Is Bianchi I a bouncing cosmology in the Wheeler-DeWitt picture?

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We provide a quantum picture for the emergence of a bouncing cosmology, according to the idea that a semiclassical behavior of the universe towards the singularity is not available in many relevant minisuperspace models. In particular, we study the Bianchi I model in vacuum adopting the isotropic Misner variable as an internal clock for the quantum evolution. The isomorphism between the Wheeler-DeWitt equation in this minisuperspace representation and the Klein-Gordon one for a relativistic scalar field allows to identify the positive and negative frequency solutions as associated to the collapsing and expanding universe respectively. We clarify how any Bianchi I localized wave packet unavoidably spreads when the singularity is approached and therefore the semiclassical description of the model evolution in the Planckian region loses its predictability. Then, we calculate the transition amplitude that a collapsing universe is turned into an expanding one, according to the standard techniques of relativistic quantum mechanics, thanks to the introduction of an ekpyroticlike matter component which mimics a "quantum" time-dependent potential term and breaks the frequency separation. In particular, the transition probability of this "quantum big bounce" acquires a maximum value when the mean values of the momenta conjugate to the anisotropies in the collapsing universe are close enough to the corresponding mean values in the expanding one, depending on the variances of the ingoing and outgoing universe wave packets. This symmetry between the prebounce and postbounce mean values reflects what happens in the semiclassical bouncing cosmology, with the difference that here the connection of the two branches takes place on a pure probabilistic level.

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I. INTRODUCTION

The presence of an initial singularity in the universe thermal history [1,2] constitutes the most relevant shortcoming of the implementation of general relativity to the cosmological problem. Since the 1970s, the idea of a possible bounce was formulated to replace the initial singularity and reconnect a collapsing universe to our expanding one in order to depict the scenario of a cyclical universe [3]. Many implementations of a big bounce scenario have been considered over the years, essentially based on suitable modifications of the Einstein theory of gravity (for recent examples, see [4–6]).

However, the justification of a bouncing cosmology as the result of a quantum gravity effect in the Planckian epoch arose when in [7] it was demonstrated that the kinematical spectrum of the geometrical operators possesses a discrete nature in the framework of loop quantum gravity (LQG). Indeed, the implementation of this formulation [8–15] to the cosmological problem provided the emergence of a big bounce with a minimal universe volume in the past being different from zero and, consequently, a regularized behavior of the energy density (for critical considerations on the so-called loop quantum cosmology (LQC) see [16–18]). The presence of a similar behavior of the universe can be also recovered when polymer quantum mechanics (PQM) [19] is applied to the cosmological degrees of freedom [20–23] (for a comprehensive review on the bouncing cosmologies in PQM and LQC see [24]).

All these descriptions of a bouncing cosmology from quantum physics mainly rely on the characterization of quasiclassical states for the universe, which outline a mean behavior as following a big bounce picture and so deviating from general relativity at sufficiently high-energy density. However, this description seems lacking when the considered quasiclassical state follows the bounce trajectory with a significant spreading that would bring the dynamics into a full quantum sector. Actually, it cannot be excluded that relevant anisotropies can arise during the evolution of a contracting isotropic universe, see for instance the so-called ekpyrotic universes [25–27] where such a problem is addressed. The emergence of non-negligible anisotropy degrees of freedom constitutes a crucial mechanism,

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through which a closed universe would pass from a Robertson-Walker geometry to a Bianchi IX one [2]. In this picture, the Kasner-like behavior of a Bianchi IX localized state would be continuously perturbed towards the bounce by the potential term, see for instance the numerical analysis in [28].

Based on these considerations, it appears more reasonable to consider the bounce as a full quantum region of the universe evolution and so apply the concept of probability amplitude associated to a transition from a collapsing universe to an expanding one. In this respect, see the pioneering work [29] for approaches based on a path-integral formulation applied to the quantum cosmology in the Euclidean sector, while for recent applications to the Lorentz sector see [30,31]. Moreover, for other quantum scenarios related to a transition from a collapsing to an expanding universe see for instance [32,33]. We also mention the study recently presented in [34], in view of its promising applications and also for the rather general paradigm that is considered. In particular, the Bianchi I quantum cosmology is investigated, focusing on the problem of time in view of the resolution of the singularity. Two different classes of time parameters are found, such that the motion (and the range of the time parameter) is unbounded (fast-gauge time) or bounded (slow-gauge time). In the latter case, the removal of the singularity is achieved by quantization thanks to the unitarity preservation.

The aim of the present analysis is investigating the possibility to have a quantum big bounce also in the Wheeler-DeWitt (WDW) approach of quantum cosmology. We study the metric canonical quantization of the Bianchi I model in vacuum, adopting the well-known Misner variables [2,35]. According to the standard literature [36], we are able to provide an isomorphism between the WDW equation and a massless Klein-Gordon one by choosing the isotropic Misner variable as the internal time. Comparing the behavior of the classical constants of motion with their corresponding quantum eigenvalues, we can interpret the negative and positive frequencies of the WDW solutions as states which describe the expanding and collapsing universe, respectively. Also, we theoretically and numerically show that the localized wave packets are subjected to a significant spreading process, in order to support the need of describing the behavior of the Bianchi I model towards the singularity as an intrinsic quantum phenomenon.

After the quantization, we include a matter term with an equation of state parameter $w > 1$ that breaks down the frequency separation, being a time-dependent potential responsible for the transition from a collapsing universe to an expanding one (i.e., the positive and negative frequency states). We remark that the standard theory of relativistic scattering processes is used, as discussed in [37], where the projection of ingoing states onto outgoing ones is described via the wave function formalism (here the WDW wave function of the universe), so that we escape the so-called third quantization of the cosmological field and all the ambiguous related issues [37,38]. In particular, we project the ingoing wave packet for the collapsing universe, that represents the exact solution of the WDW equation during the ekpyrotic phase, on to a Bianchi I expanding wave packet, according to the procedure presented in [37]. In both the universe wave packets, we use a Gaussian weight in the momenta with nonzero mean values. As a result of treating the quantum big bounce as a scattering process, the probability amplitude of transition from the collapse to the expansion is nonzero and mathematically well defined. In particular, the probability amplitude has a peaked profile, with the interpretation that the most likely transition takes place when the mean value of the momenta of the expanding wave packet is approximately equal to the mean values of the contracting one, depending on their variances. In other words, a localized collapsing state of the universe has the maximum probability to make the transition into an expanding localized state if the morphology of the latter closely resembles the packet shape of the former.

This result opens a new perspective on the physical nature of the big bounce, at least when an internal time variable can be properly recovered. Indeed, the possibility for a quantum transition in the canonical quantum dynamics phenomenologically appears as a bouncing cosmology; nevertheless, it is due to the mixing of positive and negative frequency solutions when an interaction term is included, and does not rely on the existence of a semiclassical minimal value of the universe volume, that hence is no longer essential in order to deal with a bouncing cosmology at a quantum level.

The paper is structured as follows. In Sec. II the minisuperspace of the Bianchi models is introduced, with a particular focus on the dynamics of a Bianchi I wave packet in Sec. II A. In Sec. III the procedure of scattering integrals using the wave function formalism in the Klein-Gordon theory is presented. Section [23] contains the core of the work. The transition amplitude from a contracting to an expanding Bianchi I universe thanks to the $w > 1$ matter term is developed and the existence of a quantum big bounce in the WDW theory from a probabilistic point of view is discussed. Finally, in Sec. V some concluding remarks are outlined. We note that we use $8\pi G = c = \hbar = 1$ throughout the article.

II. MINISUPERSPACE OF THE BIANCHI MODELS

Let us start our analysis by discussing the structure of the Hamiltonian constraint of the Bianchi cosmological models, i.e., anisotropic, homogeneous, and nonstationary universes, in order to outline the isomorphic feature of the minisuperspace with the relativistic quantum theory. In the following, we will concentrate our attention to the Bianchi I model, that one having zero spatial curvature.

Using the Arnowitt-Deser-Misner (ADM) formalism and the Misner variables $(\alpha, \beta_+, \beta_-)$, the line element describing a Bianchi cosmology takes the form [1,2,39]

$$ds^2 = N^2 dt^2 - e^{2\alpha}(e^{2\beta})_{ab}\sigma^a\sigma^b, \tag{1}$$

where $\beta \equiv \mathrm{diag}\{\beta_+ + \sqrt{3}\beta_-, \beta_+ - \sqrt{3}\beta_-, -2\beta_+\}$, N denotes the lapse function and all the variables are time-dependent only, due to the spatial homogeneity. The 1-forms σ^a ($a = 1, 2, 3$) reflect the specific isometry of the considered Bianchi model and in the case of Bianchi I they reduce to exact differentials.

The action describing the dynamical features of a Bianchi model takes the expression

$$S_B = \int dt(p_\alpha\dot{\alpha} + p_+\dot{\beta}_+ + p_-\dot{\beta}_- - NH), \tag{2}$$

where

$$H \equiv Ce^{-3\alpha}[-p_\alpha^2 + p_+^2 + p_-^2 + e^{4\alpha}V_B(\beta_+, \beta_-)] \tag{3}$$

in which the explicit form of the potential term V_B fixes the considered Bianchi model ($V_B \equiv 0$ for Bianchi I). Here, the dot symbol denotes the derivative with respect to t, C is a constant depending on the performed spatial integration and p_α, and p_+ and p_- are the respective conjugate momenta to the Misner variables. The isotropic variable α defines the universe volume, while β_+ and β_- are the real gravitational degrees of freedom since they correspond to the anisotropies of the model.

As already outlined in [36] for the case of a generic superspace, the variable associated to the volume has a different signature with respect to the gravitational degrees of freedom and therefore it can be interpreted as a time variable for the classical and quantum dynamics of the system. In other words, we are entitled to adopt α as the internal clock of our minisuperspace corresponding to the homogeneous cosmologies. It is worth expressing the link of the relational time α in terms of the generic time variable t by varying the action (2) with respect to the momentum p_α, namely

$$\dot{\alpha} = -2NCe^{-3\alpha}p_\alpha. \tag{4}$$

If we choose the synchronous time ($N \equiv 1$), i.e., the time coordinate in which the thermal history of the universe is preferably described, we see that for $p_\alpha < 0$ the physical space expands with time, while for $p_\alpha > 0$ it contracts as time goes. Furthermore, we note that the momentum p_α becomes a constant of motion if we deal with a Bianchi I model (for which $V_B \equiv 0$), so that its sign can be specified *a priori* and the two branches of the expanding and collapsing universe can be separated at a classical level.

Clearly, when we canonically quantize the dynamical system described in (2) and (3), all the physical content is summarized in the universe wave function $\psi = \psi(N, \alpha, \beta_\pm)$ selected by the Hamiltonian operator $\hat{H}$ that annihilates it. In this respect, the canonical implementation of the primary constraint $\hat{p}_N \equiv 0$ (p_N being the conjugate momentum to N) provides that the wave function is independent of the lapse function, while the secondary constraint, whose classical existence is ensured by the variation of the action (2) with respect to the lapse function N, reads as

$$\hat{H}\psi = [\Box + e^{4\alpha}V_B(\beta_+, \beta_-)]\psi(\alpha, \beta_\pm) = 0, \tag{5}$$

where $\Box = \partial_\alpha^2 - \partial_{\beta_+}^2 - \partial_{\beta_-}^2$. Quantizing Eq. (3), the normal ordering has been used and a global positive fact $e^{-3\alpha}$ has been removed. As we can see, the WDW equation written in the Misner variables still outlines the role of the volumelike coordinate α as the internal time of the system and the parallelism with a Klein-Gordon relativistic equation is almost immediate. Also, it is easy to check that Eq. (5) admits the probability density

$$j_0 = i(\psi^*\partial_\alpha\psi - \psi\partial_\alpha\psi^*) \tag{6}$$

in analogy with the Klein-Gordon formalism. In order to deal with a positive defined probability density j_0, we need to perform the so-called frequency separation. Actually, in the simplest case of a Bianchi I model ($V_B \equiv 0$) without any matter content, the frequency separation is easily reached since the universe wave function can be written in the plane wave basis as

$$\psi_{\omega_k}^\pm(\alpha, \beta_\pm) = e^{\mp i\omega_k\alpha}e^{i(k_+\beta_+ + k_-\beta_-)}, \tag{7}$$

where $\omega_k \equiv \sqrt{k_+^2 + k_-^2}$.

Now, if we apply the quantum operator $\hat{p}_\alpha = -i\partial_\alpha$ to the wave function $\psi_{\omega_k}^\pm$ we see that the positive frequency solution is an eigenstate with a negative eigenvalue, while the positive one is associated to the negative frequency state. Accordingly, we can interpret the positive frequency solutions as corresponding to states that describe an expanding universe, vice versa the negative frequency solutions are associated with a collapsing universe. These considerations are supported by the Ehrenfest theorem that ensures that Eq. (4) is verified by the corresponding quantum expectation values.

This interpretation of the frequency separation will allow to deal with a relativistic quantum approach to the analysis of the Bianchi I dynamics, as discussed in [37], that is based on the use of the universe wave function formalism instead of the third quantization procedure.

It is important to stress that the WDW picture is a covariant formalism in which it does not emerge a time variable clearly, in the sense of a preferred arrow of time as in the Schrödinger formulation allowed by the ADM reduction. However, in the present scheme the formal analogy between the Bianchi I WDW equation in the Misner variables and a massless Klein-Gordon one makes it is possible to identify a clock. Hence, α inherits the role of the usual parameter t in relativistic quantum mechanics, in view of its different signature in the minisupermetric with respect to the anisotropies. In other words, the isotropic variable α is responsible for the time order. As explained above, the interpretation of the quantum states depends on the sign of the eigenvalue p_α of the corresponding quantum operator $\hat{p}_\alpha$. In particular, $\psi^+_{\omega_k}$ corresponds to a state that goes from smaller to bigger values of α, i.e., it is expanding or equivalently going forward in time, whereas $\psi^-_{\omega_k}$ is contracting or going backward in time. This is picture is natural if viewed in the formalism of a relativistic wave function for a single particle in first quantization. However, the question concerning the causality relation arises, since the measurements on the physical states must prevent the light cone violation. On a classical level, particles can not have speed faster than the light value and this is summarized in the real value (zero for the massless particles) of the invariant interval. On a quantum level, the causality property of a quantum field theory is expressed by the so-called microcausality relation, a direct consequence of the Lorentz invariance of the formalism. The translation of the microcausality relation in the minisuperspace, as induced by the minisupermetric signature, appears a highly nontrivial question. Actually, in the considered model the light cone structure is not lost at all. In fact, we recall that the potential term has to be regarded as an intrinsic quantum effect, so all the momenta are constant and the classical Bianchi I dynamics follows the trajectories

$$\beta_\pm = p_\pm \alpha + \bar{\beta}_\pm, \qquad p_+^2 + p_-^2 = 1, \tag{8}$$

where $\bar{\beta}_\pm$ are constants. Therefore, the pinpoint particle describing the universe in the minisuperspace has a constant anisotropy velocity that is equal to one, so the analogy with the massless particles in standard relativistic quantum mechanics is direct. By other words, for the classical Bianchi I dynamics only the light cone surface is available whereas spacelike trajectories are forbidden, so a certain information on the causality can be still recovered. As far as we are dealing with quantum localized wave packets, the classical features of the Bianchi I model are preserved by the Ehrenfest theorem, i.e., the operator α applied to the wave packets should provide measurements preserving the causal structure. During the scattering process, the causality preservation has to be referred to the Lorentz invariance of the quantum theory with respect to the minisupermetric. We finally stress that the introduction of the potential also in the classical framework would simply reduce the velocity of the Bianchi I pinpoint particle to a subluminal one, i.e., the potential term would not imply the possibility for noncausal trajectories when described in terms of the relational clock α.

A. Wave packets behavior in the Bianchi I minisuperspace

Before proceeding on analyzing in details the big bounce as a quantum process, in this subsection we preliminary discuss the properties of the Bianchi I wave packet. We construct a superposition of the particular solutions of the form (7) by means of a generic localizing function, in order to satisfy the requirement of describing a quasiclassical state for the universe which is compatible with the frequency separation. For example, in the case of an expanding universe we have

$$\psi(\alpha, \beta_\pm) = \iint_{-\infty}^{+\infty} dk_+ dk_- A(k_+, k_-) \psi^+_{\omega_k}, \tag{9}$$

where $A(k_+, k_-)$ is commonly chosen as a Gaussian function fixed by the initial condition on the wave function at a given instant of time $\alpha = \alpha_0$.

First of all, we notice that the Bianchi I wave packet (9) is characterized by a nonlinear dispersion relation ω_k. This feature produces a spreading of the wave packet during its propagation due to the presence of a nonzero second derivative of ω_k with respect to k_+, k_-. Differently, the Friedmann-Lemaître-Robertson-Walker (FLRW) universe is not affected by this issue since it is characterized by a linear dispersion relation. In fact, if we consider Gaussian coefficients of the form

$$A(k_+, k_-) = e^{\frac{-(k_+ - \bar{k}_+)^2}{2\pi\sigma_+^2}} e^{\frac{-(k_- - \bar{k}_-)^2}{2\pi\sigma_-^2}} \tag{10}$$

in (9), we can reasonably suppose that these coefficients are significantly different from zero only in the neighborhood of $(\bar{k}_+, \bar{k}_-)$ and so justify an expansion of ω_k up to the second-order term in (k_+, k_-) that simplifies the analytical calculation of the integral. As can be easily demonstrated, a linear term in α enters in the σ of the Gaussian packet due to the second derivative of ω_k with respect to k_+, k_-. As the wave packet propagates, both the mean value and the variance change with time, producing the spreading phenomenon (see Fig. 1). This feature of the Bianchi I universe clearly prevents a satisfactory description of the dynamics towards the singularity by means of quantum expectation values on semiclassical states. More specifically, when more general cosmological models with respect to the FLRW one are considered, in view of producing a reasonable description of the universe near the Planckian region, the hypothesis of a localized state is violated.

Here, we can not avoid a discussion on the wave function interpretation in the considered theory. As in [35,40,41], we emulate the physical meaning of our states and observables from the analogy with a relativistic particle [42], which,

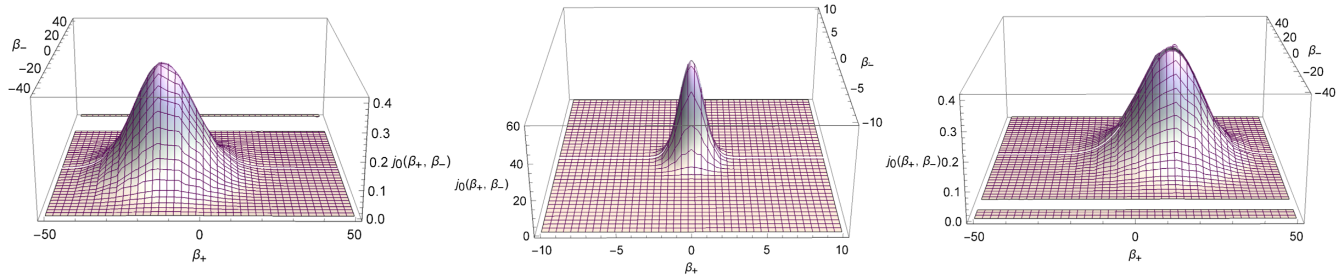

FIG. 1. 3D plots of the probability density j_0 associated to a Bianchi I wave packet containing only positive frequency plane waves. It is calculated at three different values of the relational time α ($\alpha = -10$, 0, 10, respectively).

however, is affected by subtle physical shortcomings. In fact, it is important to stress that the probability density j_0 is strictly positive for monochromatic plane waves only (see [23,43,44]). In particular, it can be easily seen that just the superposition of two different plane waves with positive energy-like eigenvalues leads to the emergence of regions in which j_0 assumes negative values. This fact is an indirect manifestation of the basic shortcoming that the Klein-Gordon equation is not a single-particle problem [37,43]. The scenario is a bit more viable, but not completely free of this limit, when we consider a Dirac equation, simply because the probability density is now always positive defined (for a Dirac-like equation in the minisuperspace see [45]). An heuristic explanation could be the fact that only one fermion can occupy a given state, due to the Pauli exclusion principle. Thus, the creation of real or virtual couples of particles-antiparticles is always relevant in relativistic quantum mechanics and only the second quantization procedure is the natural interpretative tool for the underlying physics. However, when we translate these considerations into the minisuperspace, as done here, the second quantization method (commonly dubbed third quantization approach) appears far from being physically grounded (see [40]), whereas the interpretation of the universe quantum dynamics as a single-particle problem seems more reasonable (for the discussion on multiuniverse proposals see [46–53]). Furthermore, as discussed in [23] (see also [2]), a different scenario to solve this issue could be the so-called ADM-reduction of the dynamics [54], which naturally separate the expanding and contracting branches. This is obtained at the price of fixing the time gauge and, in general, dealing with a nonlocal reduced Hamiltonian, with an associated probability density that is only globally conserved [43]. This picture, *de facto* resulting in a Salpeter-like formulation of the minisuperspace relativistic quantum dynamics, is beyond the scope of this manuscript and the proposed scheme, but could be the starting point to reformulate the quantum scenario of a cosmological scattering.

Here, we are considering the scattering theory as taking place below the couple creation threshold and accepting the single-particle representation, with the consequence of having to deal with the ill-defined probability density. This fact should be taken under serious consideration in quantum cosmology [55], since it raises the question that j_0 (properly a charge density) could not be a good candidate for a well-defined probability density through which computing expectation values of the quantum operators. Nevertheless, in our analysis the probability density j_0 remains always positive even if referred to a wave packet superposition, since the Gaussian weight privileges the peak frequency (see Fig. 1). In this work we try to go beyond the semiclassical approach to the dynamics near the singularity and so we overcome the problem of a well-defined probability density by resorting to a full quantum approach, i.e., using the notion of probability amplitude between two states.

III. THE TRANSITION AMPLITUDE IN THE WAVE FUNCTION FORMALISM

In this section we describe the formalism at the basis of the scattering amplitude calculation by following the approach presented in [37]. The Klein-Gordon equation describes relativistic particles of zero spin by means of its solutions, i.e., scalar wave functions. For the free particle the equation reads as

$$(\Box + m^2)\varphi(x) = 0, \tag{11}$$

whose solution $\varphi(x)$ can be written as a superposition of plane waves with both positive and negative frequencies

$$f_{\mathbf{p}}^{(\pm)}(x) = \frac{e^{\mp i p\cdot x}}{\sqrt{(2\pi)^2 2\omega_{\mathbf{p}}}}, \tag{12}$$

where $\omega_{\mathbf{p}} = p_0 > 0$ and $p^2 = m^2$ according to the Einstein energy condition. They form a complete set and satisfy the following orthogonality and normalization conditions

$$\int d^2x f_{\mathbf{p}'}^{(\pm)*}(x) i\overleftrightarrow{\partial}_0 f_{\mathbf{p}}^{(\pm)}(x) = \pm\delta^2(\mathbf{p}-\mathbf{p}'), \tag{13}$$

$$\int d^2x f_{\mathbf{p}'}^{(\pm)*}(x) i\overleftrightarrow{\partial}_0 f_{\mathbf{p}}^{(\mp)}(x) = 0. \tag{14}$$

The Feynman propagator for the Klein-Gordon equation has the expression

$$\Delta_F(x'-x) = \int \frac{d^3p}{(2\pi)^3} \frac{e^{-ip\cdot(x'-x)}}{p^2 - m^2 + i\epsilon} \tag{15}$$

and solves the following equation,

$$(\Box_{x'} + m^2)\Delta_F(x'-x) = -\delta^3(x'-x). \tag{16}$$

It propagates the positive-frequency parts of a generic superposition of solutions forward in time and the negative-frequency ones backward in time by construction. We notice that the possibility of creation and annihilation of single spinless particles would require a many-particle theory in interaction as developed in the quantum field theory formalism. However, it is possible to extend the propagator approach to the study of these particles coupled to source terms added to the right-hand side of (11). In particular, when an interaction term is added in Eq. (11) it becomes

$$(\Box + m^2 + V(x))\phi(x) = 0 \tag{17}$$

and the general integral has the following form

$$\phi(x) = \varphi(x) - \int d^3y \Delta_F(x-y)V(y)\phi(y), \tag{18}$$

through which the solution of (17) can be evaluated to the desired accuracy by iteration. In (18), $\varphi(x)$ is a superposition of plane waves defined as

$$\begin{aligned}\varphi(x) &= \varphi^{(+)}(x) + \varphi^{(-)}(x)\\ &= \int d^2pc_+(\mathbf{p})f_{\mathbf{p}}^{(+)} + \int d^2pc_-^*(\mathbf{p})f_{\mathbf{p}}^{(-)}.\end{aligned} \tag{19}$$

Now we can compute the transition amplitude to a particle state of given momentum p' by projecting the scattered wave emerging from the interaction onto a normalized free wave of momentum p', so that the transition probability is then given by the absolute square of this amplitude. In particular, for particles and antiparticles scattering we have

$$S_{\mathbf{p}'_+,\mathbf{p}_+} = \delta^2(\mathbf{p}'_+ - \mathbf{p}_+) - i\int d^3y f_{\mathbf{p}'_+}^{(+)*}(y)V(y)\phi(y) \tag{20}$$

and

$$S_{\mathbf{p}'_-,\mathbf{p}_-} = \delta^2(\mathbf{p}'_- - \mathbf{p}_-) - i\int d^3y f_{\mathbf{p}'_-}^{(-)*}(y)V(y)\phi(y), \tag{21}$$

respectively, whereas for pair production and annihilation we have

$$S_{\mathbf{p}_+,\mathbf{p}_-} = -i\int d^3y f_{\mathbf{p}'_+}^{(+)*}(y)V(y)\phi(y) \tag{22}$$

and

$$S_{\mathbf{p}_-,\mathbf{p}_+} = -i\int d^3y f_{\mathbf{p}'_-}^{(-)*}(y)V(y)\phi(y), \tag{23}$$

respectively. We notice that, under the hypothesis of a limited interaction region, $\phi(y)$ reduces to plane waves for $t\to-\infty$ and for $t\to+\infty$ it can be expanded in the plane waves basis with the S-matrix elements as the expansion coefficients. So, the conservation over time of the Klein-Gordon norm (13) guarantees that $\phi(y)$ can be normalized as plane waves and, if $\phi_{\mathbf{p}}(y)$ [namely the solution of (18) that reduces to a plane wave of momentum $\mathbf{p}$ for $t\to-\infty$] form a complete set, the unitarity of the operator S_{Bounce} is ensured. This legitimates $\mathcal{P} = |S_{\mathrm{Bounce}}|^2$ as a well-defined probability density.

IV. THE TRANSITION AMPLITUDE FROM A COLLAPSING TO AN EXPANDING BIANCHI I UNIVERSE

In this section we present the core of the work. First, we recall that the Bianchi I model is characterized by a primordial singularity at a classical level that is not solved in the WDW approach. Our aim is to investigate the probability of having a quantum transition from a collapsing to an expanding universe, in effort to treat the big bounce as a relativistic quantum interaction transposed to the primordial cosmology when a time-dependent interaction term is present. In this way, the big bang singularity would be solved even in the WDW formulation at a probabilistic level. All the background theory used in the following has been presented in the previous section and based on [37].

First of all, we solve the WDW equation for the Bianchi I model with a time-dependent potential

$$\hat{H}\psi = [\partial_\alpha^2 - \partial_{\beta_+}^2 - \partial_{\beta_-}^2 + \lambda e^{-3\epsilon\alpha}]\psi(\alpha,\beta_\pm) = 0, \tag{24}$$

that corresponds to (5) with $V_B \equiv 0$ and an ekpyroticlike matter component, i.e., a matter content with equation of state $P = w\rho$ where $w > 1$ [in (24) $\varepsilon = w - 1 > 0$]. Here, the ekpyrotic phase is generated by a quantum time-dependent potential that is dominant near the singularity and responsible for the transition, since it is able to mix the positive and negative frequency states. The choice of considering a fluid with equation of state $P > \rho$ is dictated by the effective value of w associated to the anisotropy variables β_+ and β_-. In fact, if we write down a Friedmann-like equation for the Bianchi I model [56], it is immediate to recognize that the effective energy density of the anisotropy degrees of freedom is associated to $w = 1$. Thus, we must take into account a matter contribution with $w > 1$, well-accounted by an ekpyrotic physics [25–27], in order to deal with a potential term which violates the frequency separation near the singularity and becomes negligible when the universe expands enough. We recall that we have chosen the natural operator ordering and that a global positive factor $e^{-3\alpha}$ has been removed before quantizing. It is important to stress that this ekpyrotic contribution is naturally designed to dominate the Planckian era, i.e., for $\alpha \to -\infty$, if present in the primordial universe dynamics. On the other hand, by considering a cosmological fluid with $w < 1$ (for instance the natural radiation contribution corresponding to $w = 1/3$), the dynamical picture would be reversed and the potential term would have dominated the late universe expansion, in clear contradiction with the presence of quantum scattering processes in a fully expanded classical universe. Furthermore, the presence of a radiation contribution as relevant in the Planckian universe is significantly questionable in this model, since it is certainly dominated by the definitely present anisotropy term.

Now we search for a solution of (24) in $L^2(\mathbb{R})$, namely of the form

$$\psi(\alpha,\beta_\pm) = \varphi(\alpha) e^{ik_+\beta_+} e^{ik_-\beta_-}, \tag{25}$$

so that (24) reduces to the following equation for the variable α

$$\partial_\alpha^2 \varphi(\alpha) + (\omega_k^2 + \lambda e^{-3\varepsilon\alpha})\varphi(\alpha) = 0, \tag{26}$$

with ω_k defined as in (7). The exact solution reads as

$$\varphi(\alpha) = c_1 \varphi^{(-)}(\alpha) + c_2 \varphi^{(+)}(\alpha), \tag{27}$$

where c_1, c_2 are integration constants and

$$\varphi^{(-)}(\alpha) = J_{-\frac{2i\omega_k}{3\varepsilon}}(2\sqrt{\lambda e^{-3\varepsilon\alpha}}/3\varepsilon)\Gamma\left(1 - \frac{2i\omega_k}{3\varepsilon}\right), \tag{28}$$

$$\varphi^{(+)}(\alpha) = J_{\frac{2i\omega_k}{3\varepsilon}}(2\sqrt{\lambda e^{-3\varepsilon\alpha}}/3\varepsilon)\Gamma\left(1 + \frac{2i\omega_k}{3\varepsilon}\right). \tag{29}$$

In (28)–(29), $J_\nu(x)$ indicates the Bessel function of the first kind and $\Gamma(x)$ the Euler gamma function. So, the general solution is

$$\psi(\alpha,\beta_\pm) = \iint_{-\infty}^{+\infty} dk_+ dk_- A(k_+,k_-)\varphi(\alpha) e^{ik_+\beta_+} e^{ik_-\beta_-}, \tag{30}$$

where $A(k_+,k_-)$ is defined as in [56]. We note that $\varphi^{(+)}(\alpha)$ and $\varphi^{(-)}(\alpha)$ reduce to a plane waves for $\alpha \to +\infty$ (except for a phase depending on ε). In other words, $\varphi(\alpha)$ has the right limit far from the singularity, since it reduces to the free solution when the $w > 1$ matter component becomes negligible. It is worth noting that the Bessel functions (corresponding for $\lambda \to 0$ to negative and positive frequency states respectively) are equally weighed in the ingoing wave packet by setting $c_1 = c_2 = 1/\sqrt{2}$. In this way, we do not privilege neither the collapsing neither the expanding configuration.

Now we compute the big bounce transition amplitude by projecting the scattered wave emerging from the interaction onto a free-universe wave packet of the form

$$\chi(\alpha,\beta_\pm) = \iint_{-\infty}^{+\infty} dk'_+ dk'_- A'(k'_+,k'_-) e^{-i\omega_{k'}\alpha} e^{ik'_+\beta_+} e^{ik'_-\beta_-}, \tag{31}$$

that consists in a superposition of only free expanding plane waves by means of Gaussian coefficients as defined in [56], where the prime symbol identifies the outgoing wave packet. In particular, by using (22) we obtain

$$S_{\rm Bounce} = -i \iiint_{-\infty}^{+\infty} d\alpha\, d\beta_+ d\beta_- \chi^*(\alpha,\beta_\pm) V(\alpha) \psi(\alpha,\beta_\pm), \tag{32}$$

where $\chi(\alpha,\beta_\pm)$ represents the free expanding universe wave packet (31), $V(\alpha) = \lambda e^{-3\varepsilon\alpha}$ and $\psi(\alpha,\beta_\pm)$ is the universe wave packet (30) that emerges from the interaction. Through the analytical calculation of the integral in the anisotropies β_+, β_- we obtain

$$\begin{aligned} S_{\rm Bounce} &= -i \iiint_{-\infty}^{+\infty} d\alpha\, d\beta_+ d\beta_- \iiiint_{-\infty}^{+\infty} dk_+ dk_- dk_+' dk_-' A(k_+,k_-) A'(k_+',k_-') V(\alpha) \varphi(\alpha) e^{i\omega_{k'}\alpha} e^{i(k_+-k_+')\beta_+} e^{i(k_- - k_-')\beta_-} \\ &= -i \int_{-\infty}^{+\infty} d\alpha \iiiint_{-\infty}^{+\infty} dk_+ dk_- dk_+' dk_-' A(k_+,k_-) A'(k_+',k_-') \delta(k_+ - k_+') \delta(k_- - k_-') V(\alpha) \varphi(\alpha) e^{i\omega_{k'}\alpha}, \end{aligned} \tag{33}$$

so the integration over k'_+, k'_- becomes trivial, thanks to the presence of the two Dirac delta functions $\delta(k'_+ - k_+)$ and $\delta(k'_- - k_-)$. We finally get

$$S_{\rm Bounce} = -i \iiint_{-\infty}^{+\infty} d\alpha\, dk_+ dk_- A(k_+,k_-) A'(k_+,k_-) V(\alpha) \varphi(\alpha) e^{i\omega_k\alpha}, \tag{34}$$

where $A(k_+, k_-)$ and $A'(k_+, k_-)$ are Gaussian distributions with different mean values and variances. We remark that the integral over the configurational variables α, β_+, β_- can be exchanged with those ones over k_+, k_- and k'_+, k'_- contained in the wave packets $\chi(\alpha \beta_+, \beta_-)$ and $\psi(\alpha \beta_+, \beta_-)$, since the integration domains are independent of all the variables. Then, the remaining integral in the variables α, k_+, k_- has been computed by means of both analytical and numerical methods. Finally, the big bounce transition probability is obtained by making the absolute square of (32) through which we get a four-variable scalar function

$$|S_{\mathrm{Bounce}}(\bar{k}'_+, \bar{k}'_-, \bar{k}_+, \bar{k}_-)|^2 \tag{35}$$

that depends only on the mean values of the momenta conjugate to the anisotropies β_+, β_- of the ingoing and outgoing states, as expected (in this calculation all the variances of the Gaussian coefficients have been set to $\sigma = 1/\sqrt{2\pi}$). In particular, by fixing the quantum numbers $\bar{k}_+, \bar{k}_-$ of the ingoing wave packet we obtain a two-variable function

$$\mathcal{P}(\bar{k}'_+, \bar{k}'_-) \tag{36}$$

describing the probability of a big bounce transition.

In Fig. 2 we present two plots that highlight the Gaussian shape of $\mathcal{P}(\bar{k}'_+, \bar{k}'_-)$, noticing that the peak of the probability density in the mean values $\bar{k}'_+$, $\bar{k}'_-$ of the outgoing wave packet occurs always in correspondence of the values assigned to the corresponding mean values $\bar{k}_+$, $\bar{k}_-$ of the ingoing wave packet. In particular, in the 3D plot we can see that the peak occurs for $(\bar{k}'_+, \bar{k}'_-) = (\bar{k}_+, \bar{k}_-) = (2, 4)$. Without loss of generality, in the 2D plots we have considered the same Gaussian distribution for the two anisotropy momenta by imposing $\bar{k} = \bar{k}_+ = \bar{k}_-$ and $\bar{k}' = \bar{k}'_+ = \bar{k}'_-$ in order to show the position of the probability peak (that occurs for $\bar{k}' = \bar{k}$) in a clearer way.

In Fig. 3 we have only considered the hypothesis of $\sigma_+ = \sigma'_+$ and $\sigma_- = \sigma'_-$, with the result that $\mathcal{P}(\bar{k}'_+, \bar{k}'_-)$ has a major variance along the direction in which the ingoing packet is widely spread (see the 3D plot) and also the position of the peak occurs no longer exactly in correspondence of the mean values $\bar{k}'_+$ and $\bar{k}'_-$ of the ingoing wave packet. As a result, when the same mean values $\bar{k}' = \bar{k}'_+ = \bar{k}'_-$ for the outgoing wave packet are considered, the probability peak occurs exactly in correspondence of the average $\bar{k}' = (\bar{k}_+ + \bar{k}_-)/2$ only when the ingoing wave packets are equally peaked, whereas when considering $\sigma_+ \neq \sigma_-$ the peak occurs near the mean value of the more localized ingoing Gaussian distribution (see the 2D plots). The relevant role of the wave packet variances on the probability peak position is even more evident in Fig. 4. In particular, in the 3D plot we have considered all the

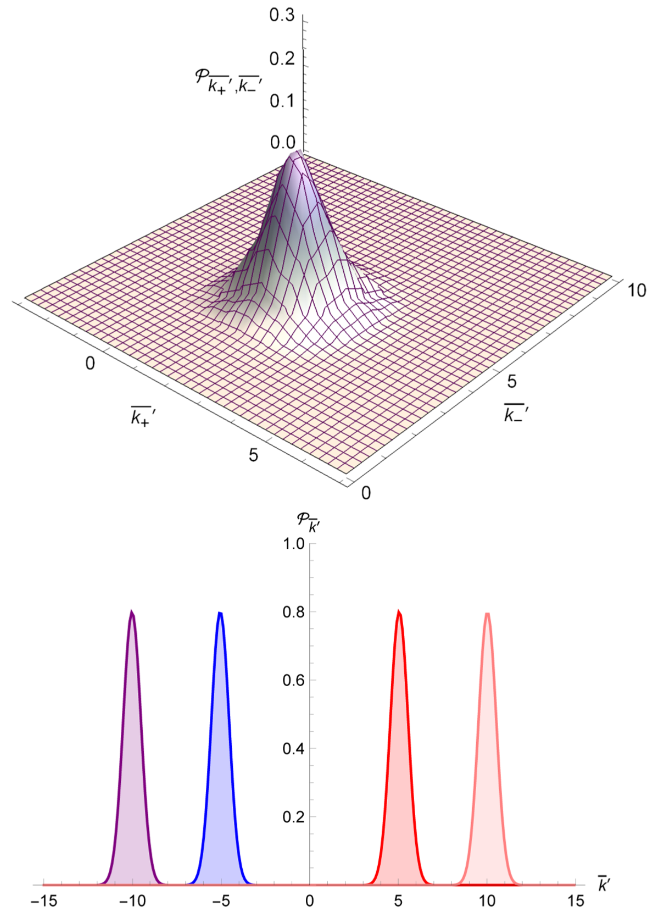

FIG. 2. Top: 3D plot of the normalized probability density $\mathcal{P}(\bar{k}'_+, \bar{k}'_-)$ of the big bounce transition. We can notice that the peak of $\mathcal{P}(\bar{k}'_+, \bar{k}'_-)$ occurs for $(\bar{k}'_+, \bar{k}'_-) = (\bar{k}_+, \bar{k}_-)$. In this graph we have considered $\lambda = 1$, $\varepsilon = 1/3$, $\bar{k}_+ = 2$, $\bar{k}_- = 4$. Bottom: 2D plots of the normalized probability density $\mathcal{P}(\bar{k}')$ of the big bounce transition for different values of $\bar{k}$. We can notice that the peak of $\mathcal{P}(\bar{k}')$ occurs for $\bar{k}' = \bar{k}$. In this graph we have considered $\lambda = 1$, $\varepsilon = 1/3$ and (from the left) $\bar{k} = -10, -5, 5, 10$.

Gaussian variances set to $\sigma = \sqrt{2\pi}$ and we note that the peak of $\mathcal{P}(\bar{k}'_+, \bar{k}'_-)$ is slightly shifted with respect to the graph presented in Fig. 2, where $\sigma = 1/\sqrt{2\pi}$. Also, in the 2D plots we can see that the peak of $\mathcal{P}(\bar{k}')$ occurs exactly in correspondence of $\bar{k}' = \bar{k}$ (here we have set $\bar{k} = 5$ for the ingoing Gaussian distributions) only when the ingoing wave packet is highly peaked, whereas the bigger the variance σ is the more appreciable the shift of the peak with respect to the value of $\bar{k}$ is.

In conclusion, we have demonstrated that the presence of the big bounce for the anisotropic Bianchi I universe can be treated at a full quantum level by means of a well-defined probability density, with different features depending on how the ingoing and outgoing wave packets are constructed. It is worth stressing that in our scattering picture the role of a time variable is played by the isotropic Misner

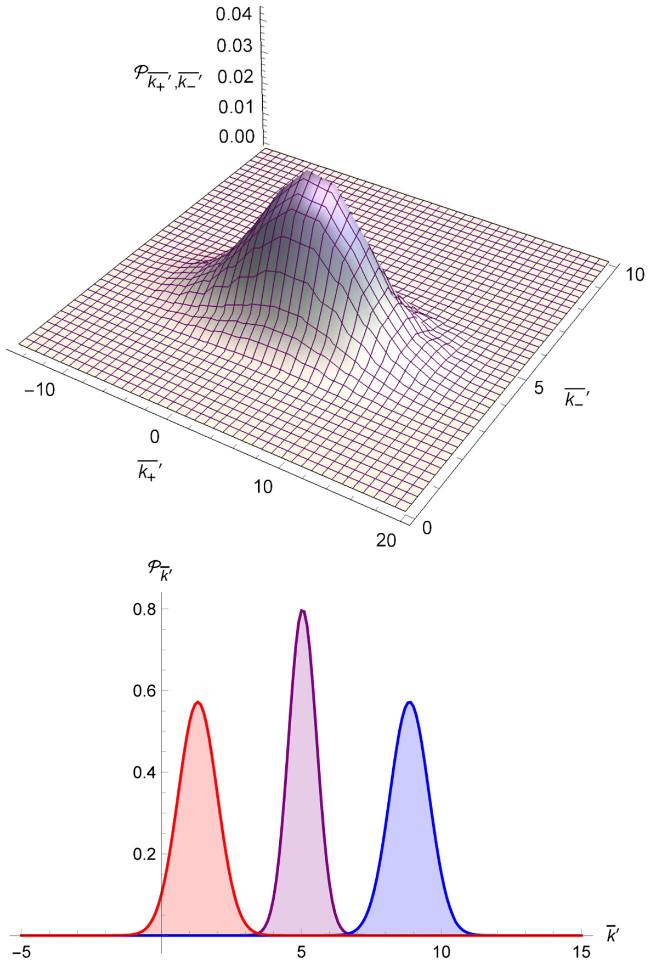

FIG. 3. 3D plot of the normalized probability density $\mathcal{P}(\bar{k}'_+, \bar{k}'_-)$ ($\bar{k}_+ = 2$, $\bar{k}_- = 4$). 2D plots of the normalized probability density $\mathcal{P}(\bar{k}')$ ($\bar{k}_+ = 1$, $\bar{k}_- = 9$ and $\sigma_+ = \sigma'_+ = 1/\sqrt{2\pi}$, $\sigma_- = \sigma'_- = \sqrt{2\pi}$ in the red plot, $\sigma_+ = \sigma'_+ = 1/\sqrt{2\pi}$, $\sigma_- = \sigma'_- = 1/\sqrt{2\pi}$ in the purple one, $\sigma_+ = \sigma'_+ = 1/\sqrt{2\pi}$, $\sigma_- = \sigma'_- = \sqrt{2\pi}$ in the blue one).

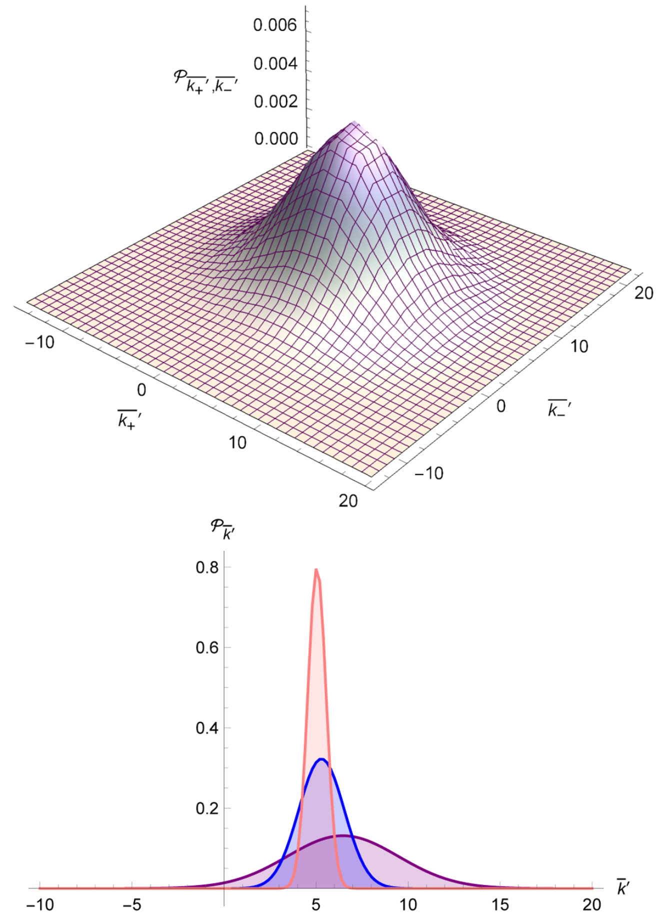

FIG. 4. Top: 3D plot of the normalized probability density $\mathcal{P}(\bar{k}'_+, \bar{k}'_-)$ of the big bounce transition for $\sigma_+ = \sigma'_+ = \sqrt{2\pi}$ and $\sigma_- = \sigma'_- = \sqrt{2\pi}$. We have considered $\lambda = 1$, $\varepsilon = 1/3$, $\bar{k}_+ = 2$, $\bar{k}_- = 4$. Bottom: 2D plots of the normalized probability density $\mathcal{P}(\bar{k}')$ of the big bounce transition for different values of the variance σ. We have considered $\lambda = 1$, $\varepsilon = 1/3$, $\bar{k} = 5$, and $\sigma = 1/\sqrt{2\pi}$ in the pink plot, $\sigma = 1$ in the blue one, $\sigma = \sqrt{2\pi}$ in the purple one.

variable α, due to the identification of the minisupermetric with a Minkowski metric tensor. A basic request for a variable to be a viable quantum clock is its monotonic behavior on a semiclassical level [57,58]. This statement suggests the idea that α can not be a proper clock in describing the quantum evolution of a bouncing cosmology, since in the collapsing and expanding branches it would provide a different time arrow [40]. However, this issue would concern a semiclassical big bounce picture and not the present analysis in which the proposed bouncing scenario is at a full quantum level, whereas the classical dynamics is singular and hence the behavior of α is monotonic. In particular, in this scheme the presence of a quantum time-dependent potential allows the coexistence of both the positive and negative energy solutions near the singularity, i.e., a mixed state, making it possible a nonzero probability transition from a collapsing to an expanding universe. Thus, the quantum resolution of the initial singularity is not related to a nonmonotonic behavior of α but to the simultaneous presence of wave packets that move forward and backward in time, due to the presence of the potential. We also remark that the picture would be perfectly time reversible in a collapsing branch, having for $\alpha \to \infty$ its collapsing asymptotic free state. Clearly, between these two separate representations we use that one in which the pure state is expanding, according to our universe phenomenology. To be thorough, despite the well-posed choice of α as time variable for the proposed scattering picture, the possibility to use a matter relational time (for instance a free massless scalar field) should be regarded as an intriguing perspective for further investigations. Actually, its concordant signature with respect to that of the anisotropies does not prevent to choose it as a clock in a genuine relational interpretation of the problem of time and, what is more, it would not be affected by any nonmonotonic behavior even in a semiclassical bouncing picture, see [59]. For other approaches to the problem of time in the WDW formalism, see also [60–64]. We finally remark that the transition we are considering is a fully quantum process, so the range of validity of the present procedure is restricted to a finite time region where the strong interaction potential is turned on. Clearly, when the universe can no longer be described by a wave function, its dynamics follows the classical trajectories that derive from (3). Moreover, the probability amplitude tends to zero by construction when $\lambda \to 0$, consistently with the fact that the transition of the quantum big bounce is possible only in the presence of a time-dependent potential able to create a mixed initial state for the collapsing universe.

An important point to be addressed in the proposed parallelism between the Bianchi I quantum cosmology and the relativistic quantum mechanics scattering is the following. In the latter, the interaction potential is significantly different from zero only for a finite time interval, before and after which the states describe free particles. In the present cosmological analysis, the interaction potential is really negligible only in the future direction, i.e., $\alpha \to +\infty$. In the past, asymptotically close to the singularity, the potential contribution explodes. However, two points should be made:

(i) the negligibility of the potential term in one of the two asymptotic time direction is enough to ensure the existence of an Hilbert space for the quantum theory [40], and

(ii) we are able to calculate an exact solution for any value of the variable α, even in the region where the potential is diverging. These two facts make the theory viable and allow to describe the transition amplitude as the direct projection of an ingoing state from $\alpha \to -\infty$ onto an outgoing state towards $\alpha \to +\infty$, disregarding the peculiar behavior of the potential term. However, the analogy between a quantum cosmological bounce and a relativistic quantum scattering would be significantly improved in the presence of a regularization of the universe volume, i.e., in the presence of a semiclassical nonsingular behavior. In fact, if the universe volume does not approach zero but a finite value, the potential term could no longer explode and it would be a transient effect, just as in quantum field theory. It is worth noting that in such a scenario a relational time must be used since the volume would be nonmonotonic and could not play the role of time. In this respect, we think that the here proposed idea of a quantum bounce as a scattering is a significant improvement of those LQC bouncing models in which the notion of a quasiclassical bounce is not applicable, but the universe volume is naturally regularized in the underlying full theory [7].

To summarize, the present scattering model has three main merits that deserve attention for further developments. The first point is having emphasized that a pure semiclassical description of a bouncing cosmology could be affected by nontrivial difficulties when analyzing the Bianchi universes, given that even the Bianchi type I is characterized by Gaussian-like spreading states. This means that the notion of a quasiclassical trajectory has to be abandoned near the Planckian era. The second merit is having shown that the epkyroticlike matter contribution is able to couple the expanding and the collapsing branches by means of the basic eigenstates, i.e., the Bessel functions, in the exact interacting solution as simultaneous components. In particular, when such a term becomes relevant we are able to calculate the exact solution of the $(1+2)$-dimensional Klein-Gordon equation, i.e., we are not using a perturbative approach, and the cross section between the two branches is naturally allowed with the same arrow of time. We stress how this aspect is closely related to the analysis presented is [34]. Finally, as a third feature to be further analyzed we observe that our picture could be extended to the so-called Belinski-Khalatnikov-Lifshitz conjecture, so leading to a notion of quantum big bounce also in the generic cosmological solution (see [65,66] and, for a careful analysis of the required additional hypotheses as well as of the technical formulation of this inhomogeneous extension, see [67]). In fact, on a qualitative level the superspace of the universe factorizes into independent minisuperspaces, i.e., small causal regions of the universe, at each point of the space (for a classical statistical and quantum discussion see [68]).

V. CONCLUDING REMARKS

In the analysis above we proposed the idea that a bouncing cosmology can emerge even in the framework of the WDW equation [2,35,41] (i.e., without introducing formalism and concepts of LQC [59]), as soon as the replacement of a collapsing universe with an expanding one is viewed on a quantum level as a transition amplitude.

We analyzed a Bianchi I model in vacuum by identifying the Misner variable α as an internal time and basing our quantum study on a parallelism with the Klein-Gordon equation. We first emphasized the isomorphism existing between the positive and negative frequency solutions and the expanding and collapsing universe, respectively. Then, we have shown that the wave packets constructed to approximate quasiclassically the evolution of the model unavoidably spread when $\alpha \to -\infty$ towards the cosmological singularity (the choice of α as time is coherent with a fast time gauge, see [34]), consistently with the behavior of a $(1+2)$-dimensional massless relativistic particle. Thus, we could infer how the behavior of the universe close enough to the initial big bang must be intrinsically a quantum phenomenon. Consequently, the absence of a quasiclassical trajectory which outlines a minimal volume is not sufficient to exclude the presence of a quantum transition from the collapsing to the expanding universe, as soon as a physical mechanism able to break down the frequency separation is taken into account.

Therefore, we considered an ekpyrotic phase in the Kasner evolution, whose presence allows to deal with a nonzero probability that the collapse is replaced by an expansion at a probabilistic level. In order to calculate this transition amplitude, having in mind to avoid any third quantization procedure, we adopted the standard method discussed in [37], which is applicable to any scattering process described in the formulation of the relativistic wave function. Thanks to the isomorphism between our model and a Klein-Gordon massless equation with a time-dependent potential, we estimated the probability amplitude associated to a collapsing wave packet that is projected onto an expanding one via the Green function.

We clearly demonstrated that the obtained probability density is well defined and has a Gaussian shape. Its maximum occurs when the mean values of the quantities k_+ and k_- (as resulting from the Gaussian packets) essentially coincide in the collapsing and expanding universe if and only if the corresponding wave packets are sufficiently localized. By increasing the variances, the position of the probability peak is shifted with respect to the case of high localization and occurs just nearby the mean values of the ingoing wave packet. We propose this result as a notion of quantum big bounce, which has also a quasiclassical symmetry in the collapsing and expanding branches when sufficiently localized wave packets (i.e., quasiclassical states) are considered. In other words, our analysis has the aim to give rise to the seeds of a new scenario for the emergence of a bouncing cosmology, given the fact that the semiclassical notion of a modified dynamics, characterized by a finite maximum for the energy density, cannot be applied in many cosmological implementations of the quantum theory since localized states naturally spread in quite general models when the singularity (or the presumed bounce) is approached.

A further development is represented by the investigation of how the scenario proposed above can be implemented in the case of a generic relational time [57], i.e., at which extent we can make a direct identification of the frequency separation with the nature of the universe volume dynamics.

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