

Smooth bounce in the affine quantization of a Bianchi I modelHervé Bergeron,^{1,*} Andrea Dapor,^{2,†} Jean Pierre Gazeau,^{3,4,‡} and Przemysław Małkiewicz^{3,5,§}¹*ISMO, UMR 8214 CNRS, Univ Paris-Sud, 91405 Orsay, France*²*University of Warsaw, Hoża 69, 00-681 Warsaw, Poland*³*APC, UMR 7164 CNRS, Univ Paris Diderot, Sorbonne Paris Cité, 75205 Paris, France*⁴*Centro Brasileiro de Pesquisas Físicas, 22290-180 Rio de Janeiro, Rio de Janeiro, Brazil*⁵*National Centre for Nuclear Research, Hoża 69, 00-681 Warsaw, Poland*

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We present the affine coherent state quantization of the Bianchi I model. As in our previous paper on quantum theory of Friedmann models, we employ a variable associated with a perfect fluid to play a role of clock. Then we deparametrize the model. A distinctive feature, absent in isotropic models, is an extra nonholonomic constraint, which survives the deparametrization and constrains the range of physical variables. The appearance of the constraint reflects the “amplification” of singularity due to anisotropy. The quantization smoothes the extra constraint and allows quantum contracting trajectories to be smoothly transformed into expanding ones. Making use of an affine coherent state we develop a semiclassical description. Figures are included to illustrate our result.

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I. INTRODUCTION

In our previous paper [1] we proposed a quantization of spatially homogeneous and isotropic spacetime, based on coherent states for the affine group (also known as wavelets). The main result of this approach was the appearance of a quantum centrifugal potential, whose effect is the regularization of the singularity, replacing the big bang with a bounce both at quantum and semiclassical levels. Moreover, the true Hamiltonian is essentially self-adjoint, and hence the dynamics is unitary and unambiguous. The results obtained in this simple model of cosmological collapse encouraged us to tackle further investigations concerning more elaborate models of the Universe.

In the present work, we study the anisotropic case of Bianchi I, allowing for more degrees of freedom in the description of spacetime. The canonical classical variables p and q introduced in [1] apply equally well to the present case, so that we can make contact with our previous result. It needs to be said that we are entering an area much less visited than the Friedmann models, and thus we should expect some new difficulties.

In the Friedmann-Robertson-Walker (FRW) case [1], apart from studying the quantum true Hamiltonian, we were also interested in the properties of quantized volume and expansion rate, as they signal the singularity by vanishing and blowing up respectively. While the quantum volume turned out to be self-adjoint, the quantum expansion rate did not. Nevertheless, it was possible to give it a semiclassical meaning through its lower symbol (i.e., its

expectation value on affine coherent states, opportunely peaked at classical phase-space points). In the present work, in addition to these quantities, we also have to deal with shear and distortion describing the anisotropic evolution. Classically, the shear and some of the scale factors blow up at the singularity. However, the existence of minimal volume for the Universe at the quantum level prevents the unbound growth of anisotropy, i.e., it smoothly evolves through the bounce. We will not provide an explicit evolution of shear and distortion at the quantum level, but confine ourselves to giving a well-behaved semiclassical Hamiltonian, which generates a well-behaved dynamics of anisotropic variables.

We should point out that, as in any Hamiltonian quantum theory of cosmology, we must choose a degree of freedom to play the role of physical time. (In the reduced phase-space scheme, this is done before quantization.) Following Schutz [2,3], we identify this internal clock with a barotropic fluid filling the Universe. This particular choice is technically attractive because the inclusion of fluid extends the phase space with canonical variables T and p_T , where the fluid’s momentum p_T is a constant of motion. Thus, it is possible to perform a reduction to the physical phase space equipped with a time-independent true Hamiltonian. This feature may be particularly useful in future analysis of a nonintegrable Bianchi IX model.

In Sec. II the geometry of the model we wish to quantize is briefly presented. Its canonical formulation is described in Sec. III, where the true Hamiltonian h is defined, and the nonholonomic constraint $h > 0$ is specified. The affine coherent state quantization of the true Hamiltonian is performed in Sec. IV without taking into account this constraint. In Sec. V we discuss different possibilities to implement the latter. It appears that the best approach

*herve.bergeron@u-psud.fr

†adapor@fuw.edu.pl

‡gazeau@apc.univ-paris7.fr

§Przemyslaw.Malkiewicz@fuw.edu.pl

consists in incorporating this constraint in the classical true Hamiltonian to be quantized. To do this, we use the procedure for coherent state quantization of distributions presented in [4]. The resulting quantum Hamiltonian is presented in Sec. VI (detailed calculations can be found in Appendix A), and its lower symbol is computed in Sec. VII. This can be thought of as an effective classical Hamiltonian accounting for quantum corrections. An approximate analytic expression for this effective Hamiltonian is used in Sec. VIII to study the effective dynamics of fundamental variables, volume, and expansion rate. Numerical analysis of the big bang singularity resolution is also presented. Section IX concludes with a discussion of some interesting issues of our results and possible future directions.

II. SPACETIME GEOMETRY

In the present work we study the anisotropic evolution of compact (say, with torus topology \mathbb{T}^3) locally flat spatial sections of the spacetime equipped with the metric

$$ds^2 = -N(t)^2 dt^2 + \sum_i a_i(t)^2 (dx^i)^2. \quad (1)$$

We fix the spatial coordinates via $\int_{\mathbb{S}^1} dx^i = 1$. The Ricci scalar reads

$$R = 2 \left[\sum_i \frac{1}{Na_i} \left(\frac{\dot{a}_i}{N} \right)_{,t} - \sum_{i>j} \left(\frac{\dot{a}_i}{Na_i} \right) \left(\frac{\dot{a}_j}{Na_j} \right) \right]. \quad (2)$$

Filled with perfect fluids, these spacetimes are singular as the world lines of comoving observers terminate within a finite proper time. Starting from a spherical chunk of space, the anisotropic evolution will deform its initial shape. Following this observation, the spacetimes are said to have cigar or barrel type singularities, with two scale factors vanishing and the other one blowing up or two scale factors reaching a finite value and the other one vanishing, respectively, at the singularity. A more detailed discussion of solutions may be found in [5].

III. CANONICAL FRAMEWORK

The Hamiltonian constraint of general relativity in the Arnowit-Deser-Misner variables (q_{ij}, p^{ij}) , equipped with the Poisson bracket $\{q_{ij}(x), p^{kl}(x')\} = 16\pi G \delta_{(i}^k \delta_{j)}^l \delta(x-x')$, reads [6]

$$H_g = \frac{1}{\kappa} \int [NC^0 + N_i C^i] d^3x, \quad (3)$$

where

$$C^0 = -\sqrt{\det(q_{ij})} \left[{}^3R + \frac{1}{\det(q_{ij})} \left(\frac{1}{2} (p_k^k)^2 - p^{ij} p_{ij} \right) \right],$$

$$C^i = -2p^{ij}_{;j} \quad (4)$$

are first-class constraints and N, N_i are Lagrange multipliers and $\kappa = 16\pi G$. The truncation of the gravitational variables to the cosmological sector translates into $q_{ij}(x) := \delta_{ij} a_i^2$ and $p^{ij}(x) := \delta_{ij} p^i$, which in turn leads to $C^i \equiv 0$ and

$$H_g = -\frac{1}{\kappa a_1 a_2 a_3} \left(\frac{1}{2} \left(\sum_i a_i^2 p^i \right)^2 - \sum_i (a_i^2 p^i)^2 \right), \quad (5)$$

where we defined

$$p^1 = -\frac{1}{N} \frac{(a_2 a_3)'}{a_1}, \quad p^2 = -\frac{1}{N} \frac{(a_3 a_1)'}{a_2},$$

$$p^3 = -\frac{1}{N} \frac{(a_1 a_2)'}{a_3}, \quad (6)$$

satisfying $\{a_i^2, p^j\} = \kappa \delta_i^j$. The Hamiltonian (5) can be brought to a simpler, diagonal form. We achieve this by Misner (canonical) parametrization of the phase space [7]: canonical pairs are given by $(\beta^0, p_0, \beta^+, p_+, \beta^-, p_-)$, where

$$\begin{pmatrix} \beta^0 \\ \beta^+ \\ \beta^- \end{pmatrix} = \begin{pmatrix} 1/3 & 1/3 & 1/3 \\ 1/6 & 1/6 & -1/3 \\ \frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{3}} & 0 \end{pmatrix} \begin{pmatrix} \ln a_1 \\ \ln a_2 \\ \ln a_3 \end{pmatrix}, \quad (7)$$

$$\begin{pmatrix} p_0 \\ p_+ \\ p_- \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -2 \\ \sqrt{3} & -\sqrt{3} & 0 \end{pmatrix} \begin{pmatrix} 2a_1^2 p_1 \\ 2a_2^2 p_2 \\ 2a_3^2 p_3 \end{pmatrix}. \quad (8)$$

In term of these variables, the gravitational Hamiltonian reads

$$H_g = \frac{1}{\kappa} N \frac{e^{-3\beta^0}}{24} (-p_0^2 + p_+^2 + p_-^2). \quad (9)$$

At this point, H_g is still a constraint. To make it into the physical true Hamiltonian, we include matter in the form of a barotropic fluid subject to the equation of state $p = w\rho$ ($w = \text{const}$). Following Schutz [2,3] we obtain for this matter the Hamiltonian

$$H_m = N \frac{P_T}{(\sqrt{q})^w} = N e^{-3w\beta^0} p_T, \quad (10)$$

where T and p_T are canonical variables associated with the fluid. In analogy with our previous work on the FRW models [1], we now replace (β^0, p_0) with the following canonical pair:

$$q := e^{\frac{3(1-w)}{2}\beta^0}, \quad p := -\frac{2}{3(1-w)}e^{-\frac{3(1-w)}{2}\beta^0}p_0, \quad (11)$$

such that $[q] = 1$, $[p] = L^2$ and $\{q, p\} = \kappa$. At the physical level we notice that this is exactly the same pair of observables which we considered for the FRW models, i.e.,

$$q = (a_1 a_2 a_3)^{\frac{1-w}{2}}, \quad p = \frac{8}{3(1-w)}(a_1 a_2 a_3)^{\frac{1+w}{2}}\Theta, \quad (12)$$

where Θ is the expansion rate. The full Hamiltonian constraint reads

$$\begin{aligned} \mathbf{H} &:= \mathbf{H}_g + \mathbf{H}_m \\ &= Nq^\mu \left(\frac{1}{24\kappa} (-\alpha^2 p^2 + q^{-2}(p_+^2 + p_-^2)) + p_T \right) \approx 0, \end{aligned} \quad (13)$$

where $\mu := -2w/(1-w)$, $\alpha := 3(1-w)/2 > 0$. Solving the constraint for p_T leads to

$$\kappa p_T = \frac{\alpha^2}{24} p^2 - \frac{1}{24} (p_+^2 + p_-^2) q^{-2}. \quad (14)$$

Upon choosing T/κ as the clock variable, we obtain the true (nonvanishing) Hamiltonian

$$\mathbf{h} = \frac{\alpha^2}{24} p^2 - \frac{1}{24} (p_+^2 + p_-^2) q^{-2} \quad (15)$$

describing the evolution of gravitational degrees of freedom $(q, p, \beta^-, p_-, \beta^+, p_+) \in \mathbb{R}_+^* \times \mathbb{R}^5$. The most important difference between (15) and the true Hamiltonian found in [1] is the appearance of the attractive potential proportional to $-q^{-2}$. We must then impose positivity of \mathbf{h} as a separate, nonholonomic constraint

$$\mathbf{h} > 0, \quad (16)$$

which classically restricts the range of gravitational variables. As a side remark, we notice that in the limit of vanishing anisotropy, $p_- \rightarrow 0$ and $p_+ \rightarrow 0$, the true Hamiltonian of the flat FRW spacetime [1] is recovered.

IV. QUANTIZATION OF TRUE HAMILTONIAN \mathbf{h}

A. Affine quantization: a compendium

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

$$(q, p)(q_0, p_0) = (qq_0, p_0/q + p), \quad q \in \mathbb{R}_+^*, p \in \mathbb{R}, \quad (17)$$

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

$$(q, p)^{-1} = \left(\frac{1}{q}, -qp \right), \quad (18)$$

Π_+ is viewed as the affine group $\text{Aff}_+(\mathbb{R})$ of the real line, and the measure $dqdp$ is left-invariant with respect to this action. The affine group $\text{Aff}_+(\mathbb{R})$ has two nonequivalent unitary irreducible representations (UIR). Both are square integrable and this is the rationale behind affine integral quantization [4]. The UIR $U_+ \equiv U$ is realized in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}_+^*, dx)$:

$$U(q, p)\psi(x) = (e^{ipx}/\sqrt{q})\psi(x/q). \quad (19)$$

Picking an *admissible* unit-norm state ψ , i.e., an element in $\mathcal{H} \cap L^2(\mathbb{R}_+^*, dx) \cap L^2(\mathbb{R}_+^*, dx/x)$, named *fiducial vector*, produces all affine coherent states (or wavelets) defined as

$$|q, p\rangle = U(q, p)|\psi\rangle. \quad (20)$$

These states in (q, p) representation, i.e., as functions $\zeta_{q,p}(q', p') := \langle q', p' | q, p \rangle$, are expected to be well peaked around their phase-space point (q, p) .

Square integrability of the UIR U and admissibility yield the resolution of the identity

$$\begin{aligned} \int_{\Pi_+} \frac{dqdp}{2\pi c_{-1}} |q, p\rangle \langle q, p| &= I, \\ \text{where } c_\gamma &:= \int_0^\infty \frac{dx}{x^{2+\gamma}} |\psi(x)|^2. \end{aligned} \quad (21)$$

The covariant integral quantization of classical observables $f(q, p)$ follows

$$f \mapsto A_f = \int_{\Pi_+} f(q, p) |q, p\rangle \langle q, p| \frac{dqdp}{2\pi c_{-1}}. \quad (22)$$

The above map is linear and transforms the constant function 1 into the identity operator and real functions into symmetric operators (provided that the integral makes sense). Also, note that this quantization procedure can be easily extended to singular functions and distributions [4]. In the sequel we restrict the choice of fiducial vector to real functions.

The map (22) yields canonical commutation rule, up to a scaling factor, for q and p . Indeed, in representation “ x ,”

$$\begin{aligned} A_p &= -i \frac{d}{dx} \equiv P, & A_q &= (c_0/c_{-1})Q, \\ Qf(x) &:= xf(x), & [A_q, A_p] &= (c_0/c_{-1})iI. \end{aligned} \quad (23)$$

Multiplication operator Q is (essentially) self-adjoint whereas P is symmetric but has no self-adjoint extension [8]. The property of the procedure which is crucial for our present purpose is the regularization of the quantum kinetic energy:

$$A_{p^2} = P^2 + \varsigma_\psi Q^{-2} \quad \text{with } \varsigma_\psi := \int_0^\infty \frac{du}{c_{-1}} u(\psi'(u))^2. \quad (24)$$

The additional term in regard with the standard canonical quantization is a centrifugal potential $\propto Q^{-2}$ whose strength depends on the fiducial vector only, and can be made as small as one wishes through an appropriate choice of ψ . If we consider the quantum dynamics of a free motion on the open half-line \mathbb{R}_+^* , it is proved [8] that the operator $P^2 = -d^2/dx^2$ alone in $L^2(\mathbb{R}_+^*, dx)$ is not essentially self-adjoint whereas the regularized operator (24) is for $\varsigma_\psi \geq 3/4$. It follows that for $\varsigma_\psi \geq 3/4$, the quantum dynamics is unitary during the entire evolution, in particular, in the passage from the motion towards the origin (contracting branch) to the motion away from it (expanding branch).

B. Quantization of Hamiltonian

We quantize the (q, p) variables introduced in (11) according to the above affine quantization framework, while for the other variables we choose the canonical quantization one since their respective phase-space geometry is the harmless plane \mathbb{R}^2 . Making use of the formulas above (see also [1]), the quantum version of the true Hamiltonian (15) is

$$h \mapsto A_h = \frac{\alpha^2}{24} P^2 + a_p^2 \frac{\alpha^2}{24} \varsigma_\psi Q^{-2} - \frac{1}{24} \frac{c_{-3}}{c_{-1}} (P_+^2 + P_-^2) Q^{-2}. \quad (25)$$

The operators P_+ and P_- are the usual momentum operators on the real line acting in $L^2(\mathbb{R}^2, d\beta^+ d\beta^-)$. Since they are self-adjoint and commute with the Hamiltonian, we can replace them with some fixed real eigenvalues, k_+ and k_- , which will remain constant during the evolution.

As in [1], we choose ψ as the function smooth in $(0, \infty)$ and rapidly decreasing at 0^+ and at the infinity:

$$\psi \equiv \psi^\nu(x) = \frac{1}{\sqrt{2xK_0(\nu)}} e^{-\frac{x}{4}(\xi_{12} + \frac{1}{x\xi_{12}})}, \quad \text{with } \nu > 0 \quad \text{and} \quad \xi_{12} = \frac{K_1(\nu)}{K_2(\nu)} > 0. \quad (26)$$

Here and in the following, $K_r(z)$ denotes the modified Bessel functions [9]. Since we deal with ratios of such

functions throughout the sequel, we adopt the convenient notation

$$\xi_{rs} = \xi_{rs}(\nu) = \frac{K_r(\nu)}{K_s(\nu)} = \frac{1}{\xi_{sr}}. \quad (27)$$

One convenient feature of such a notation is that $\xi_{rs}(\nu) \sim 1$ as $\nu \rightarrow \infty$ [a consequence of $K_r(\nu) \sim \sqrt{\pi/(2\nu)}$]. Hence, the quantum Hamiltonian (25) now reads

$$A_h = \frac{\alpha^2}{24} P^2 + a_p^2 \frac{\alpha^2}{24} \varsigma(\nu) Q^{-2} - \frac{1}{24} \xi_{21}(\nu)^2 (k_+^2 + k_-^2) Q^{-2}, \quad (28)$$

where $\varsigma(\nu) \equiv \varsigma_{\psi^\nu} = (1 + \nu \xi_{01})/4$. It is convenient to introduce the auxiliary strength parameter

$$x(\nu) := \varsigma(\nu) - \xi_{21}(\nu)^2 \frac{(k_+^2 + k_-^2)}{\alpha^2 a_p^2} \quad (29)$$

so (28) reduces to

$$A_h = \frac{\alpha^2}{24} (P^2 + x(\nu) a_p^2 Q^{-2}). \quad (30)$$

The key difficulty is the additional nonholonomic positivity constraint [also present in open ($k = -1$) FRW models], $h > 0$, to which the next section is dedicated.

V. ANALYSIS OF POSITIVITY CONSTRAINT $h > 0$

In what follows we consider different possible ways of implementing the positivity constraint (16) in the quantum theory.

A. Positivity via operator modification

The positivity requirement of the true Hamiltonian may be imposed directly on the operator A_h by just putting $x(\nu) > 0$. This leads to the condition on the amount of shear, which is expressed in terms of eigenvalues k_+ and k_- ,

$$k_+^2 + k_-^2 < \alpha^2 a_p^2 (\xi_{12})^2 \xi_{1-1} \varsigma. \quad (31)$$

The above condition reduces the space of allowed quantum states by restricting the spectral values associated with the shear operator. More precisely, the amount of anisotropy is bounded from above by the right-hand side, meaning that a highly anisotropic spacetime cannot be realized. However, there is no reason why the Universe should be so much isotropic. On the contrary, since classically the anisotropy goes as $\sim a^{-6}$ with the overall scale factor, one reasonably expects that the Universe is more and more anisotropy dominated the closer it is to the classical singularity. We

thus conclude that the above condition for the allowed amount of anisotropy in the Universe is too restrictive, and discard this approach as unphysical.

B. Positivity via domain restriction

Let us consider the eigenvalue problem for operator A_h in (30) on $L^2(\mathbb{R}_+, dx)$:

$$-\frac{d^2\psi}{dx^2} + \frac{\chi(\nu)a_p^2}{x^2}\psi = \lambda\psi. \quad (32)$$

A possible way of implementing the condition (16) is to ensure the self-adjointness of (32) and then constrain the Hilbert space to the positive eigenvalues, $\lambda > 0$. The difficulty in this approach is to implement such a Hilbertian projection in analytical computations, since it requires full knowledge of the spectral decomposition of A_h . We drop this approach for technical reasons.

C. Positivity via redefinition of classical variables

Consider the following canonical transformation:

$$q \mapsto q' := \frac{1}{2} \frac{pq}{p^2 - \mu^2/q^2}, \quad p \mapsto p' := p^2 - \frac{\mu^2}{q^2}, \quad (33)$$

$$\beta^\pm \mapsto \beta'^\pm := \beta^\pm + \frac{p_\pm}{2\alpha^2\mu} \ln\left(\frac{pq - \mu}{pq + \mu}\right),$$

$$p_\pm \mapsto p'_\pm := p_\pm, \quad (34)$$

where $\mu^2 := (p_+^2 + p_-^2)/\alpha^2$. In these new variables, the positivity constraint (16) becomes $p' > 0$. There is also another constraint, which is $|q'p'| > \mu/2$. We observe that this condition splits the physical phase space into two disconnected regions. If we now define $\tilde{q}' := q'p' - \mu/2$ and $\tilde{p}' := \ln p'$, then $(\tilde{q}', \tilde{p}') \in \mathbb{R}_+^* \times \mathbb{R}$, and the true Hamiltonian reads $\mathfrak{h} = e^{\tilde{p}'}$. The advantage here is that we do not have to impose the positivity constraint quantum mechanically, since \mathfrak{h} in this form is automatically positive definite. The disadvantage of this approach is that we lose connection with the variables used for FRW models [1]. More importantly, the expanding and contracting branches of the Universe become disconnected. For these reasons we discard also this approach.

D. Positivity via redefinition of classical expression

Another idea is to take $\theta(\mathfrak{h})\mathfrak{h}$ (where θ is the Heaviside function) as the classical true Hamiltonian, and quantize it in the spirit of an integral quantization framework [4,10]. The resulting operator $A_{\theta(\mathfrak{h})\mathfrak{h}}$ will have the positivity constraint implemented. Moreover, in this way we do not redefine the initial Hilbert space. In the next section we follow this last idea, in what we call ‘‘refined quantization’’ (as opposed to Sec. IV).

VI. REFINED QUANTIZATION OF TRUE HAMILTONIAN

A. General formula for the operator

Let us consider the simplified form of the Hamiltonian (15)

$$\mathfrak{h}_s = p^2 - \frac{k^2}{q^2} \quad (35)$$

obtained after dropping unnecessary factors, together with the positivity constraint $\mathfrak{h}_s > 0$. We derive from the decomposition $\mathfrak{h}_s = \theta(\mathfrak{h}_s)\mathfrak{h}_s + \theta(-\mathfrak{h}_s)\mathfrak{h}_s$ and the linearity of the affine integral quantization the equation

$$A_{\theta(\mathfrak{h}_s)\mathfrak{h}_s} = A_{\mathfrak{h}_s} - A_{\theta(-\mathfrak{h}_s)\mathfrak{h}_s}. \quad (36)$$

With the fiducial vector (26) and from results given in [1], we obtain for the affine quantized version of \mathfrak{h}_s in x representation:

$$\langle x' | A_{\mathfrak{h}_s} | x \rangle = \left[-\frac{d^2}{dx^2} + (\zeta(\nu) - \xi_{21}(\nu)^2 k^2) \frac{1}{x^2} \right] \delta(x - x'). \quad (37)$$

All the details about the derivation of this expression are given in Appendix A.

The second term $A_{\theta(-\mathfrak{h}_s)\mathfrak{h}_s}$ for the same fiducial vector (26), in x representation reads

$$\langle x' | A_{\theta(-\mathfrak{h}_s)\mathfrak{h}_s} | x \rangle = \frac{2}{\pi K_0(\nu) c_{-1}} \left(\frac{k \text{Re}[K_0(2\gamma)]}{\sqrt{xx'}(x-x')^2} - \frac{4\xi_{12} \sqrt{xx'} \text{Im}[\gamma K_1(2\gamma)]}{\nu (x-x')^3 (x+x')} \right), \quad (38)$$

where

$$\gamma = \frac{\nu}{4} \sqrt{\left(\frac{1}{x} + \frac{1}{x'}\right) \left(x + x' - i \frac{4k}{\nu \xi_{12}} (x - x')\right)}$$

$$= \frac{\nu}{4} \sqrt{\left(1 + \frac{1}{y}\right) \left(1 + y - i \frac{4k}{\nu \xi_{12}} (1 - y)\right)} \quad (39)$$

with $y = x'/x$. This is a nonlocal operator, and there is little chance to solve its eigenvalue problem analytically. We are not going to analyze it except for noticing that the operator $A_{\theta(\mathfrak{h}_s)\mathfrak{h}_s}$ is positive definite and as such it admits self-adjoint extension(s), e.g., Friedrich’s extension. Therefore, the existence of unitary evolution is guaranteed. In what follows we make use of the semiclassical description available in our approach based on affine coherent states.

VII. SEMICLASSICAL APPROACH

A. From Lagrangian

Inspired by Klauder's approach [11,12], we present a consistent framework allowing us to approximate the quantum Hamiltonian and its associated dynamics by making use of a semiclassical Lagrangian approach.

For a general Hamiltonian operator \mathbf{H} , the Schrödinger equation, $i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \mathbf{H} |\Psi(t)\rangle$, can be deduced from the Lagrangian:

$$\mathbf{L}(\Psi, \dot{\Psi}, \mathcal{N}) := \langle \Psi(t) | \left(i\hbar \frac{\partial}{\partial t} - \mathbf{H} \right) | \Psi(t) \rangle, \quad (40)$$

through the application of the variational principle with respect to $|\Psi(t)\rangle$. Following Klauder, we assume that $|\Psi(t)\rangle$ is an affine coherent state $|q(t), p(t)\rangle$, where $q(t)$ and $p(t)$ are some time-dependent functions. Then the Lagrangian (40) turns to the semiclassical form

$$\begin{aligned} \tilde{\mathbf{L}}(q, \dot{q}, p) &= \langle q(t), p(t) | \left(i\hbar \frac{\partial}{\partial t} - \mathbf{H} \right) | q(t), p(t) \rangle \\ &= -\xi_{02}(\nu) q \dot{p} - \langle q(t), p(t) | \mathbf{H} | q(t), p(t) \rangle. \end{aligned} \quad (41)$$

We rescale the family of coherent states to define a new family of coherent states $|q(t), p(t)\rangle^{\text{new}} := |\lambda q(t), p(t)\rangle$, where $\lambda = \xi_{20}(\nu)$. In this way, we ensure that (\dot{q}, \dot{p}) , computed as the expectation values with respect to the rescaled family, fully correspond to the classical pair, i.e., $(\dot{q}, \dot{p}) = (q, p)$. Then, we derive the semiclassical equations of motion as

$$\dot{q} = \frac{\partial}{\partial p} \check{\mathbf{H}}(q, p), \quad (42)$$

$$\dot{p} = -\frac{\partial}{\partial q} \check{\mathbf{H}}(q, p), \quad (43)$$

where $\check{\mathbf{H}}(q, p)$ is the lower symbol of \mathbf{H} , $\check{\mathbf{H}}(q, p) = \langle \lambda q(t), p(t) | \hat{\mathbf{H}} | \lambda q(t), p(t) \rangle$. We note that the

$$\langle \lambda q, p | A_{\theta(-h_s)h_s} | \lambda q, p \rangle = \frac{2}{\pi} \left(\frac{4\xi_{12}}{\lambda q \nu K_0(\nu)} \right)^2 \int_0^\infty \left(k \frac{\text{Re}[K_0(2\gamma)]}{y(1-y)^2} - \frac{4\xi_{12}}{\nu} \frac{\text{Im}[\gamma K_1(2\gamma)]}{(1-y)^3(y+1)} \right) \frac{\tilde{\gamma}^2 K_2(2\tilde{\gamma}) y^2 dy}{(y^2+1)^2 c_{-1}} \quad (44)$$

where

$$\tilde{\gamma} = \frac{\nu}{4} \sqrt{\left(1 + \frac{1}{y}\right) \left(1 + y - i \frac{4p\lambda q}{\nu \xi_{12}} (1-y)\right)}$$

and $y = x'/x$. The analytic evaluation of the above integral is rather intractable and we proceed with a numerical integration instead.

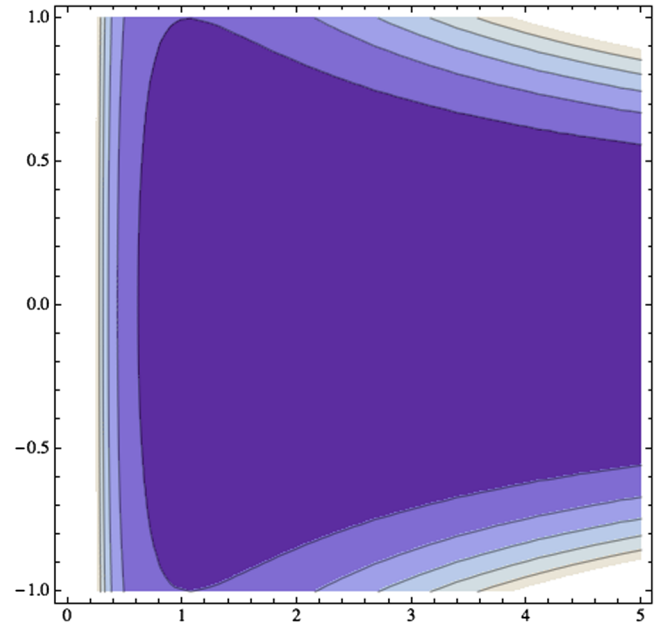


FIG. 1 (color online). The figure shows the trajectories generated by the lower symbol of the true Hamiltonian. The trajectories are clearly reversed and the bounce occurs. The parameters are chosen as $k = 10a_p$ (for the potential strength), $\nu = 3$ (for the fiducial vector).

classical relation between \dot{q} and p cannot hold any longer on the semiclassical level since this relation is now given by (42), in which classical \mathbf{H} is replaced with $\check{\mathbf{H}}$. This is viewed as the consequence of the quantum noncommutativity of basic variables. In our reconstruction of the semiclassical description of spacetime we will keep the interpretation of q as fundamentally given by (12).

We now specify $\mathbf{H} = A_{\theta(h_s)h_s}$, and $\check{\mathbf{H}} = \langle \lambda q, p | A_{\theta(h_s)h_s} | \lambda q, p \rangle$. The latter lower symbol is the basis of our semiclassical description.

B. Lower symbol

We find that the lower symbol of $A_{\theta(-h_s)h_s}$ reads

VIII. SINGULARITY RESOLUTION

A. Numerical examples

The semiclassical refined true Hamiltonian is defined as the difference of the lower symbol of (37) and the lower symbol (44). Figures 1 and 2 illustrate the singularity resolution in the half-plane (q, p) for different values of the strength k . The contour plots of the lower symbol of the

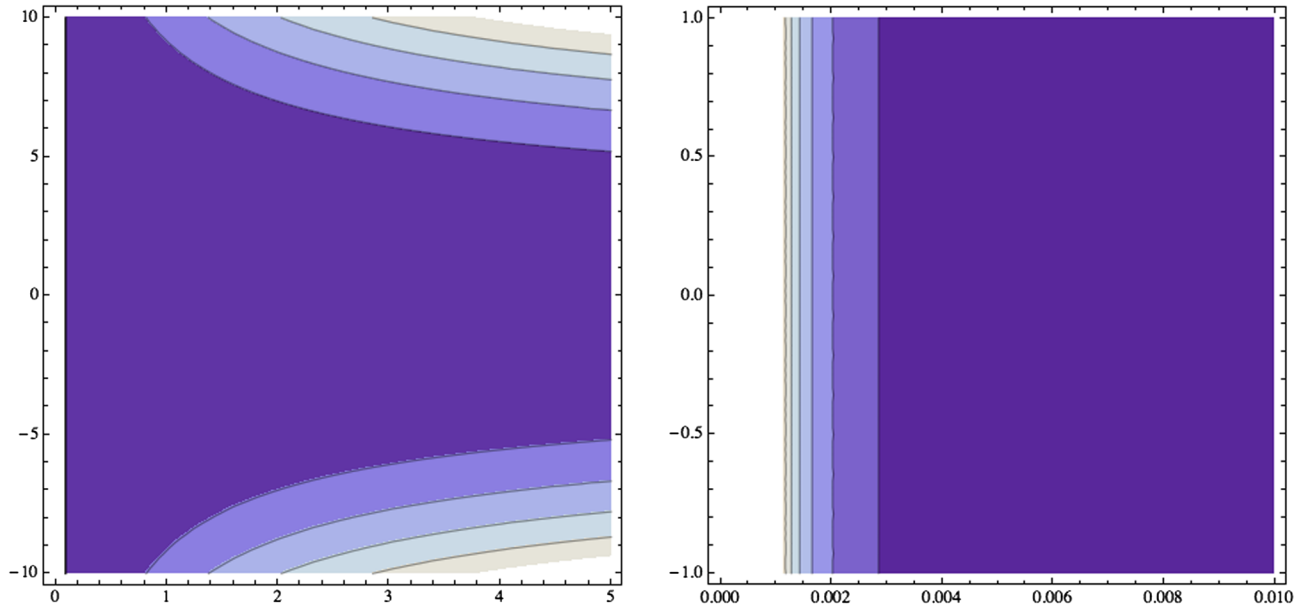


FIG. 2 (color online). Here $k = 50a_p$, the semiclassical trajectories are initially more divergent, but they are again reversed. On the left, the same scale as above. On the right, the plot is zoomed in, so that we can see the reversal of trajectories near $q = 0$.

Hamiltonian contain semiclassical trajectories as constant-value levels. The numerical computations prove that they exhibit bouncing behavior.

B. Lower symbol of the Hamiltonian

Combining the lower symbol of the operator A_{h_s} , given in Appendix A, with (44), we find that the lower symbol of the true Hamiltonian (36) has the following form:

$$\langle \lambda q, p | A_{\theta(h_s)h_s} | \lambda q, p \rangle = \frac{1}{\lambda^2 q^2} (p^2 \lambda^2 q^2 + A(\nu) - B(\nu) k^2 + F_\nu(k^2, p^2 \lambda^2 q^2)), \quad (45)$$

where

$$A(\nu) := \frac{a_p^2}{4} \xi_{10} \xi_{12} (\nu \xi_{32} - 1), \quad B(\nu) := \xi_{20}, \quad (46)$$

and

$$\frac{1}{\lambda^2 q^2} F_\nu(k^2, p^2 \lambda^2 q^2) := -\langle \lambda q, p | A_{\theta(-h_s)h_s} | \lambda q, p \rangle \quad (47)$$

is the corrective term due to the positivity constraint, for which we find the following limits:

$$\langle \lambda q, p | A_{\theta(h)h} | \lambda q, p \rangle \approx \frac{1}{\lambda^2 q^2} \frac{\alpha^2}{24} \left(p^2 \lambda^2 q^2 + A(\nu) - B(\nu) \frac{k^2}{\alpha^2} + a_\nu \left(\frac{k^2}{\alpha^2} \right) b_\nu \left(\frac{k^2}{\alpha^2}, p^2 \lambda^2 q^2 \right) \right) \equiv \tilde{h}(q, p). \quad (52)$$

$$\begin{aligned} F_\nu(0, 0) &= 0, \\ \lim_{k \rightarrow \infty} F_\nu(k^2, 0) &= -A(\nu) + B(\nu) k^2, \\ \lim_{x \rightarrow \infty} F_\nu(k^2, x) &= 0. \end{aligned} \quad (48)$$

Note that the lower symbol (45) is even in k and in pq .

Based on our numerical simulations, we can guess the following approximative form for $F_\nu(k^2, p^2 \lambda^2 q^2)$:

$$F_\nu(k^2, p^2 \lambda^2 q^2) \approx a_\nu(k^2) b_\nu(k^2, p^2 \lambda^2 q^2) \quad (49)$$

where

$$a_\nu(k^2) = -A(\nu) \frac{\lambda_1(\nu) k^2}{1 + \lambda_1(\nu) k^2} + B(\nu) k^2, \quad (50)$$

$$b_\nu(k^2, p^2 \lambda^2 q^2) = \frac{1 + \lambda_1(\nu) k^2}{1 + \lambda_1(\nu) k^2 + \lambda_2(\nu) p^2 \lambda^2 q^2}. \quad (51)$$

That this factorization is indeed a good approximation of $F_\nu(k^2, p^2 \lambda^2 q^2)$ is confirmed for $\nu = 3$ by the plots in Figs. 3(a) and 3(b) with $\lambda_1 \approx 0.3$ and $\lambda_2 \approx 0.7$.

C. Effective dynamics of q and p

Let us now restore the original physical factors α and a_p present in (25). The approximate form of the lower symbol (45) of the true Hamiltonian now reads

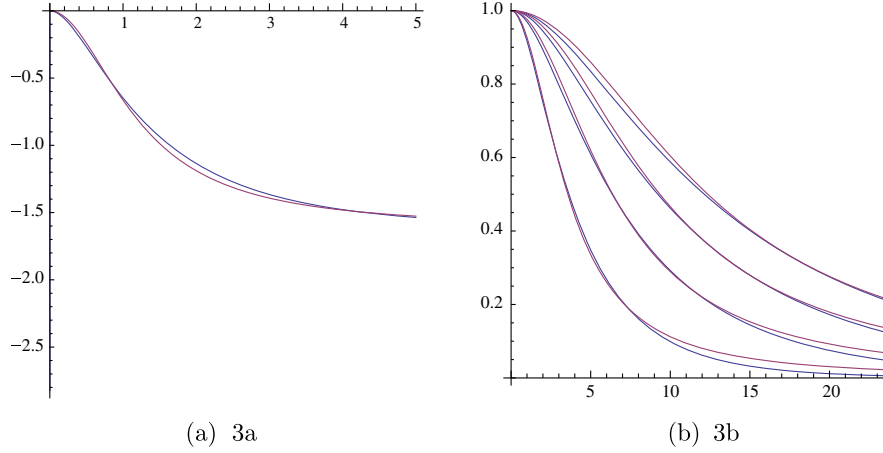


FIG. 3 (color online). (a) Plot of the exact $F_3(k^2, 0)$ in blue and its approximation $a_3(k^2)$ in red. (b) Plot of the exact $\frac{F_3(k^2, x^2)}{F_3(k^2, 0)}$ in blue and its approximation $b_3(k^2, x^2)$ in red. Plotted for $k = 1, 2, 3, 4$. Beyond the plotted range of x the effect of theta function becomes negligible due to the relatively large positive value of $\langle \lambda q, p | A_{\theta(h)\hbar} | \lambda q, p \rangle$, and the accuracy of the approximation is not very significant for reproducing the correct dynamics.

Making use of the approximation we obtain

$$\frac{d}{dT}(pq) = \{pq, \tilde{\hbar}\} = 2\tilde{\hbar} > 0 \quad (53)$$

where $\tilde{\hbar}$, our semiclassical Hamiltonian, is constant and d is defined in the preamble thus

$$pq = 2\tilde{\hbar}(T - T_{\text{bounce}}). \quad (54)$$

We set $T_{\text{bounce}} = 0$. Now we easily integrate (42)–(43) and obtain for q the expression

$$q = \sqrt{\frac{q^2 \tilde{\hbar}}{\tilde{\hbar}}} = \sqrt{\frac{1}{\tilde{\hbar}} \frac{\alpha^2}{24\lambda^2} \left(4\tilde{\hbar}^2 T^2 \lambda^2 + A(\nu) - B(\nu) \frac{k^2}{\alpha^2} + a_\nu \left(\frac{k^2}{\alpha^2} \right) b_\nu \left(\frac{k^2}{\alpha^2}, 4\tilde{\hbar}^2 T^2 \lambda^2 \right) \right)}, \quad (55)$$

where we substituted pq according to (54) and where $\tilde{\hbar}$ on the right-hand side is treated as a constant of integration. Next, we find for p

$$p = \frac{2\tilde{\hbar}T}{\sqrt{\frac{1}{\tilde{\hbar}} \frac{\alpha^2}{24\lambda^2} \left(4\tilde{\hbar}^2 T^2 \lambda^2 + A(\nu) - B(\nu) \frac{k^2}{\alpha^2} + a_\nu \left(\frac{k^2}{\alpha^2} \right) b_\nu \left(\frac{k^2}{\alpha^2}, 4\tilde{\hbar}^2 T^2 \lambda^2 \right) \right)}}. \quad (56)$$

D. Effective spacetime

From the initial definitions given in Sec. III we have

$$ds^2 = -N^2 dT^2 + (a_1 dx^1)^2 + (a_2 dx^2)^2 + (a_3 dx^3)^2, \quad (57)$$

where

$$N = -\frac{1}{q^\mu}, \quad a_1 = q_a^\mu e^{\beta^+ + \sqrt{3}\beta^-}, \\ a_2 = q_a^\mu e^{\beta^+ - \sqrt{3}\beta^-}, \quad a_3 = q_a^\mu e^{-2\beta^+}. \quad (58)$$

In order to construct the semiclassical spacetime, in addition to $q(T)$, we need the semiclassical dynamics of

β^\pm , which can be derived from the respective Hamilton equations after replacing k^2 with $p_+^2 + p_-^2$ in (52). However, the resulting formulas are involved and will be omitted. Instead we focus on the overall expansion and the total volume.

E. Effective dynamics of volume and expansion rate

The volume V and expansion rate Θ read, respectively,

$$V(T) = q_a^3, \quad \Theta(T) := \frac{1}{N} \dot{V} = -\frac{3}{\alpha} q^{\mu-1} \dot{q}. \quad (59)$$

Towards the singularity, the volume decreases until it reaches its minimal value, which is

$$V_{\min} = \left(\frac{A(\nu)}{1 + \lambda_1 \frac{k^2}{\alpha^2}} \frac{\alpha^2}{24\lambda^2 \hbar} \right)^{\frac{3}{2\alpha}}. \quad (60)$$

We note that for $k^2 = 0$ the above formula gives the minimal volume of the flat FRW universe [1]. The precise moment of the maximal value of the expansion rate, T_{Θ} , is very difficult to obtain. Let us assume that in the vicinity of the bounce, where the contraction reaches its maximal value, we may apply the following approximation:

$$q \approx \sqrt{\frac{1}{\hbar} \frac{\alpha^2}{24\lambda^2} \left(4\tilde{\hbar}^2 T^2 \lambda^2 + \frac{A(\nu)}{1 + \lambda_1(\nu) \frac{k^2}{\alpha^2}} \right)}. \quad (61)$$

Then, we find

$$T_{\Theta} \approx \pm \sqrt{\frac{1}{4\lambda^2 \tilde{\hbar}^2 (1 - \mu)} \frac{A(\nu)}{1 + \lambda_1(\nu) \frac{k^2}{\alpha^2}}}, \quad (62)$$

and

$$\begin{aligned} \Theta_{\max} &= \Theta(T_{\Theta}) \\ &\approx \pm \frac{\alpha}{4} \left(\frac{\mu - 2}{\mu - 1} \frac{\alpha^2}{24\tilde{\hbar}^2 \lambda^2} \frac{A(\nu)}{1 + \lambda_1(\nu) \frac{k^2}{\alpha^2}} \right)^{\frac{\mu-1}{2}} \sqrt{\frac{1}{1 - \mu} \frac{A(\nu)}{1 + \lambda_1(\nu) \frac{k^2}{\alpha^2}}}. \end{aligned} \quad (63)$$

IX. DISCUSSION

A. Mechanism behind the singularity resolution

In the present paper we have dealt with the anisotropic cosmological model of Bianchi I. Classically, such space-time presents a singularity which is much stronger than the one for the Friedmann models considered in our previous paper [1]. The classical trajectories in the (q, p) plane diverge as they approach the singularity $q = 0$. Indeed, the contracting and expanding branches are disconnected manifolds of the constraint surface. Therefore, one does not expect that canonical quantization may resolve such singularities.

We employ a more suitable framework, known as the affine coherent state quantization. In order to resolve the singularity with a bounce, we introduce a phase space in which the expanding and contracting branches are connected by a classically forbidden region. Classically, an extra *positivity constraint* is present, to ban that region. The affine coherent state quantization, because it can also be applied to distributions, smoothes this constraint, allowing the semiclassical trajectories to cross the classically forbidden region and join the contraction and expansion with a smooth bounce (see Fig. 1). Thus, we have obtained an anisotropic singularity resolution by a new mechanism, which is peculiar to our quantization framework. To illustrate the smoothing which takes place in the phase

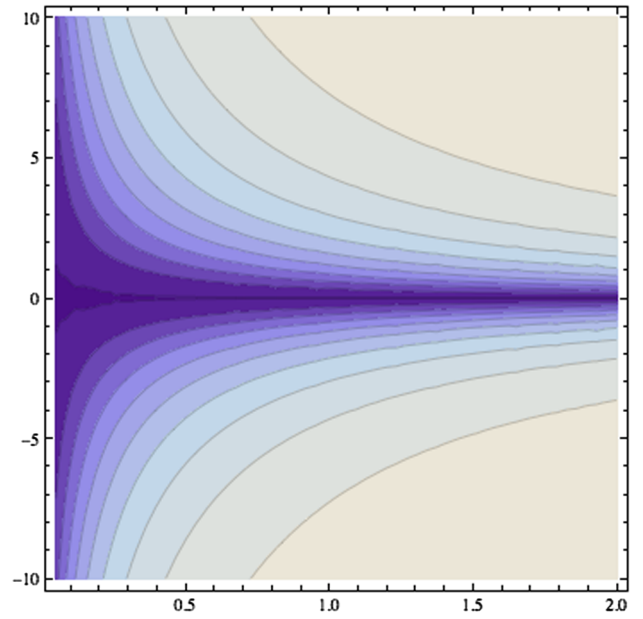


FIG. 4 (color online). Contour plot of the semiclassical expression $\langle q, p | A_{\theta} | q, p \rangle$. Here $k = 3$, q is running on the interval $[0, 2]$ and p on $[-10, 10]$. $\langle q, p | A_{\theta} | q, p \rangle$ is running on the interval $[0.74, 1]$.

space, we analyze the case of the theta function in Appendix B. Upon quantization, the theta function becomes a positive operator with a trivial kernel and its lower symbol is presented in Fig. 4. Consequently, all quantum configurations corresponding to the phase space become accessible by the physical (i.e., satisfying all the classical and quantum constraints) motion.

The present result shows that, in order to solve the singularity problem, one needs (at least partially) to impose the gravitational constraints at the quantum level. It does not mean that the Dirac approach is preferred. Rather, a combination of reducing the constraint partially on the classical level and partially on the quantum level seems to be the best option.

B. Features of the quantum bounce

We notice in formula (60) that the larger the anisotropy k^2 , the smaller the minimal volume which is reached by the collapsing universe. This straightforward observation challenges the relevance of the Planck scale to the big bounce as the change in anisotropy may make the bounce scale arbitrarily low.¹ Moreover, we notice that in (60) the minimal volume depends only on one effective constant

¹Another argument against the role of the Planck scale in dynamics of quantum cosmological models stems from the lack of a privileged time function in quantum gravity. A detailed reasoning may be found in [13]. Even for a specific choice of time, it has recently been shown [14] that quantum gravitational effects could be detected by relatively low-energy particles, provided that the spacetime is in a sufficiently nonclassical state.

$A(\nu)$, that is, the one which was present already in the isotropic models. Thus, we have obtained an extension of our previous result [1], which is exactly the “isotropic limit” of our present result. The next step in our research is to study in a similar manner other types of singularity. In farther future, we will consider the effect of the obtained singularity resolution on cosmological perturbations.

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APPENDIX A: COMPUTATION OF QUANTIZED HAMILTONIAN

The affine CS quantization (with fiducial vector ψ) of the simplified Hamiltonian $h_s = p^2 - k^2/q^2$, together with the positivity constraint $h_s > 0$, is performed through the decomposition into two terms

$$A_{\theta(h_s)h_s} = A_{h_s} - \bar{A}_{\theta(-h_s)h_s},$$

where the operators read in x representation, $\langle x'|A|x\rangle \equiv A$,

$$A_{h_s} = \int_{\Pi_+} \frac{dqdp}{2\pi} \theta\left(p^2 - \frac{k^2}{q^2}\right) \left(p^2 - \frac{k^2}{q^2}\right) e^{ip(x-x')} q^{-1} \bar{\psi}(x'/q) \psi(x/q),$$

$$A_{\theta(-h_s)h_s} = \int_{\Pi_+} \frac{dqdp}{2\pi} \theta\left(-p^2 + \frac{k^2}{q^2}\right) \left(p^2 - \frac{k^2}{q^2}\right) e^{ip(x-x')} q^{-1} \bar{\psi}(x'/q) \psi(x/q).$$

First, let us focus on the second term:

$$\begin{aligned} A_{\theta(-h_s)h_s} &= \int_{\Pi_+} \frac{dqdp}{2\pi} \theta\left(-p^2 + \frac{k^2}{q^2}\right) \left(p^2 - \frac{k^2}{q^2}\right) e^{ip(x-x')} q^{-1} \bar{\psi}(x'/q) \psi(x/q) \\ &= \int_{\Pi_+} \frac{dqdp}{2\pi} \theta(|k| - |pq|) \left(p^2 - \frac{k^2}{q^2}\right) e^{ip(x-x')} q^{-1} \bar{\psi}(x'/q) \psi(x/q) \\ &= \int_{\Pi_+} \frac{dqdp}{2\pi q^3} \theta(|k| - |P|) (P^2 - k^2) e^{i\frac{p}{q}(x-x')} q^{-1} \bar{\psi}(x'/q) \psi(x/q) \\ &= \int_0^\infty \int_{-|k|}^{|k|} \frac{dqdp}{2\pi q^3} (P^2 - k^2) e^{i\frac{p}{q}(x-x')} q^{-1} \bar{\psi}(x'/q) \psi(x/q) \\ &= \int_0^\infty \int_{-|k|}^{|k|} \frac{dqdp}{2\pi q^3} \psi(x/q) \left(-q^2 \frac{\partial^2}{\partial x^2} - k^2\right) e^{i\frac{p}{q}(x-x')} q^{-1} \bar{\psi}(x'/q) \\ &= \int_0^\infty \frac{dq}{2\pi q^3} \psi(x/q) \left(-q^2 \frac{\partial^2}{\partial x^2} - k^2\right) \frac{2 \sin\left(\frac{|k|}{q}(x-x')\right)}{x-x'} \bar{\psi}(x'/q) \\ &= \frac{2}{\pi} \int_0^\infty \frac{dq}{q} \left(\frac{k \cos\left(\frac{|k|}{q}(x-x')\right)}{q(x-x')^2} - \frac{\sin\left(\frac{|k|}{q}(x-x')\right)}{(x-x')^3}\right) \bar{\psi}(x'/q) \psi(x/q). \end{aligned}$$

Considering now the first term,

$$\begin{aligned} A_{h_s} &= \int_{\Pi_+} \frac{dqdp}{2\pi} \psi(x/q) \left(-\frac{\partial^2}{\partial x^2} - \frac{k^2}{q^2}\right) e^{ip(x-x')} q^{-1} \bar{\psi}(x'/q) \\ &= - \int_0^\infty dq \delta(x-x') q^{-1} \bar{\psi}(x'/q) [\psi_{,xx}(x/q) + 2\psi_{,x}(x/q) \partial_x + \psi(x/q) \partial_x^2] \\ &\quad - k^2 \int_0^\infty dq \delta(x-x') q^{-3} \bar{\psi}(x'/q) \psi(x/q), \end{aligned}$$

and introducing the integrals

$$\mathcal{I}_n := \int_0^\infty y^n |\psi|^2 dy, \quad \mathcal{J}_n := \int_0^\infty y^n |\psi'|^2 dy, \quad \mathcal{K}_n := \int_0^\infty y^n (\bar{\psi}\psi' - \bar{\psi}'\psi) dy,$$

we get the expression

$$A_{h_s} = \left(\mathcal{I}_{-1} P^2 + \frac{i \mathcal{K}_0}{2} (Q^{-1} P + P Q^{-1}) + (\mathcal{J}_1 - k^2 \mathcal{I}_1) Q^{-2} \right).$$

This reduces to (37) if ψ is real, since then $\mathcal{K}_0 = 0$ and we evaluate, with the notation $\xi_{rs}(\nu) = K_r(\nu)/K_s(\nu)$,

$$\frac{\mathcal{J}_1}{\mathcal{I}_{-1}} = \varsigma(\nu) = \frac{1}{4} (1 + \nu \xi_{01}(\nu)), \quad \frac{\mathcal{I}_1}{\mathcal{I}_{-1}} = \xi_{21}(\nu)^2.$$

The lower symbol of A_{h_s} is constructed out of the following partial results:

$$\langle q, p | P^2 | q, p \rangle = p^2 + \frac{1}{4} \xi_{10}(\nu) \xi_{12}(\nu) (\nu \xi_{32}(\nu) - 1) q^{-2}$$

and

$$\langle q, p | Q^{-2} | q, p \rangle = \xi_{10}(\nu) \xi_{12}(\nu) q^{-2}.$$

APPENDIX B: QUANTIZATION OF θ

The kernel of A_θ is (dimensionless)

$$\langle x | A_\theta | x' \rangle = \delta(x - x') - \frac{\xi}{2\pi K_0(\nu)} \frac{1}{x - x'} \operatorname{Im} \left[\sqrt{1 - \frac{4ikx - x'}{\xi\nu x + x'}} K_1 \left(\frac{\nu x + x'}{2\sqrt{xx'}} \sqrt{1 - \frac{4ikx - x'}{\xi\nu x + x'}} \right) \right]. \quad (\text{B1})$$

The semiclassical expression is

$$\langle q, p | A_\theta | q, p \rangle = 1 - \frac{\xi}{\pi K_0(\nu)^2} \int_0^1 \frac{dy}{\sqrt{y}(1-y)} \operatorname{Im} \left[\gamma(y, k) K_1 \left(\frac{\nu 1 + y}{2\sqrt{y}} \gamma(y, k) \right) \right] \operatorname{Re} \left[K_0 \left(\frac{\nu 1 + y}{2\sqrt{y}} \gamma(y, qp) \right) \right] \quad (\text{B2})$$

with

$$\gamma(y, a) = \sqrt{1 - \frac{4ia(1-y)}{\xi\nu(1+y)}}. \quad (\text{B3})$$

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