purely numerical constants dependent on the choice of the so-called *fiducial* vector. With the choice made in our previous paper [20], and thanks to the formula recalled in Appendix A, we have

$$\mathfrak{K}_1 = \frac{1}{4}\left(1 + \nu\frac{K_0(\nu)}{K_1(\nu)}\right), \qquad \mathfrak{K}_2 = \left(\frac{K_2(\nu)}{K_1(\nu)}\right)^2$$

$$\mathfrak{K}_3 = \frac{K_{5/3}(\nu)}{K_1(\nu)^{1/3}K_2(\nu)^{2/3}}, \qquad (22)$$

where $\nu > 0$ is a free parameter and the $K_r(\nu)$ are the modified Bessel functions [31]. Since we deal with ratios of such functions throughout the sequel, we adopt the convenient notation

$$\xi_{rs} = \xi_{rs}(\nu) = \frac{K_r(\nu)}{K_s(\nu)} = \frac{1}{\xi_{sr}}. \qquad (23)$$

One convenient feature of such a notation is that $\xi_{rs}(\nu) \sim 1$ as $\nu \to \infty$ [a consequence of $K_r(\nu) \sim \sqrt{\pi/(2\nu)}$]. Thus (22) reads

$$\mathfrak{K}_1 = \frac{1}{4}(1 + \nu\xi_{01}(\nu)), \qquad \mathfrak{K}_2 = (\xi_{21}(\nu))^2,$$

$$\mathfrak{K}_3 = (\xi_{\frac{5}{3}1})^{1/3}(\xi_{\frac{5}{3}2})^{2/3}. \qquad (24)$$

There exist many other choices of fiducial vectors yielding similar constants $\mathfrak{K}_i$. These vectors depend themselves on arbitrary parameters which can be suitably adjusted. Also, the Hamiltonian (20) itself is defined up to a multiplicative factor. It is also crucial to recall that there exists an infinite range of values for constants $\mathfrak{K}_i$, for which the symmetric $\hat{H}$ has a unique self-adjoint extension. This is proved by making use of the reasoning previously presented in [20] and recalled in Appendix A.

We make an important remark that the analysis developed in the following sections is independent of the specific numerical values given to the coefficients $\mathfrak{K}_i$ as long as the bounce happens for small enough values of q in order for the adiabatic approximation to be valid (see below). In other words, all the following results determine the qualitative features of the dynamics unambiguously and the numerical coefficients pin down the dynamics quantitatively.

B. Semiclassical Lagrangian approach

Being inspired by Klauder's approach [29], we present a consistent framework allowing one to approximate the quantum Hamiltonian and its associated dynamics (in the constraint surface) by making use of the semiclassical Lagrangian approach.

1. General setting

The quantum Hamiltonian (20) has the general form (up to constant factors)

$$\hat{H} = \mathcal{N}\left(\hat{p}^2 + \frac{K}{\hat{q}^2} + L\hat{q}^{\frac{2}{3}} - \hat{H}^{(\text{int})}(\hat{q})\right), \qquad (25)$$

where K and L are some positive constants and the q-dependent Hamiltonian $\hat{H}^{(\text{int})}(q)$ (also denoted by $\hat{H}_q$ in the previous subsection) acts on Hilbert space of states for "internal" degrees of freedom, i.e., the anisotropic ones.

The Schrödinger equation, $i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \mathcal{N}\hat{H}|\Psi(t)\rangle$, can be deduced from the Lagrangian:

$$\mathsf{L}(\Psi, \dot{\Psi}, \mathcal{N}) := \langle\Psi(t)|\left(i\hbar\frac{\partial}{\partial t} - \mathcal{N}\hat{H}\right)|\Psi(t)\rangle, \qquad (26)$$

via the variational principle with respect to $|\Psi(t)\rangle$. In order to solve the Schrödinger equation, the lapse function $\mathcal{N}$ should be fixed.

The quantum counterpart of the classical constraint $\mathsf{H} = 0$ can be obtained as follows:

$$\frac{\partial\mathsf{L}}{\partial\mathcal{N}} = \langle\Psi(t)|\hat{p}^2 + \frac{K}{\hat{q}^2} + L\hat{q}^{\frac{2}{3}} - \hat{H}^{(\text{int})}(\hat{q})|\Psi(t)\rangle = 0. \qquad (27)$$

The commonly used Dirac way of imposing a constraint, $\hat{H}|\Psi(t)\rangle = 0$, implies (27) but the reciprocal does not hold in general.

At this stage, we suppose (due to the confining character of the potential $V_{\mathfrak{n}}$) that there exists $\hat{H}^{(\text{int})}(q)$ as a self-adjoint operator (and as a function of the c-number q) with purely discrete spectral decomposition, which is of course true in its harmonic approximation,

$$\hat{H}^{(\text{int})}(q) = \sum_n E_n^{(\text{int})}(q)|\phi_n^{(\text{int})}\rangle\langle\phi_n^{(\text{int})}|. \qquad (28)$$

To present the Klauder semiclassical procedure in the most general situation (not restricted to Bianchi IX), we distinguish the two cases:

(i) $\phi_n^{(\text{int})}$ is *independent* of q, which allows a complete separation of variables, and leads to the original Born-Oppenheimer [27,28] approach;

(ii) $\phi_n^{(\text{int})}$ is *dependent* on q.

Different semiclassical approximations result depending on these choices.[1]

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[1]We first present case (i), which is simple, and later introduce the more complicated case (ii), being applied to the Bianchi-IX model.

2. Semiclassical Lagrangian approximations

(i) $\phi_n^{(\text{int})}$ independent of q.—In this case, a family of exact solutions of the time-dependent Schrödinger equation $i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$ can be introduced in the form of the tensor product

$$|\Psi(t)\rangle = |\phi(t)\rangle \otimes |\phi_n^{(\text{int})}\rangle, \qquad (29)$$

where $|\phi(t)\rangle$ is solution to the reduced time-dependent Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}|\phi(t)\rangle = \mathcal{N}\left(\hat{p}^2 + \frac{K}{\hat{q}^2} + L\hat{q}^{\frac{2}{3}} - E_n^{(\text{int})}(\hat{q})\right)|\phi(t)\rangle$$
$$=: \mathcal{N}\hat{H}_n^{\text{red}}|\phi(t)\rangle \qquad (30)$$

where $E_n^{(\text{int})}$ is the eigenvalue of $\hat{H}^{(\text{in})}$. The tensor product $|\Psi(t)\rangle$ of Eq. (29) is precisely the Born-Oppenheimer-like solution [32]. Equation (30) may be derived from a variational principle applied to the quantum Lagrangian

$$\mathsf{L}^{\text{red}}(\phi, \dot{\phi}, \mathcal{N}) := \langle\phi(t)|\left(i\hbar \frac{\partial}{\partial t} - \mathcal{N}\hat{H}_n^{\text{red}}\right)|\phi(t)\rangle. \quad (31)$$

Following Klauder [29], we assume that $|\phi(t)\rangle$ is in fact an affine coherent state. We assume in the following that the fiducial vector ψ has been chosen such that $c_0(\psi) = c_{-1}(\psi)$ in order to obtain the canonical rule $[A_q, A_p] = i\hbar$. Furthermore, we need to apply a rescaling $|q(t), p(t)\rangle \to |\lambda q(t), p(t)\rangle$ in order to ensure $\langle\lambda q(t), p(t)|A_q|q(t), p(t)\rangle = q(t)$ and $\langle\lambda q(t), p(t)|A_p|q(t), p(t)\rangle = p(t)$. The parameter λ is uniquely defined by the choice of the fiducial vector, namely $\lambda = 1/c_{-3}(\psi)$ (see Appendix A).

Therefore we replace $|\Psi(t)\rangle$ in L of Eq. (26) by

$$|\Psi(t)\rangle = |\lambda q(t), p(t)\rangle \otimes |\phi_n^{(\text{int})}\rangle, \qquad (32)$$

where $q(t)$ and $p(t)$ are some time-dependent functions. Then the Lagrangian (26) or (31) turns to assume the semiclassical form

$$\mathsf{L}^{\text{sc}}(q, \dot{q}, p, \dot{p}, \mathcal{N}) = \langle\lambda q(t), p(t)|\left(i\hbar \frac{\partial}{\partial t} - \mathcal{N}\hat{H}_n^{\text{red}}\right)$$
$$\times |\lambda q(t), p(t)\rangle$$
$$= -q\dot{p} - \mathcal{N}\langle\lambda q(t), p(t)|\hat{H}_n^{\text{red}}|\lambda q(t), p(t)\rangle \qquad (33)$$

$$= -\frac{d}{dt}(qp) + \dot{q}p - \mathcal{N}\langle\lambda q(t),$$
$$p(t)|\hat{H}_n^{\text{red}}|\lambda q(t), p(t)\rangle. \qquad (34)$$

The appearance of the first term $-q\dot{p}$ in the rhs of this equation results from the derivative of (A12) with respect to parameters q and p leading to (A31).

The semiclassical expression for the Hamiltonian is the lower symbol

$$\check{\mathsf{H}}_n^{\text{red}}(q, p) := \langle\lambda q, p|\hat{H}_n^{\text{red}}|\lambda q, p\rangle. \qquad (35)$$

It is defined by the "frozen" quantum eigenstate "n" of the internal degrees of freedom.

From this reduced Hamiltonian one derives the equations of motion together with the constraint

$$\dot{q} = \mathcal{N}\frac{\partial}{\partial p}\check{\mathsf{H}}_n^{\text{red}}(q, p), \qquad (36)$$

$$\dot{p} = -\mathcal{N}\frac{\partial}{\partial q}\check{\mathsf{H}}_n^{\text{red}}(q, p) \qquad (37)$$

$$0 = \check{\mathsf{H}}_n^{\text{red}}(q, p). \qquad (38)$$

These equations will allow us to set up Friedmann-like equations with quantum corrections for q and p.

(ii) $\phi_n^{(\text{int})}$ dependent of q.—Let us examine the general case in which the eigenstates $|\phi_n^{(\text{int})}\rangle$ depend on q. We start again from the spectral decomposition

$$\hat{H}^{(\text{int})}(q) = \sum_n E_n^{(\text{int})}(q)|\phi_n^{(\text{int})}(q)\rangle\langle\phi_n^{(\text{int})}(q)|, \qquad (39)$$

and we pick some other q-independent orthonormal basis $|e_n^{(\text{int})}\rangle$ of the internal Hilbert space $\mathcal{H}^{(\text{int})}$. This change of basis is associated with the introduction of the q-dependent unitary operator

$$U(q) := \sum_n |\phi_n^{(\text{int})}(q)\rangle\langle e_n^{(\text{int})}|, \qquad (40)$$

which allows one to deal with the analogue of the Hamiltonian (28):

$$\tilde{\mathsf{H}}^{(\text{int})}(q) = U^\dagger(q)\hat{H}^{(\text{int})}(q)U(q) = \sum_n E_n^{(\text{int})}(q)|e_n^{(\text{int})}\rangle\langle e_n^{(\text{int})}|. \qquad (41)$$

The quantum Hamiltonian (25) now has the general form

$$\hat{H} = \mathcal{N}\left(\hat{p}^2 + \frac{K}{\hat{q}^2} + L\hat{q}^{\frac{2}{3}} - U(\hat{q})\tilde{\mathsf{H}}^{(\text{int})}(\hat{q})U^\dagger(\hat{q})\right). \quad (42)$$

The difference between the Hamiltonians of cases (i) and (ii) is the presence in (ii) of the unitary operator $U(\hat{q})$ that introduces a quantum correlation (entanglement) between the internal degrees of freedom (anisotropy) and the "external" one (the scale factor). As a consequence, any solution $|\Psi(t)\rangle$ of the time-dependent Schrödinger equation $i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$ cannot be factorized as a tensor

product like $|\phi(t)\rangle \otimes |\phi^{(\text{int})}(t)\rangle$, contrarily to case (i). In our case we wish to follow Klauder's approach to build some semiclassical Lagrangian analoguous to Eq. (31). We use the previous case (i) as a starting point (as a guide) to build approximate possible forms of $|\Psi(t)\rangle$.

It is interesting to notice that the Hamiltonian $\hat{\mathsf{H}}$ of Eq. (42) is unitarily equivalent to the one that occurs in quantum electrodynamics. For this purpose let us introduce the q-dependent operator $\hat{\mathsf{A}}(q)$ acting on the Hilbert space $\mathcal{H}^{(\text{int})}$ of internal degrees of freedom as

$$\hat{\mathsf{A}}(q) = i\hbar \frac{\mathrm{d}U}{\mathrm{d}q}(q) U^\dagger(q). \qquad (43)$$

As a matter of fact, $\hat{\mathsf{A}}(q)$ is self adjoint, and the Hamiltonian $\hat{\mathsf{H}}$ of Eq. (42) reads as

$$\hat{\mathsf{H}} = \mathcal{N}U(\hat{q})\left((\hat{p} - \hat{\mathsf{A}}(\hat{q}))^2 + \frac{K}{\hat{q}^2} + L\hat{q}^{\frac{2}{3}} - \tilde{\mathsf{H}}^{(\text{int})}(\hat{q}) \right) U^\dagger(\hat{q}). \qquad (44)$$

The form (44) [i.e. modulo the unitary transformation $U(\hat{q})$] is the most general form of the Hamiltonian of a particle moving on a half line and minimally coupled to an external field. This form is also most general on the grounds of the so-called shadow principle [33]. According to the principle, at any fixed time the state of an interacting particle should be indistinguishable from the state of a free particle and the Galilean addition rule of velocities should be preserved. In particular, if we interpret $\tilde{\mathsf{H}}^{(\text{int})}(q)$ as a q-dependent electromagnetic energy (despite all the differences) and $\hat{\mathsf{A}}(q)$ as a gauge field, the problem appears (up to a unitary transformation) similar to the one of a charged particle in interaction with an electromagnetic field.

Now, using (42) and taking into account the analysis of the previous case (i), one can define different possible expressions of $|\Psi(t)\rangle$:

(a) In the first approach we keep the tensor product expression of (i), but insert the q dependence of eigenstates. This corresponds to a Born-Oppenheimer-like approximation:

$$|\Psi(t)\rangle \approx |\lambda q(t), p(t)\rangle \otimes |\phi_n^{(\text{int})}(q(t))\rangle. \qquad (45)$$

(b) The second strategy consists in introducing some (minimal) entanglement between q and internal (anisotropy) degrees of freedom. This corresponds to a Born-Huang-like approximation:

$$|\Psi(t)\rangle \approx U(\hat{q})(|\lambda q(t), p(t)\rangle \otimes |e_n^{(\text{int})}\rangle). \qquad (46)$$

(c) In the third method one keeps the tensor product approximation, but includes a general time-dependent state for the internal degrees of freedom:

$$|\Psi(t)\rangle \approx |\lambda q(t), p(t)\rangle \otimes |\phi^{(\text{int})}(t)\rangle. \qquad (47)$$

(d) The fourth strategy is the most general one. It consists in merging (b) and (c):

$$|\Psi(t)\rangle \approx U(\hat{q})(|\lambda q(t), p(t)\rangle \otimes |\phi^{(\text{int})}(t)\rangle). \qquad (48)$$

Building now the semiclassical Lagrangian in agreement with the procedure defined in (i), we can distinguish two categories in the approximations listed above.

(1) (a)–(b) are completely manageable on the semiclassical level: they involve q and p as dynamical variables, while the anisotropy degrees of freedom are frozen in some eigenstate; (a) and (b) correspond typically to adiabatic approximations.

(2) (c)–(d) are more complicated: they mix a semiclassical dynamics for (q, p) and a quantum dynamics for the anisotropy degrees of freedom. This corresponds to "vibroniclike" approximations, well known in molecular physics and quantum chemistry [34]. In our case this means that different quantum eigenstates of the anisotropy degrees of freedom are involved in the dynamics: during the evolution excitations and decays are possible, with an exchange of energy with the "classical degree of freedom" (q, p).

The Bianchi-IX Hamiltonian belongs to the general case (ii). So the different approximations (a)–(d) presented above can be tested. In this paper we restrict ourselves to the presentation of the simplest cases (a)–(b). We postpone the study of the more complicated cases (c)–(d) to future papers.

C. Semiclassical constraint

We now proceed to the spectral analysis of the operator $\hat{\mathsf{H}}$ by making use of BO-like and BH-like approximations, presented in a general form in Sec. III B, and to its semiclassical analysis through affine coherent states.

1. Born-Oppenheimer approximation

In this approximation we assume that the anisotropy degrees of freedom are frozen in some eigenstate $|\phi_n^{(\text{int})}(q(t))\rangle$, evolving adiabatically, of the q-dependent Hamiltonian $\hat{\mathsf{H}}_q$ given by (21). If we denote by $E_N(q)$ the eigenenergies of $\hat{\mathsf{H}}_q$, the reduced Hamiltonian $\hat{\mathsf{H}}_N^{\text{red}}$ of Eq. (30) reads

$$\hat{\mathsf{H}}_N^{\text{red}} = \frac{9}{4}\left(\hat{p}^2 + \frac{\hbar^2 \boldsymbol{\mathfrak{K}}_1}{\hat{q}^2} \right) + 36\mathfrak{n}^2 \boldsymbol{\mathfrak{K}}_3 \hat{q}^{2/3} - E_N(\hat{q}). \qquad (49)$$

Due to the harmonic behavior of $V_{\mathfrak{n}}$ near its minimum, i.e.,

$$V_{\mathfrak{n}}(\beta) = 8\mathfrak{n}^2(\beta_+^2 + \beta_-^2) + o(\beta_\pm^2), \qquad (50)$$

the harmonic approximation to the eigenenergies $E_N(q)$ is manageable ($N = 0, 1, \ldots$), giving

$$E_N(q) \simeq \frac{24\hbar}{q^{2/3}} \mathfrak{n} \sqrt{2\mathfrak{K}_2 \mathfrak{K}_3} (N + 1). \tag{51}$$

In fact $N = n_+ + n_-$, $n_\pm \in \mathbb{N}$. More details, including a discussion of another common approximation made for the anisotropy potential, are given in Appendix B.

We remark that the harmonic form of $E_N(q)$ is an increasingly rough approximation for large values of N, since $V_{\mathfrak{n}}$ is highly nonharmonic far from its minimum. But for small values of N, this expression is valid for any value of q. The steep wall approximation (see Appendix B) is able to give a better expression for the eigenenergies as their values go to infinity. However, both approximations do not change the main line of reasoning in what follows.

Taking into account the rescaling of affine coherent states (see Sec. III B 2), the semiclassical expression $\check{\mathsf{H}}_N^{\text{red}}$ involved in Eq. (35) is defined as

$$\check{\mathsf{H}}_N^{\text{red}}(q, p) = \langle \lambda q, p | \hat{\mathsf{H}}_N^{\text{red}} | \lambda q, p \rangle, \tag{52}$$

where $\lambda := \xi_{02}(\nu)$ is chosen to get the exact correspondence (see Sec. III B 2)

$$\langle \lambda q, p | \hat{q} | \lambda q, p \rangle = q, \qquad \langle \lambda q, p | \hat{p} | \lambda q, p \rangle = p. \tag{53}$$

Finally, we obtain

$$\check{\mathsf{H}}_N^{\text{red}}(q, p) = \frac{9}{4}\left(p^2 + \frac{\hbar^2 \mathfrak{K}_4}{q^2} \right) + 36\mathfrak{n}^2 \mathfrak{K}_5 q^{2/3}$$
$$- \frac{24\hbar}{q^{2/3}} \mathfrak{K}_6 \mathfrak{n}(N + 1), \tag{54}$$

where the three new constants $\mathfrak{K}_i = \mathfrak{K}_i(\nu)$ are given by

$$\mathfrak{K}_4 = (\xi_{10})^2 \left(\frac{\nu^2}{16} + \frac{\nu}{4}\xi_{21} + \frac{3\nu}{8}\xi_{10} + \xi_{20} \right),$$
$$\mathfrak{K}_5 = \xi_{\frac{2}{3}1} \left(\xi_{\frac{5}{3}0} \right)^{1/3} \left(\xi_{\frac{5}{3}2} \right)^{2/3},$$
$$\mathfrak{K}_6 = \sqrt{2}(\xi_{10})^{4/3}(\xi_{20})^{5/3} \left(\xi_{\frac{5}{3}1} \right)^{1/2}. \tag{55}$$

For large values of ν (typically $\nu \gtrsim 20$) we get

$$\mathfrak{K}_4 \simeq \frac{\nu^2}{16}, \qquad \mathfrak{K}_5 \simeq 1, \qquad \mathfrak{K}_6 \simeq \sqrt{2}. \tag{56}$$

2. Born-Huang approximation

In the Born-Huang approximation framework (see Sec. III B 2), we also assume that the anisotropy degrees of freedom are frozen in some eigenstate, but it is an eigenstate $|e_n^{(\text{int})}\rangle$ of the Hamiltonian $\tilde{\mathsf{H}}^{(\text{int})}(q)$ introduced in

Eq. (41). In the case of Bianchi IX, thanks to the harmonic approximation of $V_{\mathfrak{n}}(\beta)$, we can find an approximation for $\tilde{\mathsf{H}}^{(\text{int})}(q)$ and the corresponding unitary operator $U(q)$ in Eq. (40). We get

$$U(q) \simeq e^{\frac{2i}{3}(\ln q)\hat{\mathsf{D}}}, \tag{57}$$

with

$$\hat{\mathsf{D}} = \hat{\mathsf{D}}_+ + \hat{\mathsf{D}}_-, \qquad \hat{\mathsf{D}}_\pm = \frac{1}{2\hbar}(\hat{p}_\pm \hat{\beta}_\pm + \hat{\beta}_\pm \hat{p}_\pm). \tag{58}$$

The gauge field $\hat{\mathsf{A}}(q)$ given in Eq. (43) becomes

$$\hat{\mathsf{A}}(q) = -\frac{2\hbar}{3q}\hat{\mathsf{D}}. \tag{59}$$

As it is shown in Appendix B, the harmonic approximation implies that the eigenstates $|e_n^{(\text{int})}\rangle$ depend in fact on two positive integers $n_\pm$ (we use the notation $|e_{n_\pm}^{(\text{int})}\rangle$). It results in

$$\langle e_{n_\pm}^{(\text{int})} | \hat{\mathsf{D}} | e_{n_\pm}^{(\text{int})} \rangle = 0,$$
$$\langle e_{n_\pm}^{(\text{int})} | \hat{\mathsf{D}}^2 | e_{n_\pm}^{(\text{int})} \rangle = \frac{1}{2}(n_+^2 + n_-^2 + n_+ + n_- + 3). \tag{60}$$

Therefore, the expectation value $\langle \Psi(t) | \hat{\mathsf{H}} | \Psi(t) \rangle$ of the Hamiltonian $\hat{\mathsf{H}}$, as defined in (44), for $|\Psi(t)\rangle = U(\hat{q})(|\lambda q(t), p(t)\rangle \otimes |e_{n_\pm}^{(\text{int})}\rangle)$ corresponding to the case III C 2 (Born-Huang-like approximation), reads

$$\langle \Psi(t) | \hat{\mathsf{H}} | \Psi(t) \rangle = \langle \lambda q(t), p(t) | \left[\frac{9}{4}\left(\hat{p}^2 + \frac{\hbar^2(\mathfrak{K}_1 + \chi(n_+, n_-))}{\hat{q}^2} \right) \right.$$
$$\left. + 36\mathfrak{n}^2 \mathfrak{K}_3 \hat{q}^{2/3} - E_N(\hat{q}) \right] | \lambda q(t), p(t) \rangle, \tag{61}$$

with

$$N = n_+ + n_-, \quad \text{and}$$
$$\chi(n_+, n_-) = \frac{2}{9}(n_+^2 + n_-^2 + n_+ + n_- + 3). \tag{62}$$

Hence, up to the modification $\mathfrak{K}_1 \mapsto \mathfrak{K}_1 + \chi(n_+, n_-)$, we recover the previous expression of Eq. (49) for the Born-Oppenheimer-like case III C 1. From Eq. (54) we deduce the final expression of the semiclassical Hamiltonian [in the harmonic approximation of $V_{\mathfrak{n}}(\beta)$]

$$\check{\mathsf{H}}_{n_\pm}^{\mathrm{red}}(q, p) = \frac{9}{4}\left(p^2 + \frac{\hbar^2(\mathfrak{K}_4 + \mathfrak{K}_4'\chi(n_+, n_-))}{q^2}\right)$$

$$+ 36\mathfrak{n}^2\mathfrak{K}_5 q^{2/3} - \frac{24\hbar}{q^{2/3}}\mathfrak{K}_6\mathfrak{n}(N+1), \qquad (63)$$

where $\mathfrak{K}_4' = (\xi_{10})^2\xi_{20}$.

IV. SEMICLASSICAL DYNAMICS

The quantum-corrected constraint $\check{\mathsf{H}}_N^{\mathrm{red}}(q, p) = 0$ may be interpreted as a semiclassical version of the Friedmann equation. The anisotropic degrees of freedom, averaged at the quantum level, give rise to the isotropic radiation energy density. This energy gravitates like common matter and fuels the contraction. It leads to a supplementary term in the Friedmann equation, shown below.

A. Effective Friedmann-like equation

Rewritten in terms of the scale factor a, the constraint $\check{\mathsf{H}}_{av}(q, p) = 0$ reads

$$\frac{\dot{a}^2}{a^2} + k\frac{c^2}{a^2} + c^2\ell^{-2}\frac{\mathfrak{K}_4}{a^6} = \frac{8\pi G}{3c^2}\rho(a), \qquad (64)$$

where, using the Planck area $\mathfrak{a}_P = 2\pi G\hbar c^{-3}$,

$$k = \frac{\mathfrak{K}_5\mathfrak{n}^2}{4}, \qquad \ell = \frac{\mathcal{V}_0}{\mathfrak{a}_P}, \qquad \rho(a) = \mathfrak{n}\mathcal{V}_0^{-1}\mathfrak{K}_6\frac{\hbar c(N+1)}{a^4}. \tag{65}$$

The classical constraint (18) is recovered for $\hbar \to 0$. The main features of this quantum-corrected model are the following:

(i) The value of the isotropic curvature, kc^2a^{-2}, present in closed FRW models, is dressed by the quantization with a constant $\mathfrak{K}_5$, which is close enough to 1 to be ignored in qualitative considerations.

(ii) The *repulsive* potential term proportional to a^{-6}, absent in classical FRW/BIX models, is generated by the affine CS quantization.

(iii) The energy of the anisotropic oscillations is turned at the quantum level into the radiation energy, $\rho(a)$. The expression for $\rho(a)$ in terms of the quantum number N becomes a poor approximation for high values of N, due to the breakdown of harmonic approximation. Nevertheless, the dimensional analysis shows that the dependence $\rho(a) \propto \mathfrak{n}\mathcal{V}_0^{-1}\hbar ca^{-4}$ is correct for $a \to 0$.

B. Comparing classical with semiclassical constraint

The classical Friedmann equation generalized to Bianchi-IX geometry reads

$$\frac{\dot{a}^2}{a^2} + \frac{1}{6}{}^3R - \frac{1}{6}\Sigma^2 = 0, \qquad (66)$$

where ${}^3R$ and Σ^2 are respectively the curvature and shear of the spatial sections. The Bianchi-IX curvature (9) may be split into isotropic and anisotropic parts and the shear may be expressed in Misner's canonical variables as follows:

$${}^3R = 3\frac{1 - V(\beta)}{2a^2}, \qquad \Sigma^2 = \frac{p_+^2 + p_-^2}{24a^6}, \qquad (67)$$

where the anisotropic part of curvature potential $V(\beta)$, defined by (11) and (15), reads explicitly as

$$V(\beta) = \frac{e^{4\beta_+}}{3}((e^{-6\beta_+} - 2\cosh(2\sqrt{3}\beta_-))^2 - 4) + 1.$$

This way we arrive at the following form of (66):

$$\frac{\dot{a}^2}{a^2} + \frac{1}{4a^2} = \frac{1}{6}\frac{p_+^2 + p_-^2}{24a^6} + \frac{V(\beta)}{4a^2}. \qquad (68)$$

The left-hand side of (68) contains only the isotropic variables, whereas the right-hand side contains all the anisotropic terms. The first and the second term of (64), namely $\dot{a}^2a^{-2}$ and kc^2a^{-2}, correspond to the first and second term of (68), i.e. to $\dot{a}^2a^{-2}$ and $(2a)^{-2}$, respectively. The third term in (64), $c^2\ell^{-2}\mathfrak{K}_4a^{-6}$, has no corresponding term in the classical equation. It is a purely quantum effect induced by the affine CS quantization. The right-hand side of (64) describes the quantized anisotropic energy, which depends on the scale factor as a^{-4}. It corresponds to the energy of anisotropy oscillations in the rhs of (68), which depends on the scale factor roughly as a^{-6}. This difference between the right-hand sides of (64) and (68) in dependence on a is another purely quantum effect.

Concerning the curvaturelike term $\mathfrak{K}_5\mathfrak{n}^2c^2(2a)^{-2}$ in the semiclassical Eq. (64), we note that it reproduces the classical recollapse in the evolution of the vacuum Bianchi-IX model, which results from S^3 topology of this model [35]. The recollapse is included in the plots of Fig. 3. The fact that our semiclassical procedure reproduces this particular classical feature can be viewed as the confirmation of the consistency of our approach.

Furthermore, from the semiclassical Lagrangian approach developed in Sec. III B, we note that any effective matter term $F(q) = \rho(q^{2/3})$ with $\rho(a) = Ka^{-n}$ may be incorporated in the Lagrangian of Eq. (25), leading after the action minimization of Eq. (27) to a supplementary matter term $\tilde{\rho}(a) = \xi Ka^{-n} = \xi\rho(a)$, $(\xi > 0)$, in the rhs of Eq. (64). Therefore adding an effective radiative matter term like ρ_0a^{-4} (where ρ_0 is a positive constant) into the rhs of (64) would bring only a quantitative change in the semiclassical dynamics as it scales exactly as quantized anisotropy.

C. Singularity resolution

Equation (64) implies

$$kc^2 + c^2\ell^{-2}\frac{\mathfrak{K}_4}{a^4} - \frac{8\pi G}{3c^2}a^2\rho(a) \leq 0, \qquad (69)$$

which defines the allowed values assumed by a. The inequality (69) can be satisfied only for

$$(N+1)^2 \geq \frac{9}{16}\frac{\mathfrak{K}_4\mathfrak{K}_5}{\mathfrak{K}_6^2}, \qquad (70)$$

or $(N+1)^2 \geq f(\nu)$ with

$$f(\nu) := \frac{9}{32}(\xi_{02})^4(\xi_{10})^{1/3}\xi_{\frac{2}{3}1}^2\left(\frac{\nu^2}{16}+\frac{\nu}{4}\xi_{21}+\frac{3\nu}{8}\xi_{10}+\xi_{20}\right). \qquad (71)$$

The function $f(\nu)$ is strictly increasing, from 0 to $+\infty$, with $f(\nu) \simeq \frac{9}{512}\nu^2$ in the limit $\nu \to \infty$. Therefore for each value of N, there exists a bounded interval $]0,\nu_m(N)]$ for which the condition (71) holds true, with $f(\nu_m(N)) = (N+1)^2$.

For large values of N, we have $\nu_m(N) \simeq \frac{16\sqrt{2}}{3}(N+1)$, and $\nu_m(N) \geq \nu_m(0) \simeq 7.4$. Thus, for $\nu \in]0,\nu_m(0)[$ and for all $N \geq 0$, the condition (69) is satisfied. We find that $a \in [a_-, a_+]$, where

$$a_\pm^2 = \frac{8\mathfrak{a}_P}{3\mathfrak{n}\mathcal{V}_0}\frac{\mathfrak{K}_6}{\mathfrak{K}_5}(N+1)\left(1 \pm \sqrt{1 - \frac{f(\nu)}{(N+1)^2}}\right). \qquad (72)$$

Therefore, the semiclassical trajectories turn out to be *periodic*, and a is *bounded* from below by a_-. This demonstrates that the system does not have the singularity that occurs at the classical level of the FRW/BIX model. We note that $a_\pm$ is dimensionless as $\mathfrak{n}\mathcal{V}_0 \propto \mathfrak{n}^{-2}$ is homogeneous to an area. Moreover, the volume of the Universe, $a^3\mathcal{V}_0$, is independent of $\mathfrak{n}$. This proves that our result is physical.

In Fig. 3 we plot a few trajectories in the half plane (a, H). The classical closed FRW model is recovered at $\hbar = 0$ and large values of ν.

Some remarks are appropriate:
(i) The product a_-a_+ is only dependent on ν,

$$a_-a_+ = \frac{2\mathfrak{a}_P}{\mathfrak{n}\mathcal{V}_0}\sqrt{\frac{\mathfrak{K}_4}{\mathfrak{K}_5}}. \qquad (73)$$

(ii) Specifying N and $\nu = \nu_m(N)$, the relation $a_- = a_+$ holds true so we have an unusual feature of a stationary universe with finite radius.
(iii) For $N = 0$ and $\nu \in]0,\nu_m(0)[$, the model shows the effect of the quantum zero point energy of the anisotropy degrees of freedom.
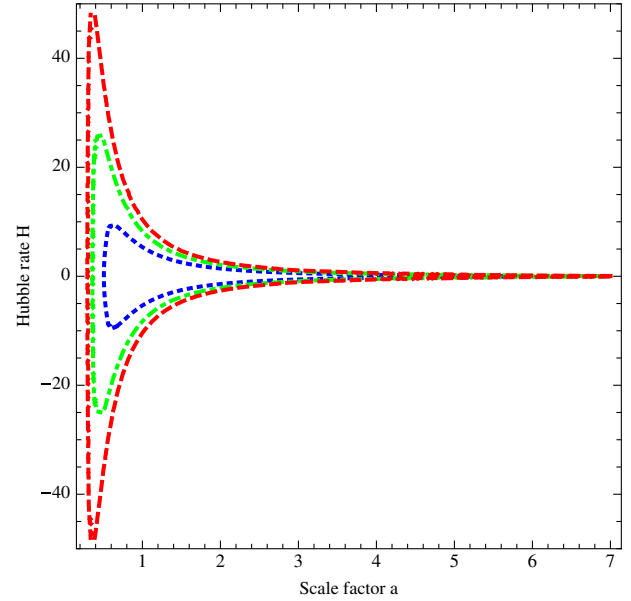

FIG. 3 (color online). Three periodic semiclassical trajectories in the half plane (a, H) from Eq. (64). They are smooth plane curves. We use standard units $\mathfrak{a}_P = c = \hbar = 1$ and choose $\nu = 3$, $\mathcal{V}_0 = 1$ [so $\mathfrak{n} = (16\pi^2)^{1/3}$], blue dotted curve for $N = 0$, green dot dashed for $N = 1$ and red dashed for $N = 2$. Each plot includes the quantum bounce (at small a) and classical recollapse (at large a).

(iv) For $\nu \in]0,\nu_m(0)[$ and all $N \geq 0$, the oscillation period T of the Universe is

$$T = \frac{4}{\mathfrak{n}c\sqrt{\mathfrak{K}_5}}a_-E\left(1 - \left(\frac{a_+}{a_-}\right)^2\right), \qquad (74)$$

where E is the complete elliptic integral of the second kind [31].

V. BEYOND ADIABATIC APPROXIMATION

As we have seen in Sec. II, when the isotropy of the closed FRW universe is perturbed, the Universe acquires the Bianchi-IX geometry and a small perturbation inevitably develops in the chaotic regime, first described in Ref. [1]. To see whether such behavior is possible at the quantum level, we now go beyond the adiabatic approximation and allow the number of particles N to grow as the Universe contracts, bounces and reexpands. We assume that the scale factor is a c-number, which evolves according to the semiclassical constraint (64) for $N = 0$. The anisotropy degrees of freedom are quantized as before but with the possibility to be excited by the time-dependent background.

We resort to the well-known fact about the harmonic oscillator that its classical and quantum dynamics of the basic variables are in one-to-one correspondence and we work in the Heisenberg picture by solving classical equations of motion. First, we find the semiclassical evolution of

a in suitable time parameter, τ. Then we use this evolution to define our wave in the time-dependent background in terms of an oscillator with "time-dependent mass." Finally, we perform numerical computations.

A. Evolution of scale factor

The semiclassical constraint (64) may be written as

$$H^2 + \frac{\Lambda_1}{a^6} + \frac{\Lambda_0}{a^2} = \frac{\Lambda_2}{a^4}. \tag{75}$$

In what follows we set $\Lambda_0 = 0$. This simplification removes the classical recollapse; the Universe expands forever now. This is a good approximation as we are not interested in the classical phase but in the quantum one during which the isotropic intrinsic curvature is assumed negligible. Moreover, we may work in natural units in which $\Lambda_1 \simeq \Lambda_2$ as both terms originate from quantum theory.

We find from (75)

$$dt = \frac{1}{\sqrt{\Lambda_2}} \frac{a^2 da}{\sqrt{a^2 - \frac{\Lambda_1}{\Lambda_2}}} \tag{76}$$

where t is the cosmological time.

The dynamics of anisotropy is given by the background-dependent Hamiltonian:

$$\mathsf{H}_{\pm} = \frac{1}{2} p_{\pm}^2 + 144\mathfrak{n}^2 a^4(\tau)\beta_{\pm}^2 \tag{77}$$

which is a part of the Hamiltonian constraint (16)–(17) if the lapse is set to $\mathcal{N} = -12a^3$. The idea of the subsequent calculations is to treat $a(\tau)$ as a fixed function of time. To obtain the correct solution $a(\tau)$, we need to adjust (76) for the choice of lapse $\mathcal{N}$. We find

$$d\tau = \frac{dt}{\mathcal{N}} = -\frac{1}{12\sqrt{\Lambda_2}} \frac{da}{a\sqrt{a^2 - \frac{\Lambda_1}{\Lambda_2}}}$$

$$= \frac{1}{12\sqrt{\Lambda_2}} d\left[\arcsin\left(\sqrt{\frac{\Lambda_1}{\Lambda_2}}a^{-1}\right)\right]; \tag{78}$$

hence

$$a(\tau) = \frac{\sqrt{\frac{\Lambda_1}{\Lambda_2}}}{\sin\left(12\sqrt{\Lambda_2}\tau + \frac{\pi}{2}\right)} \tag{79}$$

where $\tau \in \left(-\frac{\pi}{24\sqrt{\Lambda_2}}, \frac{\pi}{24\sqrt{\Lambda_2}}\right)$ and $a \in \left(+\infty, \sqrt{\frac{\Lambda_1}{\Lambda_2}}\right)$.

B. Excitation of quantum oscillator

The Hamiltonian under study is

$$\mathsf{H}_{\pm} = \frac{1}{2} p_{\pm}^2 + \frac{1}{2}\omega^2(\tau)\beta_{\pm}^2 \tag{80}$$

where $\omega = 12\sqrt{2}\mathfrak{n}a^2(\tau)$. In what follows we drop $\pm$ for brevity. The equation of motion reads

$$\frac{d^2\beta}{d\tau^2} = -\omega^2(\tau)\beta. \tag{81}$$

We work in the Heisenberg picture, and assume that

$$\hat{\beta}(\tau) = \frac{1}{\sqrt{2}}(av^*(\tau) + a^\dagger v(\tau)),$$

$$\hat{p}(\tau) = \frac{1}{\sqrt{2}}(a\acute{v}^*(\tau) + a^\dagger \acute{v}(\tau)) \tag{82}$$

where a and $a^\dagger$ are fixed operators and where $v(\tau)$ solves Eq. (81), i.e.,

$$\frac{d^2 v}{d\tau^2} = -\omega^2(\tau)v. \tag{83}$$

We demand the canonical commutation relation and obtain

$$iI = [\hat{\beta}, \hat{p}] = \left[\frac{1}{\sqrt{2}}(av^*(\tau) + a^\dagger v(\tau)), \frac{1}{\sqrt{2}}(a\acute{v}^*(\tau) + a^\dagger \acute{v}(\tau))\right]$$

$$= [a, a^\dagger]\frac{v^*\acute{v} - v\acute{v}^*}{2}. \tag{84}$$

We find from Eq. (83)

$$\frac{d}{d\tau}(v^*\acute{v} - v\acute{v}^*) = 0 \tag{85}$$

and we fix $v^*\acute{v} - v\acute{v}^* = 2i$. So a and $a^\dagger$ are annihilation and creation time-independent operators. All time dependence lies in $v(\tau)$.

The Hamiltonian now reads

$$\hat{\mathsf{H}} := \frac{1}{2}\hat{p}^2 + \frac{1}{2}\omega^2(\tau)\hat{\beta}^2$$

$$= \frac{a^2}{4}((\acute{v}^*)^2 + \omega^2(v^*)^2) + \frac{(a^\dagger)^2}{4}(\acute{v}^2 + \omega^2 v^2)$$

$$+ \frac{2a^\dagger a + 1}{4}(|\acute{v}|^2 + \omega^2|v|^2). \tag{86}$$

We set the vacuum state $|0\rangle$ for $a, a^\dagger$ to minimize the energy at some initial moment τ_0. It follows that

$$v(\tau_0) = \frac{1}{\sqrt{\omega(\tau_0)}}, \qquad \acute{v}(\tau_0) = i\sqrt{\omega(\tau_0)} \tag{87}$$

and hence

$$\hat{\mathsf{H}}(\tau_0) := \left(a^\dagger a + \frac{1}{2}\right)\omega(\tau_0) \tag{88}$$

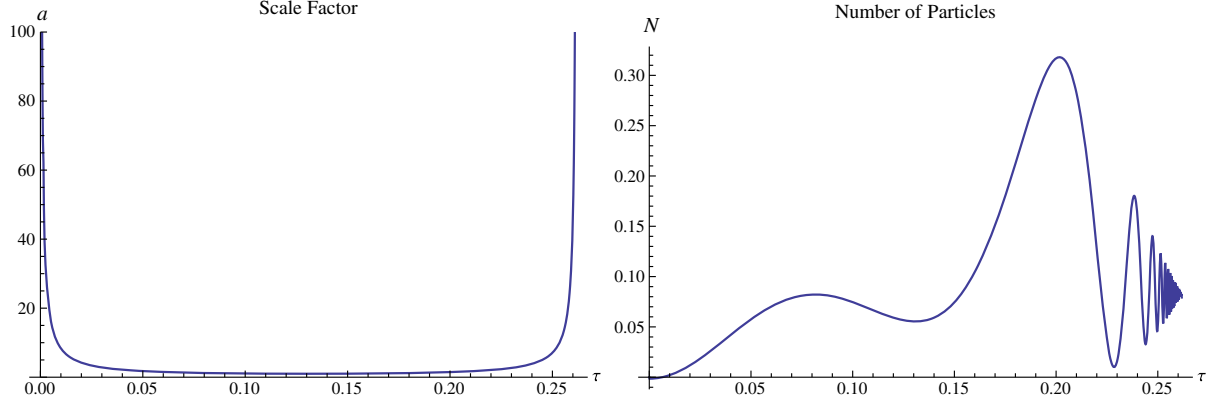where $\omega(\tau_0) = 12\sqrt{2}\mathfrak{n}a^2(\tau_0)$.

FIG. 4 (color online). The evolution of the number of particles N and the scale factor a from the contracting phase through the semiclassical bounce to the expanding phase. We fix $\Lambda_1 = 1 = \Lambda_2$, $\mathfrak{n} = 1$, and $a(\tau_0) = 10^4$.

Now, if we assume $|0\rangle$ to be the initial quantum state, and take into account both modes "$\pm$," then the number of particles N at some later time τ_1 can be found with the formula

$$\langle 0|N(\tau_1)+1|0\rangle = \frac{\langle 0|\hat{H}_+(\tau_1)+\hat{H}_-(\tau_1)|0\rangle}{\omega(\tau_1)}$$

$$= \frac{|\acute{v}|^2(\tau_1)+288\mathfrak{n}^2 a^4(\tau_1)|v|^2(\tau_1)}{24\sqrt{2}\mathfrak{n}a^2(\tau_1)}. \quad (89)$$

What remains to be solved is (83) with initial data (87).

C. Numerical results

We fix units so that $\Lambda_1 = 1 = \Lambda_2$ and also $\mathfrak{n} = 1$. So the Universe contracts from $a = \infty$, bounces at $a = 1$ and reexpands to $a = \infty$. We set the initial data as $a(\tau_0) = 10^4$. In Fig. 4 we plot the number of particles and the scale factor versus time. We also find that varying initial a from 10^4 to 10 does not affect the number of particles produced, which never exceeds 0.35.

VI. CONCLUSIONS

In this article we have examined the quantum dynamics of the vacuum Bianchi-IX model, the mixmaster universe. The Hamiltonian constraint, which consists of isotropic and anisotropic variables, has been quantized. This split of variables is crucial both for implementing our procedure and interpreting the result. Suitable coherent states, namely the ACS, have been employed to obtain some insight into the involved quantum dynamics of isotropic background. Making use of adiabatic approximation, we have identified the eigenstates for the oscillating anisotropy at its lowest excitation levels. Our procedure, developed by qualitative arguments and based on reasonable and tractable approximations, i.e. the replacement of the anisotropy potential with the harmonic potential and the Born-Oppenheimer-type evolution, is validated by considerations outside the adiabatic approximation.

The main features of our quantum model are the following: (i) the singularity avoidance due to a repulsive term regularizing the singular spacetime geometry; (ii) the reduced contraction rate of the Universe due to suppressed growth of the energy of anisotropy at the quantum level as it becomes frozen in a fixed quantum state; and (iii) the stability of quantum Friedmann-like state in the quantum Bianchi-IX model both in the contraction and expansion phase. We emphasize that the anisotropic oscillations have a nonzero ground energy level, which means that there is no true quantum FRW state.

The resolution of the singularity is due to the repulsive potential generated by the ACS quantization as in [20]. We note that our approach to "quantizing singularity" is very natural. It was developed within an appealing probabilistic interpretation of quantization procedures and, in a sense, it extends what is usually meant by canonical quantization (see Appendix A). Our approach is universal in the sense that it removes the singularity from anisotropic models, recently shown to be true also for Bianchi-I models in [36].

In our framework, due to the Born-Oppenheimer approximation, the anisotropy degrees of freedom are assumed to be in a quantum eigenstate. This property leads to the radiation energy density. In the near future, we will focus on developing our scheme to include transitions between different energy levels by more detailed computations. The Born-Huang-like approximation is just a refined version of the adiabatic approximation as shown in Sec. III B. Qualitatively, the Born-Huang-like approximation does not change the behavior of the semiclassical Hamiltonian obtained within the Born-Oppenheimer-like approximation, because the former generates a supplementary positive term $\propto q^{-2}$ that only renormalizes the term already present (due to our affine CS quantization). On the other hand, if we apply only canonical quantization to the system, then no term in q^{-2} is present at the beginning in the Born-Oppenheimer-like approximation. In that case the Born-Huang-like approximation generates a new term in the semiclassical

behavior. Since this repulsive term is responsible for the resolution of the singularity, we can say that, with or without ACS quantization, the resolution of the singularity holds true in the case of the Bianchi-IX model within the framework of the Born-Huang approximation.

We emphasize that our approach is completely different from Misner's, which was based on the so-called steep wall approximation, discussed in Appendix B. In the steep wall approximation, there is no tendency for quantum probability to be peaked in the minimum of potential, and therefore there would probably be no quantum suppression of anisotropy as it occurs for the real potential revealed in the harmonic approximation of our paper.

We have shown that the wave remains in its lowest energy states during the quantum phase. Even beyond adiabatic approximation there is no significant excitation of the wave's energy level. It is interpreted that the quantum FRW universe, unlike its classical version, is dynamically stable with respect to small isotropy perturbation. Thus, supplementing the FRW Hamiltonian with the zero-point energy originating from quantization of anisotropic degrees of freedom provides a quantum version of the Friedmann model which could be used for a study of the earliest universe.

APPENDIX A: AFFINE COHERENT STATE QUANTIZATION

Coherent state quantization is a particular approach pertaining to what is named in [30] integral quantization. When a group action is involved in the construction, one can insist on covariance aspects of the method. A detailed presentation of the subject is given in [30] and in chapter 11 of [37]. In this appendix, we give a short compendium of this approach before particularizing to the integral quantization issued from the affine group representation.

1. Covariant integral quantizations

Lie group representations [38] offer a wide range of possibilities for implementing integral quantization(s). Let G be a Lie group with left Haar measure $d\mu(g)$, and let $g \mapsto U(g)$ be a UIR of G in a Hilbert space $\mathcal{H}$. Consider a bounded operator M on $\mathcal{H}$ and suppose that the operator

$$R := \int_G \mathsf{M}(g)d\mu(g), \qquad \mathsf{M}(g) := U(g)\mathsf{M}U^\dagger(g) \quad (A1)$$

is defined in a weak sense. From the left invariance of $d\mu(g)$ we have

$$U(g_0)RU^\dagger(g_0) = \int_G \mathsf{M}(g_0 g)d\mu(g) = R, \qquad (A2)$$

so R commutes with all operators $U(g)$, $g \in G$. Thus, from Schur's lemma, $R = c_M I$ with

$$c_M = \int_G \mathrm{tr}(\rho_0 \mathsf{M}(g))d\mu(g), \qquad (A3)$$

where the unit trace positive operator ρ_0 is chosen in order to make the integral converge. This family of operators provides the resolution of the identity on $\mathcal{H}$.

$$\int_G \mathsf{M}(g)d\nu(g) = I, \qquad d\nu(g) := \frac{d\mu(g)}{c_M}, \qquad (A4)$$

and the subsequent quantization of complex-valued functions (or distributions, if well defined) on G

$$f \mapsto A_f = \int_G \mathsf{M}(g)f(g)d\nu(g). \qquad (A5)$$

This linear map, function $\mapsto$ operator in $\mathcal{H}$, is covariant in the sense that

$$U(g)A_f U^\dagger(g) = A_{\mathfrak{U}(g)f}. \qquad (A6)$$

In the case when $f \in L^2(G, d\mu(g))$, the quantity $(\mathfrak{U}(g)f)(g') := f(g^{-1}g')$ is the regular representation.

A semiclassical analysis of the operator A_f can be implemented through the study of lower symbols. Suppose that M is a density, i.e. non-negative unit trace, operator $\mathsf{M} = \rho$ on $\mathcal{H}$. Then the operators $\rho(g)$ are also density, and this allows one to build a new function $\check{f}(g)$ as

$$\check{f}(g) \equiv \check{A_f} := \int_G \mathrm{tr}(\rho(g)\rho(g'))f(g')d\nu(g'). \qquad (A7)$$

The map $f \mapsto \check{f}$ is a generalization of the Berezin or heat kernel transform on G (see [39] and references therein). One observes that the value $\check{f}(g)$ is the average about g of the original f with respect to the probability distribution on $[G, d\nu(g')]$ defined by $g' \mapsto \mathrm{tr}(\rho(g)\rho(g'))$.

Let us consider the above procedure in the case of square integrable UIRs and rank one ρ. For a square-integrable UIR U for which $|\psi\rangle$ is an admissible unit vector, i.e.,

$$c(\psi) := \int_G d\mu(g)|\langle\psi|U(g)|\psi\rangle|^2 < \infty, \qquad (A8)$$

the resolution of the identity is obeyed by the coherent states $|\psi_g\rangle = U(g)|\psi\rangle$, in a generalized sense, for the group G:

$$\int_G \rho(g)d\nu(g) = I, \qquad d\nu(g) = \frac{d\mu(g)}{c(\psi)},$$

$$\rho(g) = |\psi_g\rangle\langle\psi_g|. \qquad (A9)$$

2. The case of the affine group

As the complex plane is viewed as the phase space for the motion of a particle on the line, the half plane is viewed

as the phase space for the motion of a particle on the half line. Canonical quantization of the plane is covariant in the sense that it respects the translation symmetry of the plane through its Weyl-Heisenberg group extension. Our approach to the quantization of the half plane follows the same principle of covariance with respect the affine group structure of this geometry.

Let the upper half plane $\Pi_+ := \{(q, p)|p \in \mathbb{R}, q > 0\}$ be equipped with the measure $dq dp$. Together with the multiplication

$$(q, p)(q_0, p_0) = (qq_0, p_0/q + p), \qquad q \in \mathbb{R}_+^*, p \in \mathbb{R},$$
(A10)

the unity $(1,0)$ and the inverse

$$(q, p)^{-1} = \left(\frac{1}{q}, -qp\right),$$
(A11)

Π_+ is indeed viewed as the affine group $\text{Aff}_+(\mathbb{R})$ of the real line, and the measure $dq dp$ is left invariant with respect to this action. The affine group $\text{Aff}_+(\mathbb{R})$ has two nonequivalent UIRs [40,41]. Both are square integrable and this is the rationale behind continuous wavelet analysis (see the references in [37]). The UIR $U_+ \equiv U$ is realized in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}_+^*, dx)$:

$$U(q, p)\psi(x) = (e^{ipx}/\sqrt{q})\psi(x/q).$$
(A12)

By adopting the integral quantization scheme described above, we restrict to the specific case of rank-one density operator or projector $\rho = |\psi\rangle\langle\psi|$ where ψ is a unit-norm state in $L^2(\mathbb{R}_+^*, dx)$ which should also be in $L^2(\mathbb{R}_+^*, dx/x)$ (also called fiducial vector or wavelet). The action of UIR U produces all affine coherent states, i.e. wavelets, defined as $|q, p\rangle = U(q, p)|\psi\rangle$.

Due to the irreducibility and square integrability of the UIR U, the corresponding quantization reads as

$$f \mapsto A_f = \int_{\Pi_+} f(q, p)|q, p\rangle\langle q, p|\frac{dq dp}{2\pi c_{-1}},$$
(A13)

which arises from the resolution of the identity

$$\int_{\Pi_+} |q, p\rangle\langle q, p|\frac{dq dp}{2\pi c_{-1}} = I,$$
(A14)

where

$$c_\gamma := \int_0^\infty |\psi(x)|^2 \frac{dx}{x^{2+\gamma}}.$$
(A15)

Thus, a necessary condition to have (A14) be true is that $c_{-1} < \infty$, which explains the needed square integrability of ψ with respect to dx/x implying $\psi(0) = 0$, a well-known requirement in wavelet analysis.

The map (A13) is covariant with respect to the unitary affine action U:

$$U(q_0, p_0)A_f U^\dagger(q_0, p_0) = A_{\mathfrak{U}(q_0, p_0)f},$$
(A16)

with

$$(\mathfrak{U}(q_0, p_0)f)(q, p) = f((q_0, p_0)^{-1}(q, p))$$
$$= f\left(\frac{q}{q_0}, q_0(p - p_0)\right),$$
(A17)

$\mathfrak{U}$ being the left regular representation of the affine group. In particular, this (fundamental) property is used to prove Eq. (52).

To simplify, we pick a real fiducial vector. For the simplest functions, the affine CS quantization produces the following operators:

$$A_p = -i\frac{\partial}{\partial x} \equiv \hat{p}, \qquad A_{q^\beta} = \frac{c_{\beta-1}}{c_{-1}}\hat{q}^\beta, \qquad \hat{q}f(x) = xf(x).$$
(A18)

Whereas $A_q = (c_0/c_{-1})\hat{q}$ is self adjoint, the operator $\hat{p} = A_p$ is symmetric but has no self-adjoint extension. We check that this affine quantization is, up to a multiplicative constant, canonical, $[A_q, A_p] = ic_0/c_{-1}I$.

We obtain the exact canonical rule (i.e. $A_q = \hat{q}$ and $A_p = \hat{p}$) by imposing $c_0 = c_{-1}$. This simply corresponds to a rescaling of the fiducial vector ψ as $\psi_1(x) = \psi(x/\mu)/\sqrt{\mu}$ with $\mu = c_0/c_{-1}$. In the remainder we assume that this rescaling has been done and therefore $c_0(\psi) = c_{-1}(\psi)$.

The quantization of the product qp yields

$$A_{qp} = \frac{c_0}{c_{-1}}\frac{\hat{q}\hat{p}+\hat{p}\hat{q}}{2} = \frac{\hat{q}\hat{p}+\hat{p}\hat{q}}{2} \equiv D,$$
(A19)

where D is the dilation generator. As one of the two generators (with $\hat{q}$) of the UIR U of the affine group, it is essentially self adjoint.

The quantization of the kinetic energy gives

$$A_{p^2} = \hat{p}^2 + K\hat{q}^{-2}, \qquad K = K(\psi) = \int_0^\infty (\psi'(u))^2 u \frac{du}{c_{-1}}.$$
(A20)

Therefore, wavelet quantization prevents a quantum free particle moving on the positive line from reaching the origin. It is well known that the operator $\hat{p}^2 = -d^2/dx^2$ in $L^2(R_+^*, dx)$ is not essentially self adjoint, whereas the above regularized operator, defined on the domain of smooth function of compact support, is essentially self adjoint for $K \geq 3/4$ [42]. Then quantum dynamics of the free motion is unique.

As usual, the semiclassical aspects are included in the phase space. The quantum states and their dynamics have

phase space representations through wavelet symbols. For the state $|\phi\rangle$ one has

$$\Phi(q, p) = \langle q, p|\phi\rangle/\sqrt{2\pi}, \tag{A21}$$

with the associated probability distribution on phase space given by

$$\rho_\phi(q, p) = \frac{1}{2\pi c_{-1}}|\langle q, p|\phi\rangle|^2. \tag{A22}$$

Having the (energy) eigenstates of some quantum Hamiltonian H at our disposal, we can compute the time evolution

$$\rho_\phi(q, p, t) := \frac{1}{2\pi c_{-1}}|\langle q, p|e^{-iHt}|\phi\rangle|^2 \tag{A23}$$

for any state ϕ. The map (A7) yielding lower symbols from classical f reads in the present case (supposing that Fubini's theorem holds):

$$\check{f}(q, p) = \frac{1}{\sqrt{2\pi}c_{-1}}\int_0^\infty \frac{dq'}{qq'}\int_0^\infty dx \int_0^\infty dx' e^{ip(x'-x)}$$
$$\times F_p(q', x - x')\psi\left(\frac{x}{q}\right)\psi\left(\frac{x}{q'}\right)\psi\left(\frac{x'}{q}\right)\psi\left(\frac{x'}{q'}\right), \tag{A24}$$

where F_p stands for the partial inverse Fourier transform

$$F_p(q, x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{ipx}f(q, p). \tag{A25}$$

For functions f depending on q only, expression (A24) simplifies to a lower symbol depending on q only:

$$\check{f}(q) = \frac{1}{c_{-1}}\int_0^\infty \frac{dq'}{qq'}f(q')\int_0^\infty dx\psi^2\left(\frac{x}{q}\right)\psi^2\left(\frac{x}{q'}\right). \tag{A26}$$

For instance, any power of q is transformed into the same power up to a constant factor

$$q^\beta \mapsto \check{q^\beta} = \frac{c_{\beta-1}c_{-\beta-2}}{c_{-1}}q^\beta. \tag{A27}$$

Note that $c_{-2} = 1$ from the normalization of ψ.

We notice that $\check{q} = c_0 c_{-3}(c_{-1})^{-1}q$. If we choose the fiducial vector such that $c_0 = c_{-1}$ in order to obtain the canonical rule, it remains $\check{q} = c_{-3}q$. Using a q-rescaling of the coherent states in the definition of the symbols $\check{A}_f$ like $\check{A}_f = \langle \lambda q, p|A_f|\lambda q, p\rangle$ allows one to obtain $\check{q} = q$ if we choose $\lambda = 1/c_{-3}$. Other important symbols are

$$p \mapsto \check{p} = p, \tag{A28}$$

$$p^2 \mapsto \check{p^2} = p^2 + \frac{c(\psi)}{q^2},$$

$$c(\psi) = \int_0^\infty (\psi'(x))^2\left(1 + \frac{c_0}{c_{-1}}x\right)dx. \tag{A29}$$

$$qp \mapsto \check{qp} = \frac{c_0 c_{-3}}{c_{-1}}qp \tag{A30}$$

Another interesting formula in the semiclassical context concerns the Fubini-Study metric derived from the symbol of total differential d with respect to parameters q and p affine coherent states,

$$\langle q, p|d|q, p\rangle = iqdp\int_0^\infty (\psi(x))^2 xdx = iqdpc_{-3}, \tag{A31}$$

and from the norm squared of $d|q, p\rangle$,

$$\|d|q, p\rangle\|^2 = c_{-4}q^2 dp^2 + L\frac{dq^2}{q^2},$$

$$L = \int_0^\infty dx x^2(\psi'(x)')^2 - \frac{1}{4}. \tag{A32}$$

With Klauder's notations [29]

$$d\sigma^2(q, p) := 2[\|d|q, p\rangle\|^2 - |\langle q, p|d|q, p\rangle|^2]$$
$$= 2\left((c_{-4} - c_{-3}^2)q^2 dp^2 + L\frac{dq^2}{q^2}\right). \tag{A33}$$

APPENDIX B: QUANTUM ANISOTROPIES

1. General setting

The Hamiltonian $\hat{H}_q$ of Eq. (21) reads

$$\hat{H}_q = \mathfrak{K}_2\frac{\hat{p}_+^2 + \hat{p}_-^2}{q^2} + 36\mathfrak{K}_3 q^{2/3}V_\mathfrak{n}(\beta), \tag{B1}$$

where

$$V_\mathfrak{n}(\beta) = \frac{\mathfrak{n}^2}{3}e^{4\beta_+}([2\cosh(2\sqrt{3}\beta_-) - e^{-6\beta_+}]^2 - 4) + \mathfrak{n}^2. \tag{B2}$$

More explicitly, we have for $\hat{H}_q$ the expression

$$\hat{H}_q = \frac{2\mathfrak{K}_2\hbar^2}{q^2}\hat{\mathcal{E}}(q), \tag{B3}$$

with

$$\hat{\mathcal{E}}(q) = -\frac{1}{2}\Delta + \chi(q)V_{\mathfrak{n}}(\beta), \qquad \Delta = \partial_{\beta_+}^2 + \partial_{\beta_-}^2,$$

$$\chi(q) = \frac{18\mathfrak{K}_3}{\mathfrak{K}_2\hbar^2}q^{8/3}. \qquad (B4)$$

$V_{\mathfrak{n}}(\beta)$ possesses an absolute minimum for $\beta_\pm = 0$, and near this minimum we have

$$V_{\mathfrak{n}}(\beta) = 8(\beta_+^2 + \beta_-^2) + o(\beta_\pm^2). \qquad (B5)$$

As mentioned above, $V_{\mathfrak{n}}(\beta)$ and therefore $\hat{\mathcal{E}}(q)$ possess the symmetry C_{3v}. This group has three irreducible representations usually called A_1, A_2 and E. Therefore the eigenstates of $\hat{\mathcal{E}}(q)$ can be classified according to these representations.

2. Harmonic approximation

Using (B5) we obtain

$$\hat{\mathcal{E}}(q) \simeq -\frac{1}{2}\Delta + 8\chi(q)(\beta_+^2 + \beta_-^2). \qquad (B6)$$

Introducing the quantum numbers $n_\pm = 0, 1, \ldots$, corresponding to the independent harmonic Hamiltonians in β_+ and β_-, we deduce the harmonic approximation of the eigenvalues $e(n_+, n_-)$ of $\hat{\mathcal{E}}(q)$:

$$e(n_+, n_-) \simeq 4\sqrt{\chi(q)}(n_+ + n_- + 1), \qquad (B7)$$

which gives the approximation of the eigenvalues $E_N(q)$ of $\hat{\mathsf{H}}_q$, with $N = n_+ + n_-$,

$$E_N(q) \simeq \frac{24\hbar}{q^{2/3}}\mathfrak{n}\sqrt{2\mathfrak{K}_2\mathfrak{K}_3}(N+1). \qquad (B8)$$

3. Steep wall approximation

As mentioned above, taking into account the C_{3v} symmetry and the exponential walls of the potential, we can approximate $V_{\mathfrak{n}}(\beta)$ by an equilateral triangular box as shown on Fig. 3. The interest of this approximation is that it preserves the symmetry C_{3v} of the potential and it also possesses an explicit solution in terms of eigenstates and eigenvalues [43–45].

The size of the triangle is a free parameter that must be somehow adjusted, e.g., through some variational method.

Let us denote by b the side length of the equilateral triangle box T_b of Fig. 5, and let us denote by U_T the potential equal to 0 inside the triangle and equal to $+\infty$ outside. The stationary Schrödinger equation $-\frac{1}{2}\Delta\psi = e^{(T)}\psi$
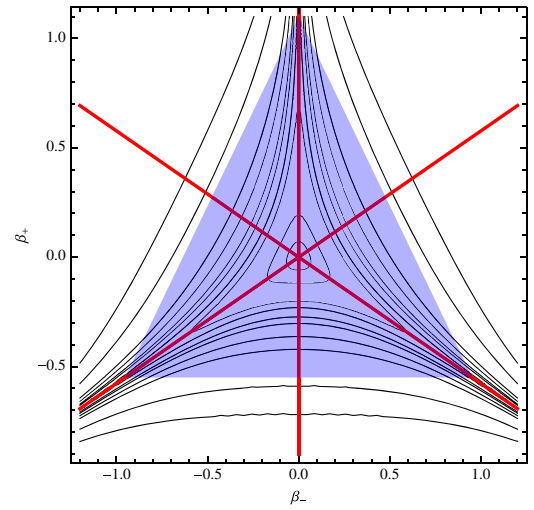

FIG. 5 (color online).   Contour plot of $V(\beta)$ near its minimum. Red lines: the three C_{3v} symmetry axes $\beta_- = 0$, $\beta_+ = \beta_-/\sqrt{3}$, $\beta_+ = -\beta_-/\sqrt{3}$. A possible triangular box approximation is in blue.

with the Dirichlet boundary conditions has the explicit solution [43–45]. The eigenvalues $e_{m,n}^{(T)}$ with $m = 0, 1, 2, \ldots$ and $n = 1, 2, \ldots$ are given by[2]

$$e_{m,n}^{(T)} = \frac{8\pi^2}{3b^2}\left(\frac{m^2}{3} + n^2 + mn\right). \qquad (B9)$$

The ground state energy is $e_{0,1}^{(T)}$. The corresponding normalized ground state wave function[3] $\psi_{0,1}$ reads [43]

$$\psi_{0,1}(\beta) = \sqrt{\frac{8}{3\sqrt{3}b^2}}\left(\sin\left(\frac{4\pi\beta_+}{b\sqrt{3}} + \frac{2\pi}{3}\right)\right.$$
$$\left. + 2\sin\left(\frac{2\pi\beta_+}{b\sqrt{3}} + \frac{\pi}{3}\right)\cos\frac{2\pi\beta_-}{b}\right), \qquad (B10)$$

where $\beta_\pm \in T_b$.

Assuming that the harmonic approximation (Sec. B 2) yields a fairly good approximation to the ground energy of $\hat{\mathcal{E}}(q)$, the length parameter b can be estimated by imposing that the two ground states coincide up to some small correction

$$e_{0,1}^{(T)} \approx 4\sqrt{\chi(q)}. \qquad (B11)$$

This relation yields

$$b \approx \sqrt{\frac{2\pi^2}{3\sqrt{\chi(q)}}}. \qquad (B12)$$

This leads to a new approximation $e(m, n)$ of the eigenvalues of $\hat{\mathcal{E}}(q)$ as

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[2]We have changed the parametrization of [43] to have independent integers.

[3]We have modified the solution $\psi_{0,1}$ of [43] in order to take into account the different origin and the orientation of the triangle.

$$e(m, n) \simeq 4\sqrt{\chi(q)}\left(\frac{m^2}{3} + n^2 + mn\right). \qquad \text{(B13)}$$

The eigenvalues E_N of $\hat{\mathsf{H}}_q$ are still given formally by

$$E_N(q) \simeq \frac{24\hbar}{q^{2/3}}\,\mathfrak{n}\,\sqrt{2\mathfrak{K}_2\mathfrak{K}_3}(N+1), \qquad \text{(B14)}$$

but now N does not reduce to a simple integer. It is given by

$$N = \frac{m^2}{3} + n^2 + mn - 1, \quad \text{with}$$
$$m = 0, 1; \ldots, n = 1, 2, \ldots \qquad \text{(B15)}$$

The last remark concerns the actual discrete spectrum of the Hamiltonian (B1) [or (B4)]. Clearly, it interpolates between the spectrum of the isotropic two-dimensional-harmonic oscillator, which is linear in N and the spectrum of the triangular steep wall which behaves like squared integers. This is reminiscent of the one-dimensional-Schrödinger operator with a symmetric Pöschl-Teller potential for which the two types, harmonic and infinite square well, of approximations hold (see for instance [46]). In this article we have privileged the harmonic side of the anisotropy potential for obvious reasons, but it seems to us that a rigorous complete mathematical analysis of the spectral properties of the operator (B1) is still lacking.

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