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Semiclassical solutions of generalized Wheeler-DeWitt cosmology

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We consider an extension of Wheeler-DeWitt minisuperspace cosmology with additional interaction terms that preserve the linear structure of the theory. General perturbative methods are developed and applied to known semiclassical solutions for a closed Universe filled with a massless scalar. The exact Feynman propagator of the free theory is derived by means of a conformal transformation in minisuperspace. As an example, a stochastic interaction term is considered, and first order perturbative corrections are computed. It is argued that such an interaction can be used to describe the interaction of the cosmological background with the microscopic d.o.f. of the gravitational field. A Helmoltz-like equation is considered for the case of interactions that do not depend on the internal time, and the corresponding Green’s kernel is obtained exactly. The possibility of linking this approach to fundamental theories of quantum gravity is investigated.

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I. INTRODUCTION

The Wheeler-DeWitt (WDW) equation represents the starting point of the canonical quantization program, also known as geometrodynamics. It was originally derived by applying Dirac’s quantization scheme to Einstein’s theory of gravity, formulated in Arnowitt-Deser-Misner variables. It has the peculiar form of a timeless Schrödinger equation, the solutions of which are functions defined on the space of three-dimensional geometries

$$H\psi = 0.$$  \hspace{1cm} (1)

The equation is a constraint imposed on physical states, encoding the invariance of the theory under reparametrization of the time variable. Together with the (spatial) diffeomorphism constraint, it expresses the principle of general covariance at the quantum level. This approach has, however, several limitations that prevented it from being accepted as a fully satisfactory theory of quantum gravity in its original formulation.1 Nonetheless, some of the issues it raises, as for instance the problem of time (i.e. the lack of a universal parameter used to describe the evolution of the gravitational field), are actually problems encountered by all fundamental (nonperturbative) approaches to quantum gravity. Others stem instead from the dubious mathematical structure of the theory. Among the most essential ones in the latter category, we mention the factor ordering problem in the Hamiltonian constraint and the construction of a physical Hilbert space.

Despite its limitations, WDW was proved to be a valuable instrument in cases where the number of degrees of freedom is restricted a priori, i.e. in minisuperspace and midisuperspace models. In particular, its application to cosmological settings has been extremely useful to gain insight into some of the deep questions raised by a quantum theory of the gravitational field, such as the problem of time [2] and the occurrence of stable macroscopic branches for the state of the Universe (as in the consistent histories approach [3]).

One of the fundamental aspects of WDW is its linearity. This is indeed a consequence of the Dirac quantization procedure and a property of any first-quantized theory. One can nonetheless find in the literature several proposals for nonlinear extensions of the geometrodynamics equation. They are in general motivated by an interpretation of $\psi$ in Eq. (1) as a field operator (rather than a function) defined on the space of geometries. This idea has been applied to cosmology and found concrete realization in the old baby universes approach [4]. More recently, a model motivated by Group Field Theory (GFT) (see Ref. [5] for a recent outline) has been proposed in Ref. [6] that retains the same spirit, taking loop quantum cosmology (LQC) [7] as a starting point.2

It is worthwhile stressing that the WDW theory can be recovered in the continuum limit (see Ref. [9] for details)

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1For a general account of the WDW theory and the problems it encounters, see e.g. Ref. [1].

2Yet another interpretation of the dynamical equation on minisuperspace has been recently advocated in Ref. [8]. According to this point of view, it should rather be interpreted as some analog of a (nonlinear) hydrodynamical equation, for which the superposition principle does not hold in general.
from a more fundamental theory such as LQC. In this sense it can be interpreted as an effective theory of quantum cosmology, valid at scales such that the fundamentally discrete structure of spacetime cannot be probed. Therefore, WDW, far from being of mere historical relevance, is rather to be considered as an important tool to extract predictions from cosmological models when a continuum, semiclassical behavior is to be expected.

In what follows we consider as a starting point the Hamiltonian constraint of LQC, leading to the free evolution of the Universe, as discussed in the GFT-inspired model [6]. Nonlinear terms are allowed, which can be interpreted as interactions between disconnected homogeneous components of an isotropic Universe (scattering processes describe topology change). Instead of resorting to a third quantized formalism built on minisuperspace models, we follow a rather conservative approach which does not postulate the existence of universes disconnected from ours. We therefore only take into account linear modifications of the theory, so as to guarantee that the superposition principle remains satisfied. Hence, these extra terms can be interpreted as self-interactions of the Universe, as well as violations of the Hamiltonian constraint.

We aim at studying the dynamics in a regime such that the free LQC dynamics (given by finite difference equations) can be approximately described in terms of differential equations. In this regime, the dynamics is given by a modified WDW equation. Since WDW is obtained in the limit of large volumes, it is clear that this effective theory cannot be used to study the dynamics of the Universe near the big bang or big crunch singularities. The additional interactions should be such that deviations from the Friedmann equation are small and will therefore be treated as small perturbations.

We consider a closed Friedmann-Lemaître-Robertson-Walker (FLRW) Universe, for which semiclassical solutions are known explicitly [10]. Corrections to the solutions arising from the extra linear interactions are obtained perturbatively. Of particular interest is the case in which the perturbation is represented by white noise. In fact, this could be a way to model the effect of the discrete structure underlying spacetime on the evolution of the macroscopically relevant degrees of freedom. It should therefore be possible to make contact, at least qualitatively, between the usual quantum cosmology and the GFT cosmology, according to which the dynamics of the Universe is that of a condensate of elementary spacetime constituents. Considering a white noise term amounts to treating the vacuum fluctuations of the gravitational field as a stochastic process, an approach motivated by an analogy with stochastic electrodynamics (SED) [11–14]. This will be done in Sec. VI. The analogy with SED has of course its limitations, since in the case at hand there is no knowledge about the dynamics of the vacuum, which should instead come from a full theory of quantum gravity. In spite of this limitation, the methods developed here are fully general, so as to allow for a perturbative analysis of the solutions of the linearly modified WDW equation for any possible form of the additional interactions.

In the present work, we restrict to a closed Universe, for which wave packet solutions were constructed in Ref. [10]. In the same work, it was shown that it is possible to construct a quantum state whose evolution mimics a solution of the classical Friedmann equation and is given by a quantum superposition of two Gaussian wave packets (one for each of the two phases of the Universe, expanding and contracting) centered on the classical trajectory. We build on the results of Ref. [10], considering the new interaction term as a perturbation and thus determining the corrections to the motion of the wave packets.

The rest of the paper is organized as follows. In Sec. II, we show how our model is motivated by LQC- and GFT-inspired cosmology [6] in the continuum limit (large volumes). In Sec. III, we review the construction of the wave packet solutions done in Ref. [10]. These solutions will be used in the subsequent sections as the unperturbed states describing the evolution of a semiclassical Universe. In Sec. IV, using the scalar field to define an internal time, we develop a framework for time-independent perturbation theory. The inverse of the Helmholtz operator corresponding to the free theory is computed exactly and turns out to depend on a real parameter, linked to the choice of the boundary conditions at the singularity. An analog of Ehrenfest’s theorem for the evolution equation of the expectation values of observables is then given. In Sec. V, the Feynman propagator of the WDW free field operator is evaluated exactly. This is accomplished by using a conformal map in minisuperspace, which reduces the problem to that of finding the Klein-Gordon propagator in a planar region with a boundary. In Sec. VI, we consider the case in which the additional interaction is given by white noise and discuss the implications for semiclassicality and the arrow of time. Finally, we review our results and their physical implications in Sec. VII.

II. FROM THE LQC FREE THEORY TO WDW

Let us briefly show how the WDW equation is recovered from the Hamiltonian constraint of LQC following Ref. [9].

3For our purposes it is convenient to consider a massless scalar field $\phi$, minimally coupled to the gravitational field. This choice has the advantage of allowing for a straightforward deparametrization of the theory, thus defining a clock. The Hamiltonian constraint has the general structure [6,9]

3The actual way in which WDW represents a large volume limit of LQC is put in clear mathematical terms in Refs. [15,16], where the analysis is based on a special class of solvable models (sLQC).
\[ \hat{K} \psi(\nu, \phi) \equiv -B(\nu)(\Theta + \partial_\phi^2)\psi(\nu, \phi) = 0, \]

(2)

where \( \psi \) is a wave function on configuration space, \( \Theta \) is a finite difference operator acting on the gravitational sector in the kinetic Hilbert space of the theory \( \mathcal{H}_{\text{kin}} \), and \( \nu \) denotes the generic eigenvalue of the volume operator. The discreteness introduced by the LQC formulation does not affect the matter sector, which is still the same as in the continuum WDW quantum theory. The gravitational sector of the Hamiltonian constraint operator of LQC in “improved dynamics”\(^4\), reads

\[ -B(\nu)\Theta \psi(\nu, \phi) \equiv A(\nu)\psi(\nu + \nu_0, \phi) + C(\nu)\psi(\nu, \phi) + D(\nu)\psi(\nu - \nu_0, \phi), \]

(3)

where the finite increment \( \nu_0 \) represents an elementary volume unit and \( A, B, C, D \) are functions which depend on the chosen quantization scheme. In order to guarantee that \( \Theta \) is symmetric\(^5\) in \( \nu \), the coefficients must satisfy the \( D(\nu) = A(\nu - \nu_0) \) condition [6]; it holds in both the \( k = 0 \) and the \( k = 1 \) case.

It is a general result of LQC that WDW can be recovered in the continuum (i.e., large volume) limit [15]. In particular, it was shown in Ref. [9] that for \( k = 1 \) one recovers the Hamiltonian constraint of Ref. [10]. In fact it turns out that \( \Theta \) can be expressed as the sum of the operator \( (\Theta_0) \) relative to the \( k = 0 \) case and a \( \phi \)-independent potential term (i.e., diagonal in the \( \nu \) basis) as

\[ \Theta = \Theta_0 + \frac{\pi G l_0^2}{3K^{4/3}} |\nu|^{4/3}. \]

(4)

In the above expression \( K = \frac{2\sqrt{3}}{3\sqrt[3]{3\sqrt{3}}} \), \( \gamma \) is the Barbero-Immirzi parameter of loop quantum gravity, \( G \) is the gravitational constant, and \( l_0 \) is the cube root of the fiducial volume of the fiducial cell on the spatial manifold in the \( k = 1 \) model. The latter can be formally sent to zero in order to recover the \( k = 0 \) case.

Restricting to wave functions \( \psi(\nu) \) which are smooth and slowly varying in \( \nu \), we obtain the WDW limit of the Hamiltonian constraint

\[ \Theta_0 \psi(\nu, \phi) = -12\pi G (\nu \partial_\nu)^2 \psi(\nu, \phi), \]

(5)

which is exactly the same constraint one obtains in WDW theory. Thus, LQC naturally recovers the factor ordering (also called covariant factor ordering, in the sense that the quantum constraint operator is of the form \( G^{AB}\nabla_A \nabla_B \)), where \( G^{AB} \) is the inverse WDW metric and \( \nabla_A \) denotes the covariant derivative associated with \( G_{AB} \) which was obtained in Ref. [2] under the requirement of field reparametrization invariance of the minisuperspace path integral. Since \( \nu \) represents a proper volume, it is proportional to the volume of a comoving cell with linear dimension equal to the scale factor \( a \),

\[ \nu \propto a^3. \]

(6)

Introducing the variable \( \alpha = \log a \), we rewrite the constraint operator \( \hat{K} \) as

\[ \hat{K} = e^{-3\alpha} \left( \frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \phi^2} - e^{4\alpha} \right). \]

(7)

Let us consider a modified dynamical equation of the form

\[ \hat{K} \psi(\nu, \phi) + \sum_{\nu'} \int d\phi' g(\nu, \nu'; \phi, \phi') \psi(\nu', \phi') = 0, \]

(8)

which, in the continuum limit \( \nu \gg \nu_0 \), leads to

\[ \left( \frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \phi^2} - e^{4\alpha} \right) \psi = -e^{3\alpha} \int d\alpha' d\phi' \frac{d\nu}{d\alpha'} g(\nu, \nu'). \]

(9)

We will assume for simplicity that the interaction \( g \) is local in minisuperspace, i.e., \( g(\nu, \nu'; \phi, \phi') = g(\nu, \phi) \delta(\nu - \nu') \delta(\phi - \phi') \). Given the properties of the Dirac delta function

\[ \delta(\nu - \nu') = \frac{d}{d\alpha} \bigg|_{\alpha'} \]

(10)

Eq. (9) reduces to a Klein-Gordon equation with space- and time-dependent potential \( e^{3\alpha} g(\alpha, \phi) \); note that \( g \) is kept completely general.

It should be pointed out that more general interaction terms than the ones considered in (8) can in principle be conceived. In fact, from the point of view of a third quantized theory of gravity, the most general equation of motion would involve nonlinear terms. However, the methods developed in this work are completely general, and their application to the study of nonlinearities in perturbation theory is straightforward, following the analogous well-known procedure in perturbative Relativistic Quantum Field Theory (RQFT). The main ingredient for such calculations is given by the Green’s function, together with the Feynman rules for the vertices associated with the
various interactions. A perturbative study of the WDW equation with an additional linear term can therefore be seen as the starting point for a more general study. Note that, even though such a generalization may seem more natural from a merely formal point of view, it makes the physical interpretation of the theory even more problematic. A linear term instead, as we will show with the example in Sec. VI, can be used to model the interaction of the degree of freedom represented by the scale factor with other microscopic degrees of freedom of the gravitational field without having to change the interpretation of $\psi$.

Since the interaction term represented by the rhs of Eq. (9) is unknown, we cannot determine an exact solution of the equation without resorting to a case by case analysis. However, since the solutions of the WDW equation in the absence of a potential are known explicitly, we will adopt a perturbative approach. The method we develop is fully general and can thus be applied for any possible choice of the function $g$.

We formally expand the wave function and the WDW operator in terms of a dimensionless parameter $\lambda$ (that serves bookkeeping purposes and will be eventually set equal to 1),

\[ \psi = \psi^{(0)} + \lambda \psi^{(1)} + \ldots, \]  
\[ \hat{T} = \hat{T}_0 + \lambda e^{3\sigma} \int g. \]

with the definitions

\[ \hat{T}_0 \equiv \left( \frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \phi^2} - e^{4\alpha} \right). \]

We therefore have

\[ \hat{T}_0 \psi^{(0)} = 0, \]  
\[ \hat{T}_0 \psi^{(1)} = -e^{3\sigma} g \psi^{(0)}. \]

The zeroth order term $\psi^{(0)}$ is a solution of the wave equation with an exponential potential, which was obtained in Ref. [10] and will be reviewed in the next section. If we were able to invert $\hat{T}_0$, we would get the wave function corrected to first order. However, finding the Green’s function is not straightforward in this case as it would be for $k = 0$ (where the kinetic operator is just the d’Alembertian, for which the Green’s kernels are well known for all possible choices of boundary conditions). Moreover, as for the d’Alembertian, the Green’s kernel will depend on the boundary conditions. The problem of determining which set of boundary conditions is more appropriate depends on the physical situation we have in mind and will be dealt with in the next sections.

At this point, we would like to point out the relation between our approach and the model in Ref. [6], where a third quantization perspective is assumed. The action on minisuperspace that was considered in Ref. [6] reads\(^6\)

\[ S[\psi] = S_{\text{free}}[\psi] + \sum_n \frac{\lambda_n}{n!} \int \! d\phi_1 \ldots d\phi_n f^{(n)}(\nu_i, \phi_i) \prod_j \psi(\nu_j, \phi_j), \]  
\[ \hat{\mathcal{C}} \]

where the first term gives the dynamics of the free theory, namely, a homogeneous and isotropic gravitational background coupled to a massless scalar field

\[ S_{\text{free}}[\psi] = \sum_{\nu} \int \! d\psi \psi(\nu, \phi) \hat{\mathcal{K}} \psi(\nu, \phi); \]

$\hat{\mathcal{K}}$ is the Hamiltonian constraint in LQC, and the terms containing the functions $f^{(n)}$ represent additional interactions that violate the constraint. This is a toy model for group field cosmology [6], given by a GFT with group $G = U(1)$ and $\nu$ a Lie algebra element. The free dynamics depends on the specific LQC model adopted. However, the continuum limit should be the same regardless of the model considered and must give the WDW equation for the corresponding three-space topology. The WDW approach to quantum cosmology should therefore be interpreted as an effective theory, valid at scales such that the discreteness introduced by the polymer quantization cannot be probed. We will show that, even from this more limited perspective, the action Eq. (16) leads to a novel effective theory of quantum cosmology that represent modifications of WDW. The validity of this approach is limited to large volumes and therefore cannot be used to study the dynamics near spacetime singularities.

It was hinted in Ref. [6] that the additional interactions could also be interpreted as interactions occurring between homogeneous patches of an inhomogeneous Universe. Another possible interpretation is that they actually represent interactions among different, separate, universes. The latter turns out to be a natural option in the framework of third quantization (see Ref. [18] and references therein), which naturally allows for topology change.\(^7\)

We restrict our attention to the quadratic term, that can be interpreted as a self-interaction of the Universe. This is in fact worth considering even without resorting to a third-quantized cosmology and can in principle be generalized to include nonlocality in minisuperspace (this situation will not be dealt with in the present work).

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\(^6\)The model was originally formulated for $k = 0$, but it admits a straightforward generalization to include the case $k = 1$.

\(^7\)For an example of topology change in the old “baby universes” literature, see e.g. Ref. [4].
III. ANALYSIS OF THE UNPERTURBED CASE

We review here the construction of wave packet solutions for the cosmological background presented in Ref. [10]. The Wheeler-DeWitt equation for a homogeneous and isotropic Universe (compact spatial topology, $k = 1$) with a massless scalar field is

\[
\left( \frac{\partial^2}{\partial \alpha^2} - \frac{\partial^2}{\partial \phi^2} - e^{4\alpha} \right) \psi(\alpha, \phi) = 0. \tag{18}
\]

We impose the boundary condition

\[
\lim_{\alpha \to \infty} \psi(\alpha, \phi) = 0, \tag{19}
\]

necessary in order to reconstruct semiclassical states describing the dynamics of a closed Universe, since regions of minisuperspace corresponding to arbitrary large scale factors are not accessible.

Equation (19) can be solved by separation of variables

\[
\psi_k(\alpha, \phi) = N_k C_k(\alpha) \varphi_k(\phi), \tag{20}
\]

leading to

\[
\frac{\partial^2}{\partial \phi^2} \varphi_k + k^2 \varphi_k = 0, \tag{21}
\]

\[
\frac{\partial^2}{\partial \alpha^2} C_k - (e^{4\alpha} - k^2) C_k = 0. \tag{22}
\]

Note that $\psi_k(\alpha, \phi)$ stands for the solution of Eq. (18) and should not be confused with the Fourier transform of $\psi$, for which we will use instead the notation $\tilde{\psi}(\alpha, k)$. In Eq. (20) above, $N_k$ is a normalization factor that depends on $k$, the value of which will be fixed later.

Let us proceed with the solutions of Eqs. (21) and (22). Equation (21) yields complex exponentials as solutions

\[
\varphi_k = e^{ik\phi}, \tag{23}
\]

while Eq. (22) has the same form as the stationary Schrödinger equation for a nonrelativistic particle in one dimension, with potential $V(\alpha) = e^{4\alpha} - k^2$ and zero energy. One then easily remarks that the particle is free for $\alpha \to -\infty$, whereas the potential barrier becomes infinitely steep as $\alpha$ takes increasingly large positive values. Given the imposed boundary condition, Eq. (22) admits as an exact solution the modified Bessel function of the second kind (also known as the MacDonald function):

\[
C_k(\alpha) = K_{ik/2} \left( \frac{e^{2\alpha}}{2} \right). \tag{24}
\]

Wave packets are then constructed as linear superpositions of the (appropriately normalized) solutions

\[
\psi(\alpha, \phi) = \int_{-\infty}^{\infty} dk \psi_k(\alpha, \phi) A(k), \tag{25}
\]

with an appropriately chosen amplitude $A(k)$. Since the $C_k(\alpha)$ are improper eigenfunctions of the (one-parameter family of) Hamiltonian operator(s) in Eq. (22), they do not belong to the space of square integrable functions on the real line $L^2(\mathbb{R})$. However, it is still possible to define some sort of normalization by fixing the oscillation amplitude of the improper eigenfunctions for $\alpha \to -\infty$. For this purpose, we recall the WKB expansion of Eq. (24),

\[
K_{ik/2} \left( \frac{e^{2\alpha}}{2} \right) = \sqrt{\frac{\pi}{2}} e^{-k} (k^2 - e^{4\alpha})^{-1/4} \times \cos \left( \frac{k}{2} \sqrt{\text{arccos} \left( \frac{k}{2e^{2\alpha}} \right) - \frac{1}{2} \sqrt{k^2 - e^{4\alpha} - \pi} \frac{4}{4}} \right), \tag{26}
\]

a very accurate approximation for large values of $k$. We therefore set

\[
\psi_k(\alpha, \phi) = e^{i\alpha \sqrt{k} K_{ik/2} \left( \frac{e^{2\alpha}}{2} \right)} e^{ik\phi}, \tag{27}
\]

which for large enough values of $k$ gives elementary waves with the same amplitude to the left of the potential barrier. Note that for small $k$ the amplitude $A(k)$ will still exhibit dependence on $k$.

Let us assume a Gaussian profile for the amplitude $A(k)$ in Eq. (25),

\[
A(k) = \frac{1}{\pi^{1/4} \sqrt{b}} e^{-\frac{(\ln k)^2}{2b^2}}, \tag{28}
\]

where $\bar{k}$ should be taken large enough so as to guarantee the normalization of the function $\psi_k(\alpha, \phi)$. One then finds that the solution has the profile shown in the Fig. 1. The solution represents a wave packet that starts propagating from a region where the potential vanishes (i.e. at the initial singularity) toward the potential barrier located approximately at $\alpha_k = \frac{1}{2} \log \bar{k}$, from where it is reflected back. For such values of $\bar{k}$, the wave packet is practically completely reflected back from the barrier. The parameter $b$ gives a measure of the semiclassicality of the state; i.e. it accounts for how much it peaks on the classical trajectory. We remark that the peak of the wave packet follows closely the classical trajectory,

\[
e^{2\alpha} = \frac{\bar{k}}{\cosh(2\phi)}, \tag{29}
\]

and refer the reader to Fig. 2.
IV. TIME-INDEPENDENT PERTURBATION POTENTIAL

In the case in which the potential in the rhs of Eq. (9) does not depend on the scalar field (that we interpret as an internal time), we can resort to time-independent perturbation theory to calculate the corrections to the wave function. Namely, we consider the representation of the operator $\hat{T}_0$ defined in Eq. (13) in Fourier space, or equivalently its action on a monochromatic wave, so that we are lead to the Helmoltz equation in the presence of a potential,

$$\left( \frac{\partial^2}{\partial \alpha^2} + k^2 - e^{4\alpha} \right) \tilde{\psi}^{(0)}(\alpha, k) = 0, \quad (30)$$

where the potential cannot be considered as a small perturbation with respect to the standard Helmoltz equation. In fact, reflection from an infinite potential barrier requires boundary conditions that are incompatible with those adopted in the free particle case. We therefore have to solve Eq. (30) exactly.

In order to compute the first perturbative corrections, we need to solve Eq. (15), which in Fourier space leads to

$$\left( \frac{\partial^2}{\partial \alpha^2} + k^2 - e^{4\alpha} \right) \tilde{\psi}^{(1)}(\alpha, k) = U(\alpha) \tilde{\psi}^{(0)}(\alpha, k), \quad (31)$$

upon defining $U(\alpha) = -e^{3\alpha} g(\alpha)$. Equation (31) is easily solved once the Green’s function of the Helmoltz operator on the lhs is known. The equation for the Green’s function is

$$\left( \frac{\partial^2}{\partial \alpha^2} + k^2 - e^{4\alpha} \right) G^k(\alpha, \alpha') = \delta(\alpha - \alpha'). \quad (32)$$

The homogeneous equation admits two linearly independent solutions, which we can use to form two distinct linear combinations that satisfy the boundary conditions at the two extrema of the interval of the real axis we are considering. The remaining free parameters are then fixed by requiring continuity of the function at $\alpha'$ and the condition on the discontinuity of the first derivative at the same point.

Equation (30) has two linearly independent solutions $p(\alpha)$ and $h(\alpha)$ given by

$$p(\alpha) = K_{\frac{3}{2}} \left( \frac{e^{2\alpha}}{2} \right) \quad (33)$$

and

$$h(\alpha) = I_{-\frac{3}{2}} \left( \frac{e^{2\alpha}}{2} \right) + I_{\frac{3}{2}} \left( \frac{e^{2\alpha}}{2} \right). \quad (34)$$

We thus make the following ansatz,

$$G^k(\alpha, \alpha') = \begin{cases} 
\gamma p(\alpha) & \alpha \geq \alpha' \\
\delta h(\alpha) + \eta p(\alpha) & \alpha < \alpha',
\end{cases} \quad (35)$$
and note that $G^h(\alpha, \alpha')$ satisfies the boundary condition Eq. (19) by construction.

Since we do not know what the boundary condition for $\alpha \to -\infty$ is, i.e. near the classical singularity,\(^8\) we will not be able to fix the values of all constants $\gamma, \delta, \eta$. We will therefore end up with a one-parameter family of Green’s functions.

The Green’s function must be continuous at the point $\alpha = \alpha'$, hence

$$\gamma p(\alpha') = \delta h(\alpha') + \eta p(\alpha').$$

Moreover, in order for its second derivative to be a Dirac delta functional, the following condition on the discontinuity of the first derivative must be satisfied:

$$\gamma p'(\alpha') - \delta h'(\alpha') - \eta p'(\alpha') = 1. \quad (37)$$

Upon introducing a new constant $\Omega = \gamma - \eta$, we can rewrite Eqs. (36) and (37) in the form of a Kramer’s system,

$$\begin{cases}
\Omega p(\alpha') - \delta h(\alpha') = 0, \\
\Omega p'(\alpha') - \delta h'(\alpha') = 1,
\end{cases}$$

which admits a unique solution, given by

$$\Omega = -\frac{h(\alpha')}{W(\alpha')}, \quad (38)$$
$$\delta = -\frac{p(\alpha')}{W(\alpha')}, \quad (39)$$

where $W(\alpha') = p(\alpha')h'(\alpha') - h(\alpha')p'(\alpha')$ is the Wronskian. Hence, the ansatz (35) is rewritten as

$$G^{h,\eta}(\alpha, \alpha') = \begin{cases}
p(\alpha) \left( \eta - \frac{h(\alpha')}{W(\alpha')} \right), & \alpha \geq \alpha' \\
-\frac{p(\alpha')}{W(\alpha')} h(\alpha) + \eta p(\alpha), & \alpha \leq \alpha'.
\end{cases}$$

where we have explicitly introduced the parameter $\eta$ in our notation for the Green’s function in order to stress its nonuniqueness. Note that the phase shift at $-\infty$ varies with $\eta$.

Hence, the solution of Eq. (31) reads

$$\tilde{\psi}^{(1)}(\alpha, k) = \int d\alpha' G^{h,\eta}(\alpha, \alpha') U(\alpha') \tilde{\psi}^{(0)}(\alpha, k). \quad (40)$$

The possibility of studying the perturbative corrections using a decomposition in monochromatic components is viable because of the validity of the superposition principle.

This is in fact preserved by additional interactions of the type considered here, which violate the constraint while preserving the linearity of the wave equation. Note that, in general, modifications of the scalar constraint in the WDW theory would be nonlinear and nonlocal, as for instance within the proposal of Ref. [8], where classical geometrodynamics arises as the hydrodynamics limit of GFT. However, such nonlinearities would spoil the superposition principle, hence making the analysis of the solutions much more involved.

The time dependence of the perturbative corrections is recovered by means of the inverse Fourier transform of Eq. (40),

$$\psi^{(1)}(\alpha, \phi) = \int \frac{dk}{2\pi} \tilde{\psi}^{(1)}(\alpha, k)e^{-ik\phi}. \quad (41)$$

Expectation values of observables can be defined using the measure determined by the time component of the Noether current $j_\phi$ as

$$\langle f \rangle = \int d\alpha f j_\phi. \quad (42)$$

The Noether current is defined as

$$j_\mu = -i \left( \psi^* \frac{\partial \psi}{\partial \phi} \cdot \psi^* \frac{\partial \psi}{\partial \alpha} \right).$$

Using the conservation of the Noether current, we can then derive an analog of the Ehrenfest theorem, namely,

$$\frac{d}{d\phi} \langle f \rangle = \int d\alpha (j_\phi \partial_\phi f + f \partial_\phi j_\phi)$$
$$= \int d\alpha (j_\phi \partial_\phi f + f \partial_\alpha j_\alpha). \quad (44)$$

When the observable $f$ does not depend explicitly on the internal time $\phi$, the first term in the integrand vanishes. Considering for instance the scale factor $a = e^\alpha$ then, after integrating by parts, we get

$$\frac{d}{d\alpha} \langle a \rangle = -\int d\alpha e^\alpha j_\alpha. \quad (45)$$

In an analogous fashion, one can show that

$$\frac{d}{d\phi} \langle a^2 \rangle = -2 \int d\alpha e^{2\alpha} j_\alpha. \quad (46)$$

Formulas (44) and (46), besides their simplicity, turn out quite handy for numerical computations, especially when dealing with time-independent observables. In fact they can be used to compute time derivatives of the averaged observables without the need for a high resolution on
the $\phi$ axis; i.e. they can be calculated using data on a single time slice. Expectation values can therefore be propagated forward or backward in time by solving first order ordinary differential equations.

V. FIRST PERTURBATIVE CORRECTION FOR TIME-DEPENDENT POTENTIALS

In the previous section, we considered a time-independent perturbation, which can be dealt with using the Helmholtz equation. This is in general not possible when the perturbation depends on the internal time. In order to study the more general case, we have to resort to different techniques to find the exact Green’s function of the operator $\hat{T}_0$. Since the potential $e^{4\kappa}$ breaks translational symmetry, Fourier analysis, which makes the determination of the propagator so straightforward in the $k=0$ case (where the Hamiltonian constraint leads to the wave equation), is of no help.

Let us perform the following change of variables,

$$X = \frac{1}{2} e^{2\kappa} \cosh(2\phi), \quad Y = \frac{1}{2} e^{2\kappa} \sinh(2\phi),$$

which represents a mapping of minisuperspace into the wedge $X > |Y|$ (Fig. 3). The minisuperspace interval (corresponding to DeWitt’s supermetric) can be expressed in the new coordinates as

$$d\phi^2 - d\alpha^2 = \frac{1}{X^2 - Y^2} (dY^2 - dX^2),$$

with $(X^2 - Y^2)^{-1}$ the conformal factor. As an immediate consequence of conformal invariance, uniformly expanding (contracting) universes are given by straight lines parallel to $X = Y$ ($X = -Y$) within the wedge. The “horizons” $X = -Y$ and $X = Y$ represent the initial and final singularities, respectively. It is worth pointing out that the classical trajectory Eq. (29) takes now the much simpler expression

$$\tilde{k} = 2X;$$

i.e. classical trajectories are represented by straight lines parallel to the $Y$ axis and with the extrema on the two singularities.

In the new coordinates $X, Y$, the operator $\hat{T}_0$ in Eq. (13) reads

$$\hat{T}_0 = (X^2 - Y^2)(\partial_X^2 - \partial_Y^2 - 4),$$

which is, up to the inverse of the conformal factor, a Klein-Gordon operator with $m^2 = 4$. This is a first step toward a perturbative solution of Eq. (15), which we rewrite below for convenience of the reader in the form

$$\hat{T}_0 \psi^{(1)} = U(\alpha, \phi) \psi^{(0)},$$

where

$$U(\alpha, \phi) = -e^{4\kappa} g(\alpha, \phi).$$

Note that the above is the same equation as the one considered in the previous section, but we are now allowing for the interaction potential to depend also on $\phi$. Given Eq. (50), we recast Eq. (51) in the form that will be used for the applications of the next section, namely,

$$\left(\partial_X^2 - \partial_Y^2 - 4\right) \psi^{(1)} = \frac{U(X, Y)}{(X^2 - Y^2)} \psi^{(0)}.$$ (53)

The formal solution to Eq. (53) is given by a convolution of the rhs with the Green’s function satisfying suitably chosen boundary conditions

$$\psi^{(1)}(X, Y) = \int dX' dY' G(X, Y; X', Y')$$

$$\times U(X', Y') \frac{\psi^{(0)}(X', Y')}{(X^2 - Y^2)}.$$ (54)

The Green’s function of the Klein-Gordon operator in free space is well known for any dimension $D$ (see e.g. Ref. [22]). In $D = 2$ it is formally given by

$$G(X, Y; X', Y') = \int \frac{d^2 k}{(2\pi)^2} \frac{e^{-i(k_s(Y-Y')-k_l(X-X'))}}{(k_s^2 - k_l^2 - 4)}$$

and satisfies the equation

$$\left(\partial_X^2 - \partial_Y^2 - 4\right)G(X, Y; X', Y') = \delta(X - X') \delta(Y - Y').$$ (56)

Evaluating (55) explicitly using Feynman’s integration contour, which is a preferred choice in the context of a third quantization, we get [22,23]

$$G(X, Y; X', Y') = -\frac{1}{4} \frac{\theta(s) H_0^{(2)}(2\sqrt{s})}{2\sqrt{s}}$$

$$- \frac{i}{2\pi} \theta(-s) K_0(2\sqrt{-s}),$$ (57)

where we introduced the notation $s = (Y - Y')^2 - (X - X')^2$ for the interval. However, the present situation is distinguished from the free case, since there is a physical boundary represented by the edges of the wedge. The boundary conditions must be therefore appropriately discussed. A preferred choice is the one that leads to the Feynman boundary conditions in the physical coordinates $(\alpha, \phi)$. In the following, we will see the form that these conditions take in the new coordinate system, finding the

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Recall that any two metrics on a two-dimensional manifold are related by a conformal transformation.

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Notice that here $Y$ plays the role of time.
transformation laws of the operators that annihilate progressive and regressive waves.

We begin by noticing that the generator of dilations in the $(X, Y)$ plane acts as a tangential derivative along the edges

$$X\partial_X + Y\partial_Y = \partial_t.$$  \hfill (58)

Moreover on the upper edge $X = Y$ (corresponding to the big crunch), we have

$$\partial_t|_{X=Y} = \frac{1}{4}(\partial_\alpha + \partial_\phi).$$  \hfill (59)

while on the lower edge (corresponding to the initial singularity), we have

$$\partial_t|_{X=-Y} = \frac{1}{4}(\partial_\alpha - \partial_\phi).$$  \hfill (60)

Therefore, the boundary conditions

$$\partial_t|_{X=Y} G = \partial_t|_{X=-Y} G = 0$$  \hfill (61)

are equivalent to the statement that the Green’s function is a positive (negative) frequency solution of the wave equation at the final (initial) singularity. This is in agreement with the Feynman prescription and with the fact that the potential $e^{\alpha}$ vanishes at the singularity $\alpha \to -\infty$.

There is a striking analogy with the classical electrostatics problem of determining the potential generated by a point charge inside a wedge formed by two conducting plates (in fact it is well known that the electric field is normal to the surface of a conductor, so that the tangential derivative of the potential vanishes). The similarity goes beyond the boundary conditions and holds also at the level of the dynamical equation. In fact, after performing a Wick rotation $Y \to -iY$, Eq. (56) becomes the Laplace equation with a constant mass term, while the operator $\partial_t$ defined in Eq. (58) keeps its form.

After performing the Wick rotation, the problem can be solved with the method of images. Given a source (charge) at point $P_0 = (r', \theta')$, three image charges as in Fig. 4 are needed to guarantee that the boundary conditions are met. The Euclidean Green’s function as a function of the point $Q = (r, \theta)$ and source $P_0$ (hence, $m = 2$) is shown to be given by

$$G(r, \theta, r', \theta') = \frac{1}{2\pi} \left( K_0(mP_0Q) - K_0(mP_1Q) + K_0(mP_3Q) - K_0(mP_5Q) \right).$$  \hfill (62)

The quantities $P_jQ$ represent the Euclidean distances between the charges and the point $Q$. The Lorentzian Green’s function is then recovered by Wick rotating all the $Y$ time coordinates, i.e. those of $Q$ and of the $P_j$’s. In order to obtain this solution, we treated the two edges symmetrically, thus maintaining time reversal symmetry. The Green’s function with a source $P_0$ within the wedge vanishes when $Q$ is on either of the two edges. In fact, this can be seen as a more satisfactory way of realizing DeWitt’s boundary condition, regarding it as a property of correlators rather than of states.\footnote{DeWitt originally proposed the vanishing of the wave function of the Universe at singular metrics on superspace, suggesting in this way that the singularity problem would be solved \textit{a priori} with an appropriate choice of the boundary conditions. However, there are cases (see the discussion in Refs. [24,25]) where DeWitt’s proposal does not lead to a well-posed boundary value problem and actually overconstrains the dynamics. For instance, the solution given in Ref. [10] that we discussed in Sec. III satisfies it for $\alpha \to \infty$ but not at the initial singularity, since all the elementary solutions $C_k(\alpha)$ are indefinitely oscillating in that region. Imposing the same condition on the Green’s function does not seem to lead to such difficulties.}
VI. TREATING THE INTERACTION AS WHITE NOISE

The methods developed in the previous sections are completely general and can be applied to any choice of the extra interaction terms using Eq. (54). In this section we will consider, as a particularly simple example, the case in which the additional interaction is given by white noise. Besides the mathematical simplicity, there are also physical motivations for doing so. In fact, we can make the assumption that the additional terms that violate the Hamiltonian constraint can be used to model the effect of the underlying discreteness of spacetime on the evolution of the Universe.

Some approaches to quantum gravity (for instance GFT) suggest that an appropriate description of the gravitational interaction at a fundamental level is to be given in the language of third quantization [26]. At this stage, one might make an analogy with the derivation of the Lamb shift in QED and effective stochastic approaches. As it is well known, the effect stems from the second quantized nature of the electromagnetic field. However, the same prediction can also be obtained if one holds the electromagnetic field as classical but imposes ad hoc conditions on the statistical distribution of its modes, which necessarily has to be the same as that corresponding to the vacuum state of QED. In this way, the instability of excited energy levels in atoms and the Lamb shift are seen as a result of the interaction of the electron with a stochastic background electromagnetic field [11,13]. However, in the present context, we will not resort to a third quantization of the gravitational field but instead put in ad hoc stochastic terms arising from interactions with degrees of freedom other than the scale factor. Certainly, our position here is weaker than that of SED (see Refs. [12,14] and the works cited above), since a fundamental third quantized theory of gravity has not yet been developed to such an extent so as to make observable predictions in cosmology. Therefore, we are unable to give details about the statistical distribution of the gravitational degrees of freedom in what would correspond to the vacuum state. Our model should henceforth be considered as purely phenomenological, and its link to the full theory will be clarified only when the construction of the latter will eventually be completed.

To be more specific, we treat the function $g$ in the perturbation as white noise. Stochastic noise is used to describe the interaction of a system with other degrees of freedom regarded as an environment.\textsuperscript{12} Hence, we write

\begin{equation}
\left\langle g(\alpha, \phi) g(\alpha', \phi') \right\rangle = 0,
\end{equation}

\begin{equation}
\left\langle g(\alpha, \phi) g(\alpha', \phi') \right\rangle = \epsilon \delta(\alpha - \alpha') \delta(\phi - \phi'),
\end{equation}

where $\langle \_ \_ \rangle$ denotes an ensemble average and $\epsilon$ is a parameter which can be regarded as the magnitude of the noise. It is straightforward to see that

\begin{equation}
\left\langle \psi^{(1)} \right\rangle = 0,
\end{equation}

which means that the ensemble average of the corrections to the wave function vanishes.

A more interesting quantity is represented by the second moment

\begin{equation}
\mathcal{F}(X_1, Y_1; X_2, Y_2) = \left\langle \left( \psi^{(1)}(X_1, Y_1) \right)^* \psi^{(1)}(X_2, Y_2) \right\rangle.
\end{equation}

In fact when evaluated at the same two points $\mathcal{F}(X, Y) \equiv \mathcal{F}(X, Y; X, Y)$, it represents the variance of the statistical fluctuations of the wave function at the point $(X, Y)$. Using Eqs. (15), (64), and (66), we get

\begin{equation}
\left\langle \left| \psi^{(1)}(X, Y) \right|^2 \right\rangle = \mathcal{F}(X, Y) = 16 \epsilon \int_{X \geq |Y|} dX dY' (X^2 - Y'^2)^2 |\psi^{(0)}|^2 \times (X', Y')^2 |G(X - X', Y - Y')|^2.
\end{equation}

In order to obtain the correct expression of the integrand, one needs to use the transformation properties of the Dirac distribution, yielding

\begin{equation}
\left\langle g(\alpha, \phi) g(\alpha', \phi') \right\rangle = 2 \epsilon (X^2 - Y^2) \delta(X - X') \delta(Y - Y').
\end{equation}

Notice the resemblance of Eq. (66) with the two-point function evaluated to first order using Feynman rules for a scalar field in two dimensions interacting with a potential $(X^2 - Y^2)^2 |\psi^{(0)}|^2$. Following this analogy, the variance $\mathcal{F}$ can be seen as a vacuum bubble.

Equation (67) implies that a white noise interaction is such that the different contributions to the modulus square of the perturbations add up incoherently. Moreover, the perturbative corrections receive contributions from all regions of minisuperspace where the unperturbed wave function is supported.

A discussion about the implications of the results of this section is now in order. The boundary conditions (61) imposed on the Green’s function (62) treat the two directions of the internal time $\phi$ symmetrically. Therefore, the amplitude for a Universe expanding from $X = -Y$ to the point with coordinates $(X_0, Y_0)$ is the same as that for having a collapsing Universe (or anti-Universe, notice the close analogy with CPT symmetry in ordinary RQFT) going from $(X_0, Y_0)$ to $X = -Y$. It is also clear

12For a derivation of the Schrödinger-Langevin equation using the methods of stochastic quantization, we refer the reader to Ref. [27]. We are not aware of other existing works suggesting the application of stochastic methods to quantum cosmology. There are, however, applications to the fields of classical cosmology and inflation, and the interested reader is referred to the published literature.
from (67) and the property $G(X - X', Y - Y') = G(X - X', Y' - Y)$ that
\[ \tilde{F}(X, Y) = \tilde{F}(X, -Y). \tag{69} \]

Therefore, fluctuations in the perturbed wave function are symmetric under time inversion. This result can be seen to hold more generally for any interaction function $g(\alpha, \phi)$ which respects this same symmetry property. In such cases, the arrow of time is thus determined by the unperturbed solution for the background and points toward the direction in which the Universe expands, in agreement with the interpretation of Ref. [10]. Whether this cosmological arrow of time agrees with the thermodynamic one, defined by the direction of growth of inhomogeneities, remains an open problem in LQC.\(^{13}\) The suggestive idea of such an identification between the two fundamental arrows of time is old and was first proposed by Hawking [30] in the context of the sum-over-geometries approach to quantum cosmology, but later disproved by Page [31]. Their arguments are based on the formal properties of the wave function of the Universe, defined by a path integral over compact Euclidean metrics (hence, with no boundary). However, it is not clear whether they have a counterpart in other approaches to quantum cosmology, such as the one we considered in this work. In order to be able to provide a satisfactory answer to this question, one must not neglect the role played by inhomogeneities. Their dynamics might in fact display interesting features especially where quantum effects become more relevant, i.e. close to the singularities and at the turning point. In particular, the symmetry (or the lack thereof) of the dynamics around the latter will be crucial, since that is the point where the cosmological arrow of time defined by the background undergoes an inversion [30].

Another important aspect concerns the semiclassical properties of the perturbed states that we constructed. From Fig. 5 one sees that the perturbation at a fixed $\phi$ is a rapidly decreasing function of $\alpha$ with Gaussian tails. Therefore, the result of a white noise perturbation on a wave packet solution of the WDW equation is still a wave packet. The position of the peak of the perturbation, like that of the unperturbed state, is a monotonically increasing function of $\phi$ for negative values of $\phi$, while it is monotonically decreasing for positive $\phi$. In this sense we can regard the perturbed state as retaining the property of semiclassicality of the unperturbed state. It is therefore possible to perform the classical limit, which can be obtained when $\hbar \to 0$ or equivalently by considering infinitesimally narrow unperturbed wave packets $\psi^{(0)}$, i.e. in the limit $b \to 0$. More precisely, one should compute expectation values of physical observables (e.g. the scale factor) on the perturbed state $\psi^{(0)} + \psi^{(1)}$ and perform an asymptotic expansion near $\hbar = 0$. One can also simultaneously expand around $\epsilon = 0$, and the classical dynamics would then be seen to get corrections in the form of additional terms involving powers of $\epsilon$ and $\hbar$, to be interpreted as stochastic and quantum effects, respectively (or a combination of the two).

VII. CONCLUSIONS

Motivated by LQC and GFT, we considered an extension of WDW minisuperspace cosmology with additional interaction terms representing a self-interaction of the Universe. Such terms can be seen as a particular case of the model considered in Ref. [6], which was proposed as an approach to quantum dynamics of inhomogeneous cosmology. In general, inhomogeneities would lead to nonlinear
differential equations for the quantum field. This is indeed the case when the “wave function” of the Universe is interpreted as a quantum field or even as a classical field describing the hydrodynamics limit of GFT.

In the framework of a first quantized cosmology, we only considered linear modifications of the theory in order to secure the validity of the superposition principle. Our work represents indeed a first step toward a more general study, that should take into account nonlinear and possibly nonlocal interactions in minisuperspace. However, the way such terms arise, their exact form, and even the precise way in which minisuperspace dynamics is derived from fundamental theories of quantum gravity should be dictated from the full theory itself.

Assuming that the additional interactions are such that deviations from the Friedmann equation are small, we developed general perturbative methods which allowed us to solve the modified WDW equation. We considered a closed FLRW Universe filled with a massless scalar field to define an internal time, for which wave packets solutions are known explicitly and propagate with no dispersion. A modified WDW equation was then obtained in the large volume limit of a particular GFT-inspired extension of LQC for a closed FLRW Universe. Perturbative methods were then used to find the corrections given by self-interactions of the Universe to the exact solution given in Ref. [10]. To this end, the Feynman propagator of the WDW equation was evaluated exactly by means of a conformal map in minisuperspace and (after a Wick rotation) using the method of the image charges that is familiar from electrostatics. This is potentially interesting as a basic building block for any future perturbative analysis of nonlinear minisuperspace dynamics for a closed Universe. Our choice of the boundary conditions satisfied by the Green’s function is compatible with a cosmological arrow of time given by the expansion of the Universe.

A Helmoltz-like equation was obtained from WDW when the extra interaction did not depend on the internal time. Its Green’s kernel was evaluated exactly and turned out to depend on a free parameter $\eta$ related to the choice of boundary conditions. Further research must be carried over to link $\eta$ to different boundary proposals.

We illustrated our perturbative approach in the simple and physically motivated case in which the perturbation was presented by white noise. In this phenomenological model, the stochastic interaction term can be seen as describing the interaction of the cosmological background with other degrees of freedom of the gravitational field. Calculating the variance of the statistical fluctuations of the wave function, we found that a white noise interaction is such that the different contributions to the modulus square of the perturbations add up incoherently and that the perturbed wave function retains the property of semiclassicality. Furthermore, the width of the perturbation of the wave function reaches a minimum at recollapse.

**APPENDIX A: WKB APPROXIMATION OF THE ELEMENTARY SOLUTIONS AND ASYMPTOTICS OF THE WAVE PACKETS**

Since Eq. (22) has the form of a time-independent Schrödinger equation, it is possible to construct approximate solutions using the WKB method (Fig. 6).

For a given $k$, we divide the real line in three regions, with a neighborhood of the classical turning point in the middle. The classical turning point is defined as the point where the potential is equal to the energy

$$\alpha_k = \frac{1}{2} \log k.$$  \hspace{1cm} (A1)

The WKB solution to first order in the classically allowed region $\left[ -\infty, \alpha_k - \epsilon \right]$ (with $\epsilon$ an appropriately chosen real number, see below) is

$$C_k^I = \frac{2}{(k^2 - e^{\alpha k})^{1/4}} \cos \left( \frac{1}{2} \sqrt{k^2 - e^{\alpha k}} \right) - \frac{k}{2} \coth \left( \frac{k}{\sqrt{k^2 - e^{\alpha k}}} + \frac{\pi}{4} \right).$$  \hspace{1cm} (A2)

and reduces to a plane wave in the allowed region for $\alpha \ll \alpha_k$. The presence of the barrier fixes the amplitude and the phase relation of the incoming and the reflected wave through the matching conditions.

The solution in the classically forbidden region $\left[ \alpha_k - \epsilon, \alpha_k + \epsilon \right]$ is instead exponentially decreasing as it penetrates the potential barrier and reads

$$C_k^{III} = \frac{1}{(e^{\alpha k} - k^2)^{1/4}} \exp \left( -\frac{1}{2} \sqrt{e^{\alpha k} - k^2} \right) + \frac{k}{2} \arctan \left( \frac{k}{\sqrt{e^{\alpha k} - k^2}} \right).$$  \hspace{1cm} (A3)

Finally, in the intermediate region $\left[ \alpha_k - \epsilon, \alpha_k + \epsilon \right]$, any semiclassical method would break down, and hence the Schrödinger equation must be solved exactly using the linearized potential

$$V(\alpha) = V(\alpha_k) + V'(\alpha_k)(\alpha - \alpha_k) = 4e^{\alpha_k} (\alpha - \alpha_k) = 4k^2 (\alpha - \alpha_k).$$  \hspace{1cm} (A4)

In this intermediate regime, Eq. (22) can be rewritten as the well-known Airy equation

$$\frac{d^2 C_k^I}{d t^2} - t C_k^I = 0,$$  \hspace{1cm} (A5)

where the variable $t$ is defined as

$$t = (4k^2)^{1/2}(\alpha - \alpha_k).$$  \hspace{1cm} (A6)
Of the two independent solutions of Eq. (A5), only the Airy function \( \text{Ai}(t) \) satisfies the boundary condition, and hence we conclude that

\[
C''_k = c \text{Ai}(t), \quad \text{(A7)}
\]

where \( c \) is a constant that has to be determined by matching the asymptotics of \( \text{Ai}(t) \) with the WKB approximations on both sides of the turning point. Hence, we get that for \( t \ll 0 \)

\[
\text{Ai}(t) \approx \frac{\cos \left( \frac{4}{3} |t|^{3/2} - \frac{\pi}{4} \right)}{\sqrt{\pi} |t|^{1/4}}, \quad \text{(A8)}
\]

while for \( t \gg 0 \)

\[
\text{Ai}(t) \approx \frac{e^{-3^{1/2}}}{2\sqrt{\pi} t^{1/4}}. \quad \text{(A9)}
\]

We thus fix \( c = 2\sqrt{\pi} \). Note that the arbitrariness in the choice of \( \epsilon \) can be solved, e.g. by requiring the point \( \alpha_k - \epsilon \) to coincide with the first zero of the Airy function.

The WKB approximation improves at large values of \( k \), as one should expect from a method that is semiclassical in spirit. Yet it allows one to capture some effects that are genuinely quantum, such as the barrier penetration and the tunneling effect.

From the approximate solution we have just found, we can construct wave packets as in Ref. [10]. We thence restrict our attention to the classically allowed region and the corresponding approximate solutions, i.e. \( C''_k(\alpha) \) for \( \alpha \ll \alpha_k = \frac{1}{4} \log k \), and compute the integral in Eq. (25). If the Gaussian representing the amplitudes of the monochromatic modes is narrow peaked, i.e. its variance \( b^2 \) is small enough, we can approximate the amplitude in Eq. (A2) with that corresponding to the mode with the mean frequency \( \bar{k} \). Thus, introducing the constant

\[
c_{\bar{k}} = \frac{2}{(k^2 - e^{4\alpha})^{1/4}} \frac{1}{\sqrt{\pi}^{1/4} \sqrt{b}}, \quad \text{(A10)}
\]

we have

\[
\psi(\alpha, \phi) = c_{\bar{k}} \int_{-\infty}^{\infty} dk e^{-\frac{(k^2 - e^{4\alpha})^{1/4}}{\sqrt{\pi}^{1/4} \sqrt{b}}} \cos \left( \frac{1}{2} \sqrt{k^2 - e^{4\alpha}} \right) e^{ik\phi}.
\]

Moreover,

\[
k \text{arccoth} \left( \frac{k}{\sqrt{k^2 - e^{4\alpha}}} \right) = k \text{arccos} \frac{k}{e^{2\alpha}} = k \text{arccos} \frac{\bar{k}}{e^{2\alpha}}.
\]

The last approximation in the equation above holds as the derivative of the inverse hyperbolic function turns out to be much smaller than unity in the allowed region. Furthermore, the term approximated in Eq. (A12) dominates over the square root in the argument of the cosine in

![FIG. 6. The thick and the dot-dashed curve represent the WKB approximation of the wave function in the classically allowed and in the forbidden regions, respectively. They both diverge at the classical turning point. The Airy function is represented by the dashed curve. The value \( k = 220 \) was chosen.](image-url)
the integrand in the rhs of Eq. (A11), so we can consider the latter as a constant. Hence, we can write

$$\psi(\alpha, \phi) \approx c_{\Psi} \int_{-\infty}^{\infty} dk e^{-\frac{i(k-k')^2}{2\sigma^2}} \cos(\Lambda k + \delta) e^{ik\phi}, \quad (A13)$$

where we have introduced the notation

$$\Lambda \equiv \frac{1}{2} \arccos \frac{\tilde{k}}{e^{2\sigma^2}}, \quad (A14)$$

$$\delta \equiv \frac{1}{2} \sqrt{\tilde{k}^2 - e^{4\sigma^2} - \pi^2}, \quad (A15)$$

for convenience. Using Euler's formula we can express the cosine in the integrand in the rhs of Eq. (A13) in terms of complex exponentials and evaluate $\psi(\alpha, \phi)$. In fact, defining

$$P_k \equiv e^{i(k(\Lambda + \phi) + \delta)} \quad \text{and} \quad Q_k \equiv e^{-i(k(\Lambda - \phi) + \delta)}, \quad (A16)$$

we have

$$\psi(\alpha, \phi) \approx c_{\Psi} \int_{-\infty}^{\infty} dk e^{-\frac{i(k-k')^2}{2\sigma^2}} (e^{i(k-k')(\Lambda + \phi)} P_k + e^{-i(k-k')(\Lambda - \phi)} Q_k). \quad (A17)$$

Shifting variables and performing the Gaussian integrations, we get the result as in Ref. [10],

$$\psi(\alpha, \phi) \approx c_{\Psi} \int_{-\infty}^{\infty} d\tilde{k} \left( e^{-\frac{\tilde{k}^2}{2\sigma^2}} (P_{\tilde{k}} + Q_{\tilde{k}}) \right). \quad (A18)$$

### APPENDIX B: ORTHOGONALITY OF THE MACDONALD FUNCTIONS

It was proved in Refs. [32–34] that

$$\int_0^{\pi} \frac{dx}{x} K_{\nu}(kx) K_{\nu'}(kx) = \frac{\pi^2}{\nu} \delta(\nu - \nu') / 2 \sinh(\pi \nu), \quad (B1)$$

which expresses the orthogonality of the Macdonald functions of imaginary order. Performing a change of variables, the above formula can be recast in the form

$$\int_{-\infty}^{\infty} da K_{\tilde{k}}^2 \left( e^{2\tilde{a}k} \right) K_{\tilde{k}'}^2 \left( e^{2\tilde{a}k'} \right) = \frac{\pi^2}{\tilde{h}} \delta(h - h') / \sinh(\pi \tilde{h}), \quad (B2)$$

which is convenient for the applications considered in this work. For large values of $k$, it is equivalent to the normalization used in Sec. II,

$$\int_{-\infty}^{\infty} d\alpha \psi^*(\alpha, \phi) \psi(\alpha, \phi) = \frac{\pi^2}{2} \delta(k - k'). \quad (B3)$$
SEMICLASSICAL SOLUTIONS OF GENERALIZED …


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