Semiclassical momentum representation in quantum cosmology

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(Dated: May 1, 2015)

We develop a framework to obtain semiclassical solutions of the Wheeler-DeWitt equation in the momentum representation. Unlike in the standard WKB approximation, these solutions are valid in the vicinity of turning points. We derive and describe their regime of validity in detail, and compare them with usual semiclassical solutions. This not only gives us approximate solutions of the Wheeler-DeWitt equation, it also allows us to describe the physics of matter fields, and under which conditions they perceive a classical background near the turning point. This framework has a key application in tackling the problem of time. It allows us to use curvature as a time variable, and control the corresponding domain of validity, i.e. under which conditions it provides a good clock. We consider several applications, and in particular show how this allows us to obtain semiclassical solutions of the Wheeler-DeWitt equation parametrized by York time.

PACS numbers: 98.80.Qc 04.62.+v 04.60.-m

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I. INTRODUCTION

Despite our lack of a complete theory of quantum gravity, quantum fluctuations of the gravitational field can still be tracked down in some approximate regimes. For this reason, semiclassical approximations play a key role in attempts to characterize quantum gravitational effects, and WKB methods were developed early on in canonical quantum gravity studies [1]. Such methods are not only useful to obtain corrections to classical general relativity [2], they are also a crucial tool to tackle conceptual problems such as the problem of time [3, 4] or the emergence of a classical background metric [5–8]. Unfortunately, standard WKB techniques fail drastically near a turning point.

Surprisingly, turning points in quantum gravity have been very poorly studied [9, 10]. However, turning points are not exotic and they arise in various cases: In cosmology, when the Universe undergoes a bounce [11, 12], or recollapses due to its spatial curvature [13], but also in black hole evaporation scenarios such as in 1+1 dimensions [9, 14]. In this work, we construct a method to obtain semiclassical solutions that are valid close to turning points. In standard approaches the wave function takes the spatial metric and matter degrees of freedom as arguments. Instead of this metric representation, we work here in a momentum representation. Since metric variables are canonically conjugated to extrinsic curvature variables, the wave function will now take curvature degrees of freedom as arguments. We shall present a general framework to obtain these semiclassical solutions, compare them with the metric representation, and carefully discuss their regime of validity.

It is known that an internal variable can play the role of time efficiently only if its quantum fluctuations are small enough. Such a result has been obtained from a variety of approaches: Internal correlations [15], effective techniques [16], or matter transitions [17, 18]. The semiclassical solutions we obtain are parametrized by the extrinsic curvature. As we show, when these solutions are valid, the extrinsic curvature provides a good time variable. By coupling our solutions to internal (matter) degrees of freedom, we demonstrate the difference between our semiclassical regime and the background field approximation, where the geometry is treated entirely classically. We then apply our framework to examples, and in particular to the York construction of an “intrinsic time”. York time played a key role in the demonstration of the well-posedness of the Cauchy problem in general relativity [19]. It is also a central ingredient in some recent modified gravity theories [20], and was recently used in cosmological settings [21, 22]. Here we show that our method exactly allows us to control the approximation necessary for York time to be a good time variable at the quantum level.

In the first section, we discuss the Wheeler-DeWitt equation, and the various semiclassical approximations. In a second section, we discuss key points of our construction, namely its link with metric representation and the generic structure near a turning point. In the last section, we present applications of our framework.

II. WHEELER-DEWITT EQUATION AND MOMENTUM-REPRESENTATION

A. Minisuperspace Wheeler-DeWitt equation

When we restrict ourselves to cosmological systems (homogeneous and isotropic), gravitational degrees of freedom reduce to a single one. The set of possible metrics in this minisuperspace sector is then given by

\[ ds^2 = N^2(t)dt^2 - a^2(t)d\Omega_K^2, \] (1)
where $d\Omega_2^K$ is a fixed spatial metric of constant curvature $K$. The coupled system of matter and gravity is then governed by the minisuperspace action

$$S = \frac{V_U}{2G} \int \left( -\frac{a\dot{a}^2}{N} - \frac{V(a)N}{a} \right) dt + V_U \int \left( \sum_j \pi_j \dot{\phi}_j - H_{\text{mat}}(a; \phi_j) \right) dt. \tag{2}$$

$V(a) = -Ka^2 + \Lambda a^4$ is the Wheeler-DeWitt superpotential, $H_{\text{mat}}(a; \phi_j)$ the Hamiltonian density of matter fields, and $V_U$ the volume of the Universe. After canonical quantization, the quantum dynamics is given by a single Hamiltonian constraint: the Wheeler-DeWitt equation.

$$\left[ \frac{G^2}{aV_U^2} \partial_a \partial_a + V(a) + 2Ga\dot{H}_{\text{mat}} \right] \Psi(a, \phi_j) = 0. \tag{3}$$

At this level, the matter Hamiltonian is very general, containing all matter degrees of freedom, but also gravitational perturbations. For a Universe filled with a single scalar field in a potential $V_{\text{scal}}$, it reads

$$\dot{H}_{\text{mat}} = \frac{1}{2a^3} \left( -\partial_\phi^2 + a^6 V_{\text{scal}}(\phi) \right). \tag{4}$$

In this work, we shall make the (drastic) assumption that the Universe is filled with fields at equilibrium. This means that we assume the wave function to factorize as $|\Psi(a)\rangle = |\Psi(a)\rangle_{\text{mat}}$, where $|\text{mat}\rangle$ is the state of matter fields in equilibrium (we shall relax this assumption in section II C). Doing so, we can replace $\dot{H}_{\text{mat}}$ by its mean value $\langle \dot{H}_{\text{mat}} \rangle$. In general, matter energy density is given by two main contributions

$$\langle \dot{H}_{\text{mat}} \rangle = \rho_m + \rho_r/a. \tag{5}$$

$\rho_m$ is the energy density of non-relativistic matter and $\rho_r$ that of massless (radiation) fields. This applies at equilibrium, when equipartition is valid. On the contrary, during inflation, under slow roll conditions, the main contribution of the inflaton comes from the potential part, i.e. $\langle \dot{H}_{\text{mat}} \rangle = a^3 V_{\text{scal}}(\phi)/2$ (and $\phi \sim \text{const.}$), giving a cosmological constant contribution.

In Eq. (3), the operator ordering has been chosen to be the Laplace-Beltrami ordering. This guarantees that the Wheeler-DeWitt equation is independent of the way we parametrized the geometry in Eq. (1). In other words, the Wheeler-DeWitt equation is coordinate independent on superspace. We assume a general parametrization, where the geometry is governed by a single metric variable $h$, that is, $a = a(h)$ in Eq. (1). In terms of $h$, the Wheeler-DeWitt equation takes the very general form

$$\left[ -\partial_h^2 + W(h) \right] \Psi(h) = 0. \tag{6}$$

For this, we first notice that $\partial_a \partial_a = (a_h)^{-1} \partial_h a(a_h)^{-1} \partial_h$. Then, we redefine the wave function as

$$\Psi(a) \rightarrow \frac{\Psi(h)}{\sqrt{a(h)/a_h(h)}}. \tag{7}$$

1 To lighten the notations, we have redefined the gravitational coupling constant $G = \frac{4\pi G_N}{a}$, where $G_N$ is the standard Newton constant, and $\Lambda = 3\Lambda$ the standard cosmological constant.

2 $V_U$ appears as a global factor in the classical action, and therefore, does not affect the classical trajectories. At the quantum level, as we shall see, the volume changes the regime of validity of the semiclassical approximation: the bigger Universe, the more classical it is. In fact, all the error bounds we provide in this work scale as $V_U^{-1}$. This fact was used in a different context to advocate for the efficiency of effective equation of loop quantum cosmology.

\[ \text{[References]} \]
By applying this change of wave function to Eq. (3), we obtain the pseudo-potential

\[ W(h) = -a_h^2 V^2 \left( \frac{1}{G^2} \right) \left( V(a) + 2 G a \rho_m + 2 G \rho_r \right) + V^2 \frac{3 a^2 a_h a_{hh}}{4 G^2 a^2 a_{h}^2} \left( V(a) + 2 G a \rho_m + 2 G \rho_r \right) W_{cl}(h) + V^2 \frac{2 a^2 a_h a_{h}^2}{4 G^2 a^2 a_{h}^2} W_q(h). \]  

(8)

We see that the pseudo-potential contains two contributions. The first one is the classical pseudo-potential \( W_{cl} \), written in terms of the general metric variable \( h \). The second is the “quantum pseudo-potential” \( W_q \). This contribution directly comes from the non-commuting character of \( a \) and \( \partial_h \). While \( W_{cl} \) is insensitive to a specific choice of ordering for the Wheeler-DeWitt equation, \( W_q \) is directly affected. For a given \( a(h) \), there is always a choice of ordering such that \( W_q \) is zero. The pseudo-potential we derived in Eq. (8) corresponds to the Laplace-Beltrami quantum pseudo-potential.

**B. The momentum-WKB approximation**

We shall now analyze the Wheeler-DeWitt equation under its very general form (6) so as to build semiclassical solutions. The standard procedure consists in obtaining WKB modes. Those are given by

\[ \chi(h) = e^{i \int p_{cl}(h') dh'} \sqrt{2 p_{cl}(h)}. \]  

(9)

We denote the WKB modes by \( \chi \) rather than \( \Psi \) so as to keep in mind that \( \chi \) constitutes an approximate solution. \( p_{cl} \) is the (classical) conjugate momentum of \( h \), and obeys the Hamilton-Jacobi equation

\[ p_{cl}(h)^2 + W(h) = 0. \]  

(10)

Eq. (9) provides a semiclassical solution of the Wheeler-DeWitt equation (6), and have been extensively studied in the literature (see [2, 3] and references therein). However, Eq. (9) is not an exact solution. It provides a good approximation when

\[ \text{Er}_h(h) = \left| \frac{\partial_h p_{cl}}{p_{cl}^2} \right| \ll 1. \]  

(11)

The error function \( \text{Er}_h \) gives a bound on the local error due to the WKB approximation [26]. However, when considering a scattering problem, the accumulated error might be much smaller, due to destructive interference effects [17, 26]. As far as scattering is concerned, the criterion (11) is rather conservative. In order to keep the discussion general, we shall stick to this criterion, which guarantees that the error is at most of the order of \( \text{Er}_h \).

Unfortunately, the WKB approximation of Eq. (9) breaks down in many physically relevant situations. In particular, it fails dramatically near a turning point [3, 27], where \( p_{cl} = 0 \), or equivalently, \( W(h) = 0 \). Notice that the notion of turning point is classically independent of our choice of metric variable \( h \), i.e. of the function \( a(h) \). Indeed, we see from Eq. (8) that if \( W_{cl} \) vanishes at some point, it does for any function \( a(h) \), since different \( W_{cl} \) for different \( a(h) \) are proportional. \( W_q \) on the other hand might affect the location (or presence) of a turning point, although its contribution is often subdominant with respect to \( W_{cl} \).

We shall now focus on cases where there is a turning point. To switch to the momentum representation, we take the Fourier transform of the wave function

\[ \tilde{\Psi}(p_h) = \int \Psi(h) e^{-ip_h h} \frac{dh}{\sqrt{2\pi}}. \]  

(12)
Assuming that this Fourier transform is well defined has nontrivial consequences. First, we assumed that we integrate over all real values of $h$. This creates difficulties if one wishes to use $a$ itself as the metric variable (we shall return to that point in section III B). Second, Eq. (12) implies that we discard the growing mode in the classically forbidden side of the turning point. This is often assumed [13], and is necessary to recover the background field approximation near a turning point. After the Fourier transform, the wave function obeys the Wheeler-DeWitt equation in the momentum representation, i.e.

$$\left[p_h^2 + W(h_{cl}(p_h))\right] \tilde{\Psi}(p_h) = 0.$$  \hspace{1cm} (13)

To obtain semiclassical solutions for this equation, we assume a semiclassical ansatz

$$\tilde{\Psi}(p_h) = A(p_h) \exp \left(-i \int_{p_h}^{p_h} h_{cl}(p)dp\right).$$  \hspace{1cm} (14)

The key point is that this expression gives a good approximation when the amplitude is a slowly varying function of $p$. Therefore, we shall solve Eq. (13) using a gradient expansion. The phase of Eq. (14) is the classical action, and is obtained from the Hamilton-Jacobi equation

$$p_h^2 + W(h_{cl}(p_h)) = 0.$$  \hspace{1cm} (15)

This is the same equation as (10), except that we now solve for $h$ as a function of $p_h$ instead of the converse. If the pseudo-potential is monotonic, the solution $h_{cl}(p_h)$ is unique. If $W(h)$ vanishes, say at $h = h_{tp}$, there is a turning point. The region where $W(h)$ is positive (without loss of generality, we assume it for $h < h_{tp}$) is classically forbidden. Hence, when $p_h$ runs from $-\infty$ to $+\infty$, $h_{cl}(p_h)$ goes from $+\infty$ to $h_{tp}$ and back again.

Before using any approximation, the ansatz (14) simply defines the amplitude $A(p_h)$. When applied to Eq. (13), it gives

$$\left[p_h^2 + W(h_{cl}(p_h)) + i\partial_{p_h}\right] A(p_h) = 0.$$  \hspace{1cm} (16)

Since the amplitude is assumed to vary slowly, we expand the operator in Eq. (16) in powers of $i\partial_{p_h}$. For this, As we detail in Appendix A, one must use a Taylor expansion of functions of non-commuting arguments. Here, the first order expansion reads

$$W(h_{cl}(p_h) + i\partial_{p_h}) = W(h_{cl}(p_h)) + W'(h_{cl}(p_h))i\partial_{p_h} + \frac{i}{2} W''(h_{cl}(p_h))h_{cl}'(p_h) + O \left(\partial_{p_h}^2\right).$$  \hspace{1cm} (17)

(By convention, $W' = \partial_h W$ and $h_{cl}' = \partial_{p_h} h_{cl}$.) Using this, Eq. (16) becomes

$$\left[p_h^2 + W(h_{cl}(p_h)) + W'(h_{cl}(p_h))i\partial_{p_h} + \frac{i}{2} W''(h_{cl}(p_h))h_{cl}'(p_h)\right] A(p_h) = 0.$$  \hspace{1cm} (18)

When sorting these terms in gradients, we see that the first order one is nothing else than the classical Hamilton-Jacobi equation (15). The second order part of Eq. (18) gives the amplitude

$$A(p_h) = |W'(h_{cl}(p_h))|^{-1/2}.$$  \hspace{1cm} (19)

We then deduce the semiclassical solution of the Wheeler-DeWitt equation

$$\tilde{\chi}(p_h) = \frac{e^{-i \int h_{cl}(p_h)dp_h}}{\sqrt{|W'|}}.$$  \hspace{1cm} (20)
Postulating (20) as an exact solution amounts to “choosing time before quantization” [3]. In other words, this is what one obtains if one first solves the Hamilton-Jacobi equation for \( h_{\text{cl}} \) and then quantizes. This is not what we obtain starting from the Wheeler-DeWitt equation (3). As we show in appendix A, (20) is a good approximation if we have

\[
E_{r_p}(p_h) = \left| \frac{W''_{\text{cl}}(p_h)}{W'} \right| \ll 1, \tag{21}
\]

where \( W \) and its derivatives are evaluated at \( h = h_{\text{cl}}(p_h) \). It is remarkable that this condition cannot be guessed from the somewhat naive statement that the WKB approximation is valid when the “phase varies much more slowly than the amplitude”, which would lead to an analog of Eq. (11) like \( |W''/(h_{\text{cl}}W')| \ll 1 \). In addition, Eq. (21) shows that the error vanishes on the turning point. Of course a statement like “momentum WKB is exact on a turning point” has no meaning; the error must be small on a sufficiently large interval. But in a close vicinity of the turning point, momentum WKB is always a good approximation.

In the above construction, the prefix “semi” of “semiclassical” should not be taken lightly. Indeed, semiclassical solutions of Eq. (20) still encode many quantum features of the gravitational field. In particular, no classical background metric exists at the level of equation (20). In fact, the validity of our construction, governed by Eq. (21), is independent of internal (i.e., matter fields) degrees of freedom. As we shall now see, this is not the case when considering the classical background limit. In order to recover a classical space-time, we shall use matter fields as probes. They will experience a classical background as long as energy changes are small.

C. The background as perceived by matter fields

To physically interpret the semiclassical solutions obtained in Eq. (20), we use a matter field as a probe. In other words we ask, how do matter fields perceive the wave function of the gravitational degrees of freedom? For this we consider a massive field, i.e. \( V_{\text{scal}}(\phi) = M\phi^2 \) in Eq. (4). To simplify the discussion, we assume that this field evolves adiabatically, that is, no particle production occurs while the Universe expands. This might be a bad approximation in realistic scenarios. However, it drastically simplifies the discussion, without altering the main conclusions. In [10], we considered particle production due to interactions and the conclusions we shall draw are maintained. In the adiabatic limit, matter states are adequately described by their decomposition in the adiabatic Fock basis [28, 29]. To build this basis, we consider the instantaneous eigenvectors of the matter Hamiltonian

\[
\hat{H}_{\text{mat}} |n\rangle = M_n |n\rangle. \tag{22}
\]

The quantum number \( n \) is conserved in the adiabatic limit \(^3\). Hence, the Wheeler-DeWitt equation (3) decouples into several second order ODEs, one for each value of \( n \). We then apply all the preceding results using several pseudo-potentials

\[
W_n(h) = -a_h^2 \frac{V(a)}{G^2} \left( V(a) + 2GaMn \right) + W_q(h). \tag{23}
\]

For each pseudo-potential, we construct the semiclassical solution \( \tilde{\chi}_n(p_h) \) using Eq. (20) and the corresponding Hamilton-Jacobi solution \( h_n(p_h) \). We then obtain the general semiclassical

\(^3\) Notice that the \( n + 1/2 \) of the standard harmonic oscillator reduces here to \( n \) after renormalization of the Hamiltonian by normal ordering [24].
solution of the Wheeler-DeWitt equation as
\[ \tilde{\Psi}(p_h) = \sum_n c_n e^{-i \int h_n(p_h') dp_h'} \sqrt{|W'_n|} |n\rangle, \quad (24) \]
where \( c_n \) are constants. Such a solution is an arbitrary superposition of matter eigenstates associated with a semiclassical state for the gravitational degrees of freedom. When adopting the point of view of matter, the interpretation of this solution is rather clear. The semiclassical wave function for gravity is analogous to \( e^{-i E_n t} \), i.e. it describes the “time evolution”, where \( p_h \) plays the role of time. From this point of view, there are several crucial advantages with respect to standard discussions of the WKB interpretation of quantum cosmology \([2, 3, 30]\). First, since we obtained semiclassical solutions in the momentum representation, they are perfectly adequate to describe physics near a turning point (as shown by Eq. (21)). Second, we can consider not only one semiclassical solution, but a superposition of several of them. In other words, Eq. (24) does not describe matter in a single background. Each matter state perceives its own background. Third, one is not restricted to consider one matter eigenstate, but any superposition of eigenstates. In the presence of interactions or non-adiabaticities, quantum transitions occur between these matter states. Quantum transitions have been discussed in \([17, 18]\) in the metric representation and in \([10]\) in the momentum representation. The notion of a single background metric emerges from Eq. (24) only when the spread in matter energy is small, i.e., \( \Delta E \ll \bar{E} \). By considering energy changes at first order around its mean value, we have
\[ h_n(p_h) \simeq \bar{h}(p_h) + \partial_E h(p_h)(E_n - \bar{E}), \quad (25) \]
where \( \bar{h}(p_h) \) is the solution of the Hamilton-Jacobi equation (15) for \( E = \bar{E} \). The first factor in the second term gives rise to the background notion of time via the Hamilton-Jacobi relation
\[ t(p_h) = \int \partial_E h(p_h') dp_h'. \quad (26) \]
This is exactly what is needed to change the phase of Eq. (24) from \( \int dp_h' \) into \( \int dt' \). Therefore the solution (24) becomes
\[ \tilde{\Psi}(p_h) = e^{-i \int \bar{h}(p_h') dp_h' + i \int E(t') dt'} \sqrt{|W'_n|} \sum_n c_n e^{-i \int E_n(t') dt'} |n\rangle. \quad (27) \]
This now corresponds to a superposition of matter eigenstates living in a background metric characterized by \( \bar{p}_h(t) \) from Eq. (26), where the geometry is sourced by the mean value of matter energy \( \bar{E} \). The time \( t \) that emerges from Eq. (26) coincides with the “WKB time” \([2, 3, 30]\) and our procedure is perfectly valid near a turning point. Indeed, we recognize in Eq. (27) the standard from of a Born-Oppenheimer approximation, where \( \tilde{\Psi} = \tilde{\chi}(p_h)\psi(\phi; p_h) \), i.e. the wave function of the heavy part factorizes. A key aspect of this approach is that \( t \) is really the time as perceived by matter field. It arises as the conjugate momentum of matter energy \(^4\). We underline once more that no background time (or metric) exists at the level of Eq. (24). Hence using \( p_h \) as a time variable is more fundamental than using the WKB time \( t \) of (26). However, one still needs to consider a semiclassical approximation to have a sensible notion of evolution, as a phase for each matter state. This is even clearer when considering quantum transitions,

\(^4\) Of course, even in a fixed background, there are many choices of a time coordinate. The choice comes here from the identification of matter energy in the Hamiltonian constraint. By defining for instance \( aH_{\text{mat}} \) instead of \( H_{\text{mat}} \), one obtains the conformal time instead of the co-moving time \([10, 31]\).
as Eq. (24) induces a unitary evolution for these transitions. In [10], it was obtained that the evolution is unitary when the momentum WKB approximation is valid and the various $h_n(p_h)$ describing semiclassical trajectories have the same monotonicity in $p_h$.

At this point, we emphasize that we do not claim that $p_h$ is a fundamentally better variable, or “time”. Very similar conclusions to that drawn in section II C were obtained using WKB methods in metric representation [2, 5, 7, 18, 30]. However, the validity conditions in both representations are quite different, as shown by comparing Eqs. (11) and (21). In particular, close to a turning point, $p_h$ is the most semiclassical variable, and hence gives the best time variable.

We now discuss the validity of the background field approximation, i.e., of Eq. (25). Since the matter Hamiltonian appears linearly in the total Hamiltonian constraint, so does the matter energy in the pseudo-potential of Eq. (8). Using the definition of the Hamilton-Jacobi solution $h_{cl}$, we compute the condition for the first order expansion in the energy change $\Delta E$:

$$\frac{\Delta E \partial^2_{E} h_{cl}}{\partial E h_{cl}} = \frac{\Delta E |W''\partial_E W - W''(\partial_E W)'|}{W''} \ll 1.$$ (28)

Unlike Eq. (21), this condition depends on the matter degrees of freedom through the energy fluctuations $\Delta E$. In a large Universe, the total inertia of gravity, governed by $\bar{E}$ is much larger than energy changes, since the former is proportional to the total mass of all the particles and the latter of the mass of a single particle. Therefore, there is generally a hierarchy between the two approximations encoded in Eq. (21) and Eq. (25). The semiclassical approximation is in general much better than the (more drastic) classical background approximation. This means that the solutions of Eq. (20) are not only useful to recover quantum field theory in curved space-time, but they also encode some quantum corrections.

III. METRIC REPRESENTATION AND BOUNDARY CONDITIONS

A. Inverse Fourier transform at the saddle point approximation

Having obtained semiclassical solutions in the momentum representation, it is instructive to relate them to semiclassical solutions in the metric representation. For this, we start from $\tilde{\chi}(p_h)$ of Eq. (20) and compute its Fourier transform

$$\Psi(h) = \int e^{-i \int h_{cl}(p'_h) dp'_h + ihp_h} \frac{1}{\sqrt{2\pi |W|}} dp_h.$$ (29)

This integral gives a (semiclassical) solution in the metric representation, but whose validity is controlled by Eq. (21) rather than Eq. (11). In particular, it is valid across a turning point. As we shall now see, when both (21) and (11) are valid, this integral coincides with usual WKB solutions as in Eq. (9). To show this, we evaluate the integral using the saddle point method [32]. At each value of $h$, the value of the saddle point $p_h = p_*(h)$ solves the equation

$$h = h_{cl}(p_*(h)).$$ (30)

Hence, $p_*(h)$ is nothing else than the classical momentum function $p_*(h) = p_{cl}(h)$, solution of the Hamilton-Jacobi equation [10]. Moreover, the phase evaluated at the saddle point gives the Legendre transform of the action $\int h_{cl}(p'_h) dp'_h$; that is, the action in the metric representation. Indeed, from a change of integration variable $p'_h = p_{cl}(h')$ and an integration by parts follow the identity

$$\int p_{cl}(h) dp_h + hp_{cl}(h) = \int^{h} p_{cl}(h') dh'.$$ (31)
The result of the integration (29) at the saddle point approximation then gives
\[ \Psi(h) = e^{i \int h' p_{cl}(h') dh'} \sqrt{|h_{cl}' W'(h)|}, \] 
where the irrelevant global phase has been discarded. Moreover, deriving Eq. (15) with respect to \( p_h \) shows that \( h_{cl}' W' = -2p_h \). Therefore, the prefactor arising from the saddle point approximation is exactly what is needed to obtain the WKB amplitude in metric representation and Eq. (32) simply becomes \( \Psi(h) = \chi(h) \).

When there is a turning point, there are two solutions of the Hamilton-Jacobi equation (30) and therefore one must sum over these two saddle point contributions. Moreover, the Hamilton-Jacobi equation (15), equivalent to (30), is invariant under \( p_{cl} \rightarrow -p_{cl} \). Hence if \( p_{cl}(h) \) is one solution, the other is \( -p_{cl}(h) \). The result for the wave function becomes
\[ \Psi(h) = e^{i \int h' p_{cl}(h') dh' - \frac{i \pi}{4}} \sqrt{2|p_{cl}(h)|} + e^{-i \int h' p_{cl}(h') dh' + \frac{i \pi}{4}} \sqrt{2|p_{cl}(h)|}. \]

One solution represents a contracting Universe, while the other an expanding one. Of course, one can only obtain this expression far away from the turning point. Indeed, the validity condition for the saddle point approximation basically reduces to Eq. (11), which is valid away from the turning point.

B. Behavior of the wave function near the singularity \( a = 0 \)

A standard choice to parametrize the metric is \( \alpha = \ln(a) \) [27], which presents several advantages. First, the quantum potential of Eq. (8) vanishes, and second, while the wave function is only defined for positive values of \( a \), \( \alpha \) runs from \(-\infty \) to \( +\infty \). However, one could be willing to work directly with the scale factor \( a \), as it allows several simplifications (such as the super potential becoming polynomial). Classically, the scale factor is restricted to \( a > 0 \). Quantum mechanically, it is an open issue whether one would like to keep this constraint or not [3]. This question is the minisuperspace manifestation of a more general issue in quantum gravity, and referred to as the spatial metric reconstruction problem [3]. When constructing the momentum representation in Eq. (12), we had to consider all real values of \( a \) and this question appears to be important for our construction.

The main problem of considering negative values of \( a \) is an interpretational one. What meaning should one give to \( a < 0 \)? As emphasized in section II C, we adopt here the point of view of matter. In particular, we are not trying to answer a question such as “what is the probability of \( a \) having such value”. Hence, \( a \) should not necessarily be interpreted as part of a metric at the fundamental level, but only in the regime where matter fields approximately propagate as in a classical background. Since we considered scenarios with a turning point, we always have \( a > 0 \) in the semiclassical limit. To further support this, we evaluate the semiclassical wave function obtained in the momentum representation at \( a = 0 \). From Eq. (29), it follows that
\[ \Psi_{a=0} = \int \frac{e^{-i \int a_{cl}(p') dp'}}{\sqrt{2\pi |W|}} dp. \]

Because \( a = 0 \) is within the classically forbidden region, the saddle point \( p_s \) is complex. As a consequence, the value of the wave function is exponentially small
\[ |\Psi_{a=0}|^2 \sim \frac{e^{-\text{Im} \int p_s a_{cl}(p') dp'}}{2\pi |W_p'|}. \]
This means that whether we want to impose that $\Psi$ only has support on $a > 0$ or not, the difference between the two choices is exponentially suppressed. Of course, the above equation is valid only if the turning point lies “far enough” from $a = 0$, more precisely, if Eq. (11) is valid near $a = 0$. If it is not the case, then imposing boundary conditions such as $\Psi_{a=0} = 0$ will deform the wave function and make the momentum semiclassical solution of Eq. (20) a bad approximation. In such a case, the most reasonable method is presumably to use a different metric variable such as $\alpha$.

C. Turning point vicinity

In a small neighborhood of a bounce, the pseudo-potential is well approximated by a linear function

$$W(h) = -\kappa(h - h_{tp}), \quad (36)$$

where the bounce occurs at $h = h_{tp}$. With this pseudo-potential, the Wheeler-DeWitt equation (13) becomes

$$\left[ p_h^2 - i\kappa \partial_{p_h} + \kappa h_{tp} \right] \tilde{\Psi}(p_h) = 0. \quad (37)$$

Since it involves only a first order derivative in $p_h$, the momentum-WKB approximation is exact. The solution of Eq. (37) is given by

$$\tilde{\Psi}(p_h) = \kappa^{-1/2} \exp \left( -i(p_h^3/(3\kappa) + h_{tp}p_h) \right), \quad (38)$$

where the normalization constant is chosen to be the same as in Eq. (20). It is now instructive to use the procedure of section II and relate this solution to WKB solutions in metric representation. From Eq. (29), we write the wave function in the metric representation as

$$\Psi(h) = \int \exp \left( -i(p_h^3/(3\kappa) + h_{tp}p_h) + ip_hh \right) \frac{dp_h}{\sqrt{2\pi \kappa}}. \quad (39)$$

This is the integral representation of an Airy function [32]. Hence,

$$\Psi(h) = \sqrt{\frac{2\pi}{\kappa^{1/3}}} \text{Ai} \left( -\kappa^{1/3}(h - h_{tp}) \right). \quad (40)$$

On the right side $(h - h_{tp} > 0)$, when going far from the turning point, the Airy function reduces to a sum of oscillatory terms.

$$\Psi(h) \sim \frac{e^{i\frac{2}{3}\kappa^2|h-h_{tp}|^{3/2}} - \frac{2}{3} i}{\sqrt{2\kappa^{1/2}|h-h_{tp}|^{1/2}}} + \frac{e^{-i\frac{2}{3}\kappa^2|h-h_{tp}|^{3/2} - \frac{2}{3} i}}{\sqrt{2\kappa^{1/2}|h-h_{tp}|^{1/2}}}. \quad (41)$$

We recognize the sum of two semiclassical solutions, obtained from Eq. (9). As in Eq. (33), one describes a contracting Universe and the other an expanding one. On the other side of the turning point, for $h - h_{tp} < 0$, the wave function decays exponentially. This corresponds to the classically forbidden region, i.e., the Universe undergoes a bounce and hence never reaches very small densities. Note that in the scenario of a recollasping Universe, the discussion above is the same \textit{modulo} the replacement $W \rightarrow -W$, that is, the classically forbidden region lies at large volumes. What we learn here is that close to the turning point, the wave function cannot be approximated by semiclassical solutions in the metric representation. Far from the turning point, when $|h - h_{tp}| \gtrsim \kappa^{1/3}$, Eq. (11) becomes valid and one can interpret the solution as a superposition of two semiclassical solutions. ($\kappa^{1/3}$ corresponds to the “region of validity of
WKB” of [9]. This shows how one can go from the momentum representation “back” to the metric representation. However, this is by no means a necessity. The solution in the momentum representation (38) is valid everywhere, unlike Eq. (41). As discussed in section II C one can then use this representation to follow the evolution of matter states all along. This example also illustrates the limitations of the proposal to extend the WKB notion of time beyond the condition (11). In this approach, one uses the phase of the wave function as a time. But Eq. (40) is purely real, and no such construction is possible in this case. On the contrary, in the momentum representation, the wave function is semiclassical and \( p_h \) is a perfectly viable time variable.

IV. APPLICATIONS

A. An exactly solvable example

We now apply the preceding results in several simple examples. This illustrates how the procedure is implemented, and what are the ingredients that make the semiclassical solution (20) valid. We consider a Universe with a positive cosmological constant and filled with non-relativistic quantum matter at equilibrium. The energy density of the quantum matter is assumed to be negative. This induces a repulsive gravitational force that will generate a bounce. Using the metric variable \( h = \alpha = \ln(a) \), the potential then becomes

\[
W(\alpha) = -\frac{V_U^2}{G^2} \left( e^{6\alpha} - 2G\rho_q e^{3\alpha} \right),
\]

(42)

where \( \rho_q > 0 \) so that \(-\rho_q\) is the energy density of quantum matter. To build semiclassical solutions, we first solve the Hamilton-Jacobi equation (15). we obtain

\[
\alpha_{cl}(p_\alpha) = \frac{1}{3} \ln \left( \frac{G\rho_q}{\Lambda} + \frac{G\rho_q}{\Lambda} \sqrt{1 + \frac{\Lambda p_\alpha^2}{V_U^2 \rho_q^2}} \right).
\]

(43)

We see that \( \alpha_{cl} \) decreases from \(+\infty\) to \( \alpha_{tp} = \ln \left( 2G\rho_q / \Lambda \right) / 3 \) where the bounce occurs, and then increases back to \(+\infty\). We then directly obtain the semiclassical solution of the Wheeler-DeWitt equation using our momentum-WKB expression (20). Note that with the pseudo-potential (42), the Hamilton-Jacobi equation (15) possesses an infinite number of solutions. However, we easily see from the variations of \( W \) that there is a unique solution such that \( \alpha_{cl}(p_\alpha) \) is real. Similarly, at the quantum level, Eq. (13) possesses derivatives in \( p_\alpha \) at all orders. However, by using a semiclassical treatment, we basically neglect all other solutions except the one corresponding to the unique real solution of the Hamilton-Jacobi equation (15).

We now discuss the validity of the semiclassical approximation. For this we use the error function of Eq. (21) with the pseudo-potential (42). It is easy to see that \( Er_p(p_h) \to 0 \) for both \( p_\alpha \to 0 \) and \( p_\alpha \to \infty \). Therefore, the semiclassical solution Eq. (20) is a very good approximation both near the bounce and far from it. The error thus grows from the vicinity of the bounce to a maximum value and then decreases to zero. A quick computation shows that the maximum error is, up to a numerical factor of order 1, given by

\[
Er_{p_{\max}} = \frac{\Lambda^{1/2}}{V_U \rho_q},
\]

(44)

\footnote{Our solution (40) corresponds to the function \( v_\lambda \) of reference [9], and described in their section 2.3, but it was not identified as an Airy function.}
see Fig. 1. On can also consider the fluctuations of matter energy $\delta \rho$ around the mean value $\rho_q$. Using Eq. (28), we see that the background field approximation is valid all along if

$$\frac{\delta \rho \Lambda}{\rho_q} \ll 1.$$  \hspace{1cm} (45)

We point out that, modulo the discussion of section III B, the same error bounds are obtained when using $a$ instead of $\alpha$ as a geometric variable.

![Figure 1: Plot of the error function $E_{p}(x)/E_{p_{\text{max}}}$ as a function of $x = \Lambda^{1/2} p_a / V_U \rho_q$.](image)

**B. Cosmology with York time**

In canonical general relativity, one can define an intrinsic notion of time using the trace of the extrinsic curvature. The obtained time parameter, known as York time, is the conjugate momentum to the volume element $\sqrt{g}$. In minisuperspace, $\sqrt{g} = a^{1/3}$, and hence we apply our results using $h = a^3$, $p_h$ giving York time. Indeed, using the action Eq. (2) written in terms of $h = a^3$, one finds

$$p_h = -\frac{V_U}{3GNa},$$  \hspace{1cm} (46)

and therefore, $p_h = V_U T$ \hspace{0.5cm} (21). From Eq. (8), we deduce the pseudo-potential

$$W(h) = \frac{V_U^2}{9G^2} \left( \Lambda - \frac{K}{h^{2/3}} + \frac{2G \rho_m}{h} + \frac{2G \rho_r}{h^{4/3}} \right) - \frac{V_U^2}{4G^2 h^2}.$$  \hspace{1cm} (47)

A peculiarity of cosmology with York time is that the pseudo-potential becomes flat for large $h$. Hence, $T$ will vary slowly and one expects the semiclassical approximation \hspace{0.5cm} (20) to become inaccurate. This can be confirmed using the validity condition of Eq. \hspace{0.5cm} (21). Hence, York time might be a good time variable to follow the evolution of the state through the turning point, but it will eventually become a bad time variable. On the contrary, the volume, or $h$, will
asymptotically be better and better, since metric WKB becomes exact for $h \to \infty$. Therefore, an accurate description will in this case involve a mix between representations. To illustrate this, we investigate again the preceding example, i.e. a cosmological constant and $\rho_m = -\rho_q$ (and neglecting $W_q \propto h^{-2}$). Once again, the Hamilton-Jacobi equation \cite{15} is fairly simple to solve, and we obtain

\[ h_{cl}(T) = \frac{2G\rho_q}{\Lambda - (3GT)^2}. \]  

(48)

As in the preceding example, the Universe contracts, bounces at $T = 0$ and expands again. However, we see here that $h_{cl} \to \infty$ at a finite value of $T$ (a behavior that was previously noticed in \cite{22}). This is simply due to the fact that the extrinsic curvature is given by $\dot{a}/a$, which is constant in a De Sitter space-time. This means that the Universe reaches a state of infinite volume in a finite York time. However, this should not be interpreted literally. As one can see from the results of section II C, any matter field will experience its proper time, at least in the background field limit. In other words, it will oscillate an infinite number of times before $h$ reaches $\infty$.

We now analyze the validity regime of the semiclassical approximation. Near the turning point ($h_{cl} = 2G\rho_q/\Lambda$), the momentum representation is accurate. When increasing $T^2$, $E_r$ grows until the approximation breaks down. On the contrary, $E_r$ is very large close to the turning point, but decreases with increasing values of $T^2$. At some value $T_{cr}$, or equivalently, $h_{cr} = h_{cl}(T_{cr})$, the two error bounds cross (see Fig. 2). Applying this definition, one finds

\[ h_{cr} = \frac{3G\rho_q}{\Lambda} = \frac{3}{2} h_{tp}. \]  

(49)

On one side of this crossing, the momentum representation offers the best approximation, on the other side, the metric one is more accurate.

To obtain a globally defined solution, say using $h$ as a variable, we build

\[ \Psi(h) = \Theta(h - h_{cr}) \int \tilde{\chi}(T)e^{ihT} dT \sqrt{2\pi} + \Theta(h_{cr} - h)\chi(h), \]  

(50)
where $\tilde{\chi}$ is given by Eq. (20) and $\chi$ by Eq. (9). Now two remarks are in order. First, by construction, the error made in this approximate solution is bounded by the minimum of the error functions (11) and (21). A short computation shows that $\mathcal{E}_r \propto \frac{\Lambda^{1/2}}{\rho q}$. When $\mathcal{E}_r \ll 1$, Eq. (50) is a good approximation everywhere, i.e. close to the turning point and asymptotically. Second, from the results of section II C, we conclude that $\psi$ is smooth, and that the precise value of $h_{cr}$ does not matter at leading order. Indeed, both expressions coincide when both error terms are small, which is the case in a vicinity of $h_{cr}$.

It is noticeable that the maximum error obtained using Eq. (50) coincides with the one of section IV A. This suggests that there exists a more general framework, allowing us to obtain semiclassical states in a representation independent manner, i.e. irrespectively of $a(h)$ or momentum vs. metric representation. The natural direction to obtain such a framework would be to use a covariant approach, i.e. path integral methods. Unfortunately, if semiclassical solutions can be obtained via saddle point methods, to obtain precise characterizations of their validity is a very difficult task. In molecular physics, where similar questions arise, this point seems to remain unclear (see [34] and the discussion in section IV A of [35]).

V. CONCLUSION

In this work, we developed a general framework to obtain semiclassical solutions of the Wheeler-DeWitt equation in the momentum representation, that is using curvature as an argument of the wave function. This provides solutions whose domain of validity are orthogonal to the standard WKB approximation, and in particular, are valid around turning points. We showed this by providing a bound for the error made by our semiclassical approximation and compared it with the WKB one, see Eqs. (21) and (11). When both approximations hold, we show that they give equivalent results (see section III A). In section II C we coupled these solutions to internal (matter) degrees of freedom allowing to draw several conclusions. First, when the momentum semiclassical approximation is valid, the curvature provides a good clock parametrizing the evolution of matter states. Second, our framework allows us to consider superpositions of matter states that are coupled to different semiclassical states of the gravitational field. Third, only when the energy spread of matter states is small, does one recover a classical background space-time.

We then applied our framework to several cases. We detailed the generic features in the vicinity of turning points, and discussed the wave function structure near the singular point $a = 0$. In section IV we showed how to apply our framework to the use of York time starting from the Wheeler-DeWitt equation. Unlike in the “choosing time before quantization” approach [3], where one first solves the Hamiltonian constraint for the desired variable and then quantizes, we control here under which conditions this ad hoc procedure is a good approximation to the general Wheeler-DeWitt equation. Since York time is the conjugate momentum to the volume element [19], our framework directly gives semiclassical solutions parametrized by York time, and allows to control their validity regime. The study of our examples also hints toward the existence of a unified framework, allowing us to minimize the error of the semiclassical approximation. We also believe our results are directly applicable to loop quantum cosmology, in the so-called $b$-representation [36].

Acknowledgments

I thank Casey Tomlin and Edward Wilson-Ewing for useful comments on this manuscript.
Appendix A: Gradient expansions

1. Noncommutative Taylor expansion

In this appendix, we shall give a proof of the noncommutative expansion used in section 1113. (To simplify, we drop the indices used in the core of the text, i.e. $p_n = p$ and $h_{cl}(p) = h(p).$)

The aim is to expand the operator $W(h(p) + i\partial_p)$ in powers of $i\partial_p$. Note that this operator is perfectly well defined. It can be built rigorously as the composition of the multiplication operator $M_W : \psi(z) \to W(z)\psi(z)$, with the Fourier operator $F$ and the (unitary) multiplication operator $M_{\text{exp}} : \psi(z) \to \exp(-i \int h(z)dz)\psi(z)$. We then define

$$W(h(p) + i\partial_p) = M_{\text{exp}}^\dagger M_W F M_{\text{exp}}.$$  

To obtain its Taylor expansion, we assume that the function $W(z)$ is analytic, and possesses the following series representation

$$W(z) = \sum_{n \in \mathbb{N}} \alpha_n z^n.$$  

The operator we wish to expand is therefore given by

$$W(h(p) + i\partial_p) = \sum_{n \in \mathbb{N}} \alpha_n (h(p) + i\partial_p)^n.$$  

Expanding this equation in powers of $i\partial_p$ is a well defined procedure. By expanding the series term by term, we shall see that it is rather easy to sort out the various powers of $i\partial_p$. The delicate point however, is to understand the validity of a truncation of the series, as being a “good approximation” of the full operator. In the next subsection, we return to that point and characterize the error made by such a truncation using a next-to-leading order computation. Back to Eq. (A3), its $n$-th term gives

$$(h(p) + i\partial_p)^n = h(p)^n + \sum_{m=0}^{n-1} h(p)^{n-1-m}i\partial_p h(p)^m + O(\partial_p^2).$$  

The second term contains all the possible orderings of $i\partial_p$ and $h(p)$. To simplify it, we notice that

$$\sum_{m=0}^{n-1} h(p)^m i\partial_p h(p)^{n-1-m} = \sum_{m=0}^{n-1} (h(p)^{n-1}i\partial_p + imh(p)^{n-2}h'(p)),$$

$$= nh(p)^{n-1}i\partial_p + \frac{i}{2} n(n-1)h(p)^{n-2}h'(p),$$

where the well-known identity $\sum_{m=1}^{n-1} m = n(n-1)/2$ has been used. Plugging this result in Eq. (A3) and summing up, we directly obtain

$$W(h(p) + i\partial_p) = W(h(p)) + W'(h(p))i\partial_p + \frac{i}{2} W''(h(p))h'(p) + O(\partial_p^2).$$  

This can also be written in a more symmetric way as

$$W(h(p) + i\partial_p) = W(h(p)) + \frac{1}{2} \left(W'(h(p))i\partial_p + i\partial_p W'(h(p))\right) + O(\partial_p^2).$$  

This form shows that the first order term is simply the only ordering that preserves the hermitian character of the operator $W(h(p) + i\partial_p)$. 


2. Next-to-leading order and error function

By using the same method as before, a lengthy but straightforward calculation gives the second order expansion of Eq. (A7)

\[ O(\partial_p^2) = \frac{1}{4} i\partial_p W''(h(p))i\partial_p + \frac{1}{8} ((i\partial_p)^2 W''(h(p)) + W''(h(p))(i\partial_p)^2) + O(\partial_p^3). \] (A8)

From this, one can obtain an estimation of the error due to the semiclassical approximation, that is, the validity condition (21). For this, we decompose a solution of the Wheeler-DeWitt equation (13) as

\[ \tilde{\Psi}(p) = \tilde{\chi}(p)(1 + \epsilon(p)). \] (A9)

\[ \tilde{\chi} \] is the semiclassical solution (20), and \( \epsilon \) encodes the corrections. A next-to-leading order gradient expansion of the Wheeler-DeWitt equation (13) gives an equation on the error function.

\[ W'A(p)i\epsilon'(p) + \frac{1}{4} i\partial_p W''i\partial_p A(p) + \frac{1}{8} ((i\partial_p)^2 W'' + W''(i\partial_p)^2) A(p) = 0, \] (A10)

where \( A \) is the semiclassical amplitude of Eq. (20) and \( W \) and its derivatives are evaluated on \( h = h(p) \). To ease the discussion, we assume \( W'' > 0 \) and since \( A(p) = W'(p)^{-1/2} \), we directly obtain \( \epsilon'(p) \) in terms of \( W \) and its derivatives.

\[ \epsilon'(p) = i \frac{4W'W''W''h' + 6W'W''h'' - 9W''h'^2 - 4W^{(3)}W'^2}{32W'^3}. \] (A11)

Although \( \epsilon \) is a local function of \( p \), what is relevant to characterize the semiclassical approximation is the accumulated error. Starting at a point \( p = p_0 \), \( \chi \) always matches an exact solution of the Wheeler-DeWitt equation (with appropriate initial conditions). At a later point \( p_1 \), the relative error is then bounded by \( \int_{p_0}^{p_1} |\epsilon'(p)|dp \) (see for instance [26, 32] for the standard WKB approximation, and the appendix of [37] in a context of higher order differential equations). If the variations of \( \epsilon' \) are smooth enough, this integral is bounded by the maximum value of \( \epsilon \). In addition, if the derivatives of the potential are well sorted, all terms in Eq. (A11) contribute to the same order. The numerical factors of the various terms above are thus irrelevant, and one can tune them to integrate \( \epsilon'(p) \) in a simple manner. Doing so, we obtain the estimate for the error function as

\[ \epsilon(p) \simeq i \frac{W'^{1/2}}{W'.} \] (A12)

The criterion of Eq. (21) is then simply \( |\epsilon| \ll 1 \). Note that this condition is very general. In fact it would still apply if the constraint where of the form \( Q(p) + W(h) = 0 \) rather than \( p^2 + W(h) \). In our case, one can use the Hamilton-Jacobi equation \( p^2 + W(h(p)) = 0 \) to rewrite (A12) and eliminate \( h' \). This gives alternative forms

\[ \epsilon(p) \simeq -i \frac{2W'^{1/2}}{W'^{3/2}} \simeq -i \frac{2W'^{1/2}}{W'^{3/2}}. \] (A13)

The last form presents the advantage to express the error function only in terms of \( W \) and its derivatives.

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