

Semiclassical approximation of the Wheeler–DeWitt equation: arbitrary orders and the question of unitarity

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Abstract We extend the Born–Oppenheimer type of approximation scheme for the Wheeler–DeWitt equation of canonical quantum gravity to arbitrary orders in the inverse Planck mass squared. We discuss in detail the origin of unitarity violation in this scheme and show that unitarity can be restored by an appropriate modification which requires back reaction from matter onto the gravitational sector. In our analysis, we heavily rely on the gauge aspects of the standard Born–Oppenheimer scheme in molecular physics.

Keywords Canonical quantum gravity · Semiclassical approximation · Wheeler–DeWitt equation · Born–Oppenheimer approximation

1 Introduction

In the search for a more fundamental theory, it is of the utmost importance to understand the connection of the new theory with existing and empirically established theories. This holds, in particular, for the goal of constructing a theory of quantum gravity. By now, various approaches exist, but there is no agreement on which is the right one [1]. One necessary requirement for any approach is that its semiclassical limit contains

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classical gravity and quantum field theory in a background spacetime. Understanding this limit could also enable one to go beyond it and calculate quantum gravitational correction terms that can potentially be observed and could thus serve as a test for the theory.

One conservative but promising approach is canonical quantum gravity in the metric variables. Unlike, for example, string theory, this is not a unified theory of all interactions. But it is still expected to give reliable information about gravity in the quantum realm [2]: if one rewrites Einstein's equations into Hamilton–Jacobi form and formulates (in the spirit of what Schrödinger did for mechanics in 1926) quantum wave equations from which the Hamilton–Jacobi form can be recovered in the WKB limit, one necessarily arrives at the equations of quantum geometrodynamics. These equations should thus hold, at least approximately, as long as the linear structure of quantum theory remains valid. It should then be possible to extract meaningful predictions from this framework such as the ones discussed here, which concern quantum gravitational *corrections* to the limit of quantum field theory in curved spacetime.

The central equations of canonical quantum gravity are four local constraints—the Wheeler–DeWitt equation and three momentum (diffeomorphism) constraints. Their semiclassical limit has already been studied in a variety of ways, see [1] and the references therein. What we want to add here are essentially two things. First, we want to extend the previous expansion scheme of [3] to arbitrary orders in the appropriate parameters. And second, we want to comment on the issue whether quantum gravitational correction terms break the usual unitarity of quantum theory or not. The latter point is clarified by drawing an analogy with the gauge structure of the Born–Oppenheimer approach in molecular physics.

To be more concrete, we consider the Wheeler–DeWitt equation in the following form¹:

$$\left[-\frac{\hbar^2}{2M} \left(G_{ab} \frac{\delta^2}{\delta h_a \delta h_b} + g_a \frac{\delta}{\delta h_a} \right) + MV(h_a) + H_m(h_a, \phi) \right] \Psi[h_a, \phi] = 0. \quad (1)$$

Here, indices a, b, \dots represent a symmetric double index and h_a denotes the spatial three-metric; G_{ab} is the DeWitt metric. The variable ϕ represents a (bosonic) matter field with Hamiltonian H_m that only depends parametrically on h_a . The parameter $M := c^2/32\pi G \approx 1.34 \times 10^{25}$ kg/m is related to the square of the (reduced) Planck mass $M_P = \sqrt{\hbar c/8\pi G}$ by $M = cM_P^2/4\hbar$; M resp. $M/\hbar \approx 1.27 \times 10^{59}$ s/m³ will be the appropriate formal parameter for the Born–Oppenheimer scheme below. Finally, $V := -2c^2 \sqrt{\det h_a} R$ denotes the gravitational potential with R as the three-dimensional Ricci scalar. The functions g_a are introduced to parameterize factor ordering ambiguities. In the arguments of the wave functionals, we will often suppress the indices of the three-metric for simplicity.

The limit of quantum field theory in curved spacetime has been derived by two different but closely related expansion schemes. One is a direct expansion with respect to the parameter M in (1) [3], the other is a more or less direct application of the

¹ There is no need to address the momentum constraints here, because their sole purpose is to guarantee the invariance of the wave functional under three-dimensional coordinate transformations.

molecular Born–Oppenheimer scheme [4,5]; its main difference lies in the treatment of back reaction on the gravitational sector and the preservation or violation of unitarity in the matter sector. A recent comparison can be found in [6] and in the Appendix of [7].

In the first approach, the correct limits of classical gravity and the functional Schrödinger equation of quantum field theory in a fixed curved background can be obtained from (1) by making the ansatz [1,3]

$$\Psi[h, \phi] = \chi[h]\psi[h, \phi], \quad (2)$$

together with a WKB-like expansion in M^{-1} for χ and ψ .² For the Wheeler–DeWitt equation, this approach resembles the traditional Born–Oppenheimer ansatz of molecular physics with zero total energy.³ There is, however, an important difference to molecular physics. We use the ansatz in (2) to derive a semiclassical limit for ψ alone, accompanied by the recovery of a semiclassical (WKB) time parameter (more precisely, a local many-fingered time) through a corresponding functional χ . We also want to interpret ψ by itself as a meaningful wave functional. We do so by deriving its functional Schrödinger equation from (1), which results from a choice of functional χ . We then face the problem of choosing a reasonable χ .

This problem becomes more apparent by noting that the solution of (1), Ψ , is invariant under a rescaling of χ and ψ of the form $\chi \rightarrow e^A \chi$, $\psi \rightarrow e^{-A} \psi$ for an arbitrary complex valued functional $A[h]$. Since in the semiclassical approximation to quantum gravity a time parameter is defined through a functional depending on h (see below), the freedom to choose a “gauge” $A[h]$ will influence the time evolution of both χ and ψ and can thus have consequences for unitarity. By unitarity we here mean the conservation of the standard Schrödinger inner product for the matter wave function ψ with respect to semiclassical (WKB) time. Note that the gauge freedom of $A[h]$ is the same as the one that leads to the gauge theory of molecular physics (see for example, [10,11]), although there one restricts to transformations that leave ψ normalized to unity, that is, A is purely imaginary, and the gauge group is the unitary group, see Sect. 2 for more details. As we want to interpret such a ψ and the equation governing its evolution physically, we need a guiding principle for the choice of an appropriate gauge $A[h]$. Such a principle will be proposed and applied in the present paper.

Our paper is organized as follows. In Sect. 2, we outline the underlying gauge structure of the Born–Oppenheimer scheme, which is crucial for our discussion. In Sect. 3, we follow the ansatz of [3] where χ is taken to be a solution to the vacuum Wheeler–DeWitt equation. Within this framework, we derive a formal expression containing *all* quantum gravitational corrections at successive orders of M^{-1} . In Sect. 4, we then

² Note that Born and Oppenheimer in their classic paper [8] did not perform a WKB-like expansion, but a Taylor-series-like expansion in the small parameter $\kappa = \sqrt{\frac{m_{\text{electron}}}{m_{\text{nucleus}}}}$.

³ An exact description would require in addition a sum over a complete set of eigenstates ψ_n , but we stay in the regime of the *adiabatic* approximation where the off-diagonal terms of the Mead–Berry connection are neglected, similar to the ansatz of Born and Oppenheimer [8]. This neglect can be justified by the process of decoherence [9].

show how to choose χ such that ψ obeys a unitary time evolution, and demonstrate the similarity of the calculations in the functional Schrödinger picture for ψ to the traditional Born–Oppenheimer approach, where one considers the equation for χ (the “nuclear wave function”) after restricting the gauge group to the unitary group (i.e. with $A[h]$ purely imaginary). Both of these approaches will yield the correct limits of classical gravity and quantum field theory in a fixed curved background spacetime, but the quantum gravitational corrections will turn out to be different. The last section contains a brief summary and an outlook on possible applications.

2 Lessons from molecular physics

In this section, we start by following the standard treatment presented, for example, in [10, 11] and continue by making further elaborations which are relevant for the unitarity issue.

In the Born–Oppenheimer approximation of molecular physics, one considers molecules which consist of interacting nuclei and electrons. Because the nuclei are more massive and move slower than the electrons, one can divide the total system into a slow part (nuclei) and a fast part (electrons). These two parts are only weakly coupled and suitable for a perturbative treatment with a naturally arising small parameter defined by the mass ratio of electrons and nuclei.⁴

The total Schrödinger equation for a molecule reads

$$i\hbar\partial_t |\Psi\rangle = (T_{\text{nuc}} + T_{\text{el}} + V) |\Psi\rangle. \quad (3)$$

Here, T_{nuc} and T_{el} denote the kinetic energy operators of nuclei and electrons, respectively, and V stands for all nuclei–nuclei, electron–electron, and nuclei–electron interactions.

For every fixed nuclear position R , we can choose a complete set $|n(R)\rangle$, $n = 1, \dots, N$,⁵ for the electronic part of the quantum state. In these states, R appears as a parameter only. To be more general, we should also include time t into this state. We hence have a basis $|n(R, t)\rangle$ for each fixed nuclear configuration R and fixed time t . Let us denote the nuclear configuration space as \mathcal{S} , such that the whole ‘background space’ is $\mathcal{S} \otimes \mathbb{R}$.

By the assumption of completeness for every configuration R we can write for the total state

$$|\Psi(t)\rangle = \sum_n \int dR' \chi^n(R', t) |R'\rangle |n(R', t)\rangle \quad (4)$$

⁴ While the traditional Born–Oppenheimer approximation is based on this separation, there exist approaches that treat nuclei and electrons on the same footing [12]. It would be interesting to apply them to quantum gravity.

⁵ In realistic cases, N will be infinite.

with a set of components $\chi^n(R, t)$. Defining

$$|\psi(R, t)\rangle := \langle R|\Psi\rangle = \sum_n \chi^n(R, t) |n(R, t)\rangle, \tag{5}$$

we get by multiplying (3) with $\langle R|$ and using (4) the following Schrödinger equation for $|\psi(R, t)\rangle$:

$$i\hbar \partial_t |\psi(R, t)\rangle = \left(\frac{-\hbar^2}{2M} \nabla_R^2 + H_0(R, t) \right) |\psi(R, t)\rangle, \tag{6}$$

where

$$H_0(R, t) := T_{\text{el}}(R) + V(R). \tag{7}$$

The mass M denotes some average mass (e.g. the reduced mass) of the nuclei, and the label R a vector of all nuclear coordinates, which are in general mass weighted. For simplicity, we abbreviate the state $|n(R, t)\rangle$ by $|n\rangle$. If we define

$$\begin{aligned} \chi &= (\chi^1, \chi^2, \dots)^T, \\ \mathbf{e} &= (|1\rangle, |2\rangle, \dots), \end{aligned} \tag{8}$$

we can write $|\psi\rangle$, Eq. (5), as

$$|\psi\rangle = \mathbf{e}\chi. \tag{9}$$

Like any such product, $|\psi\rangle$ possesses a $\text{GL}(N, \mathbb{C})$ invariance of the form

$$\begin{aligned} \chi &\rightarrow C^{-1}\chi \\ \mathbf{e} &\rightarrow \mathbf{e} C \end{aligned} \tag{10}$$

for an arbitrary non-degenerate matrix $C(R, t) \in \text{GL}(N, \mathbb{C})$.

The gauge group of molecular physics is obtained by choosing $\{|n\rangle\}$ to form a local *orthonormal* basis; in this way, $\text{GL}(N, \mathbb{C})$ is reduced to the unitary group $\text{U}(N, \mathbb{C})$. The usual Born–Oppenheimer approach uses for the $\{|n\rangle\}$ the *stationary*⁶ orthonormalized eigenstates of the ‘electronic’ Hamiltonian H_0 defined in (7). This corresponds to choosing a particular representative of the unitarily equivalent set of orthonormal bases $\{|n\rangle\}$.

Let us consider the time-dependent Schrödinger equation (6). Inserting

$$|\psi\rangle = \sum_m \chi^m |m\rangle$$

⁶ These are the states without the time-dependent phase $e^{-\frac{i}{\hbar} E(R)t}$.

[which is a shorthand writing of (5)] and contracting with $\langle n |$ from the left, we get by the orthonormality of the $|n\rangle$ the following equations for the χ^n :

$$i\hbar \dot{\chi}^n + i\hbar \sum_m \chi^m \langle n | \partial_t | m \rangle = \sum_m \left(-\frac{\hbar^2}{2M} \langle n | \nabla_R^2 | m \rangle + H_0^n{}_m \right) \chi^m, \tag{11}$$

where the Laplacian ∇_R^2 acts on everything on its right, and $H_0^n{}_m := \langle n | H_0 | m \rangle$. It is appropriate to define the following quantities:

$$\begin{aligned} \tau^n{}_{im} &:= \langle n | \partial_t | m \rangle \\ \epsilon^n{}_m &:= \langle n | \partial_t + \frac{i}{\hbar} H_0 | m \rangle. \end{aligned} \tag{12}$$

The τ are the usual Mead–Berry connections [10, 11].⁷ As we will show here, see (20) below, τ and ϵ together lead to a single connection on $\mathcal{S} \otimes \mathbb{R}$. We note that both τ and ϵ are skew-Hermitian; considered as a connection, they thus have the unitary group as gauge group.

If we use again the column vector notation introduced in (8), we find for χ the equation

$$i\hbar (\partial_t + \epsilon) \chi = \left(\frac{-\hbar^2}{2M} (\nabla + \tau)^2 \right) \chi. \tag{13}$$

Note that τ and ϵ are now matrices that appear as connections on $\mathcal{S} \otimes \mathbb{R}$.⁸ Equation (13) is a consistency condition on the nuclear wave functions χ , which has to be satisfied if the $|n\rangle$ are orthonormal for every point in $\mathcal{S} \otimes \mathbb{R}$.

We note that in the usual Born–Oppenheimer framework, one chooses *time-independent* eigenstates with $H_0 |n\rangle = e_n |n\rangle$ (without the factor $e^{-i/\hbar e_n(R)t}$). For these states $\partial_t |n\rangle = 0$, and hence $\epsilon^n{}_m = \frac{i}{\hbar} \delta_m^n e_n$. Equation (13) then reduces to the time-dependent form of the Born–Oppenheimer approach:

$$i\hbar \partial_t \chi = \left(\frac{-\hbar^2}{2M} (\nabla + \tau)^2 + e \right) \chi, \tag{14}$$

with $e = \text{diag}(e_1, e_2, \dots)$. One usually also considers the stationary Schrödinger equation for the full state. In this case, the full eigenvalue E occurs on the left-hand side of (11). Equation (13) then reduces to the well-known form [10, 11]

$$E \chi = \left(\frac{-\hbar^2}{2M} (\nabla + \tau)^2 + e \right) \chi. \tag{15}$$

One can interpret (14) and (15) as resulting from a choice of gauge in (13). All these equations are unitarily related.

⁷ Sometimes the imaginary unit is included in the definition.

⁸ To our knowledge, one has in the literature so far only interpreted τ as a connection.

Let us check that the connections defined in (12) indeed transform correctly under a unitary transformation (as also done e.g. in [10] for τ alone). Writing again the basis $|n\rangle$ as a row vector, and $\mathbf{e} = (|1\rangle, |2\rangle, \dots)$, we have again $|\psi\rangle = \mathbf{e}\chi$. The modified Schrödinger equation (13) should be invariant under all transformations that leave \mathbf{e} orthonormal (in the quantum sense), that is, under unitary transformations depending on nuclear coordinates and time. For a unitary transformation of the form

$$|k\rangle \rightarrow |k\rangle U_n^k, \tag{16}$$

the corresponding bra transforms such that the orthonormality $\langle n|m\rangle = \delta_m^n$ is preserved:

$$\langle k| \rightarrow U_n^{*k} \langle k| = U_k^{\dagger n} \langle k|. \tag{17}$$

In order for $|\psi\rangle$ to be invariant under such a transformation, we have to demand that χ transforms just as $\langle n|$:

$$\chi^k \rightarrow U_k^{\dagger n} \chi^k. \tag{18}$$

In vector notation this reads

$$\begin{aligned} \mathbf{e} &\rightarrow \mathbf{e}U, \\ \chi &\rightarrow U^\dagger \chi. \end{aligned}$$

Let us now see how the τ and ϵ -matrices transform under gauge transformations. We find

$$\begin{aligned} \tau_m^n &\rightarrow \tilde{\tau}_m^n = U_p^{\dagger n} \langle p(R)|\nabla|q(R)\rangle U_m^q \\ &= U_p^{\dagger n} \tau_p^q U_m^q + U_p^{\dagger m} \nabla U_p^q, \\ \epsilon_m^n &\rightarrow \tilde{\epsilon}_m^n = \epsilon_m^n + U_k^{\dagger n} \partial_t U_n^k, \end{aligned} \tag{19}$$

which are the correct transformation laws for a connection. If we now define a ‘space-time connection’ ω as

$$\begin{aligned} \omega_{0n}^m &= \epsilon_n^m \\ \omega_{in}^m &= \tau_{in}^m, \end{aligned} \tag{20}$$

we see that ω transforms as a connection on $\mathcal{S} \otimes \mathbb{R}$. We note again that the gauge group is the unitary group, as the connection ω is skew-Hermitian. This is the same group that leaves the form of Eq. (13) invariant.

A natural question to ask is if the fibre bundle defined by the connection in (20) is trivial, that is, if the theory defined by (13) is unitarily equivalent to a theory with $\tau = \epsilon = 0$. It turns out that the answer is *no*. If we consider the curvature Θ associated with the spacetime connection (20), we find after some calculations that its non-zero components read

$$\Theta_{ni0}^m = \frac{i}{\hbar} D_i H_0^m{}_n,$$

where D_i denotes the covariant derivative with respect to the connection defined by ω . Even if we choose a frame with $\tau = 0$ (and thus have $D_i = \partial_i$), we see that Θ would only vanish if H_0 was independent of R , which is clearly not the case.

How do we interpret the result $\Theta \neq 0$? It means that there is no choice of frame, that is, of orthonormal bases $|n\rangle$, such that χ obeys the equation of free nuclei. This is physically very natural: an interacting theory is not unitarily equivalent to a free theory. With a view on quantum gravity, one should note, however, that we actually started with a $\text{GL}(N, \mathbb{C})$ invariance, so using this larger invariance one can certainly choose χ to obey a free Schrödinger equation. Yet this would spoil the normalization of the $|n\rangle$. In other words: if we put χ in a state with $\tau = \epsilon = 0$, normalization of the $|n\rangle$ cannot be imposed for all configurations on $\mathcal{S} \otimes \mathbb{R}$. This will become important for the situation in quantum gravity, to which we will now turn.

3 Semiclassical limit with vacuum gravity background

3.1 Quantum gravitational corrections to the functional Schrödinger equation

In this subsection, we will extend the scheme developed in [3] to higher orders. We start by defining the quantity

$$\rho_\chi := \frac{1}{\chi} \left[-\frac{\hbar^2}{2M} \left(G_{ab} \frac{\delta^2}{\delta h_a \delta h_b} + g_a \frac{\delta}{\delta h_a} \right) + MV \right] \chi, \quad (21)$$

which corresponds to the pure gravitational part in (1). The scheme employed in [3] corresponds to choosing a wave functional χ (i.e. fixing a gauge) in (2) with $\rho_\chi = 0$. That is, the arising picture is one in which the semiclassical background is a solution of the vacuum Einstein field equations on which the quantum matter fields described by ψ propagate. One can, of course, generalize the scheme in order to accommodate matter degrees of freedom that contribute to $\rho_\chi = 0$ and thus represent a semiclassical matter part. In such a case, the approximation scheme does not proceed with respect to M^{-1} , but with respect to another appropriate parameter; recent examples are the cases of de Sitter inflation [13] and of slow-roll inflation [14].

It is important to note that even though $\rho_\chi = 0$ resembles the vacuum Wheeler–DeWitt equation, one has to be careful in interpreting this χ as a physically meaningful functional within our framework. For example, it would be hard to interpret a similar choice in molecular physics: without the interactions of electrons and nuclei, no stable molecule could exist. For the gravitational case, the situation is not as severe: it is certainly consistent to have a vacuum solution of the Einstein equations on which the (metric-dependent) matter fields evolve. Still, the choice $\rho_\chi = 0$ neglects possible back reaction terms from the matter sector to the ‘background’ part.

If we make a WKB-like ansatz analogously to [3],

$$\chi = \exp \left[\frac{iM}{\hbar} \sum_{j=0}^{\infty} \left(\frac{\hbar}{iM} \right)^j \sigma_j \right] =: \exp \left[\frac{iM}{\hbar} (\sigma_0 + P) \right], \quad (22)$$

Table 1 Equations for the σ_j at consecutive orders of M^{-1}

Order	Equation for σ_j
M	$\frac{1}{2}G_{ab} \frac{\delta\sigma_0}{\delta h_a} \frac{\delta\sigma_0}{\delta h_b} + V = 0$
M^0	$G_{ab} \frac{\delta\sigma_0}{\delta h_a} \frac{\delta\sigma_1}{\delta h_a} + \frac{1}{2}G_{ab} \frac{\delta^2\sigma_0}{\delta h_a\delta h_b} + \frac{1}{2}g_a \frac{\delta\sigma_0}{\delta h_a} = 0$
M^{-1}	$G_{ab} \frac{\delta\sigma_0}{\delta h_a} \frac{\delta\sigma_2}{\delta h_b} + \frac{1}{2}G_{ab} \frac{\delta\sigma_1}{\delta h_a} \frac{\delta\sigma_1}{\delta h_b} + \frac{1}{2}G_{ab} \frac{\delta^2\sigma_1}{\delta h_a\delta h_b} + \frac{1}{2}g_a \frac{\delta\sigma_1}{\delta h_a} = 0$
M^{-2}	$G_{ab} \frac{\delta\sigma_0}{\delta h_a} \frac{\delta\sigma_3}{\delta h_b} + G_{ab} \frac{\delta\sigma_1}{\delta h_a} \frac{\delta\sigma_2}{\delta h_b} + \frac{1}{2}G_{ab} \frac{\delta^2\sigma_2}{\delta h_a\delta h_b} + \frac{1}{2}g_a \frac{\delta\sigma_2}{\delta h_a} = 0$
M^{-3}	$G_{ab} \frac{\delta\sigma_0}{\delta h_a} \frac{\delta\sigma_4}{\delta h_a} + G_{ab} \frac{\delta\sigma_1}{\delta h_a} \frac{\delta\sigma_3}{\delta h_b} + \frac{1}{2}G_{ab} \frac{\delta\sigma_2}{\delta h_a} \frac{\delta\sigma_2}{\delta h_b} + \frac{1}{2}G_{ab} \frac{\delta^2\sigma_3}{\delta h_a\delta h_b} + \frac{1}{2}g_a \frac{\delta\sigma_3}{\delta h_a} = 0$

One recognizes that the highest order only enters via the τ -derivative

that is,

$$P := \sum_{j=1}^{\infty} \left(\frac{\hbar}{iM} \right)^j \sigma_j, \tag{23}$$

we get at orders M^1 and M^0 of the equation $\rho_\chi = 0$ the following equations, respectively,

$$\frac{1}{2}G_{ab} \frac{\delta\sigma_0}{\delta h_a} \frac{\delta\sigma_0}{\delta h_b} + V = 0, \tag{24}$$

$$G_{ab} \frac{\delta\sigma_0}{\delta h_a} \frac{\delta\sigma_1}{\delta h_b} + \frac{1}{2}G_{ab} \frac{\delta^2\sigma_0}{\delta h_a\delta h_b} + \frac{1}{2}g_a \frac{\delta\sigma_0}{\delta h_a} = 0. \tag{25}$$

Equation (24) is the Hamilton–Jacobi equation for vacuum gravity and is equivalent (because it is a functional equation) to all Einstein field equations [15]. Note, however, that this equation only determines the magnitude of the gradient of σ_0 (in terms of the DeWitt metric), not its direction.

One can now define a local time derivative similar to [3] as⁹

$$\frac{\delta}{\delta\tau} := G_{ab} \frac{\delta\sigma_0}{\delta h_a} \frac{\delta}{\delta h_b}. \tag{26}$$

The many-fingered time $\tau(x)$ is not a scalar, but becomes one after spatial integration [1]. With this definition, it follows from (24) that the τ - τ component of the DeWitt metric becomes $G_{\tau\tau} = -1/2V$.¹⁰ It is interesting to note that all orders of $\rho_\chi = 0$ will lead to equations that determine only the gradients of the other σ_j 's along the τ -direction, $\delta\sigma_j/\delta\tau$, and not the other components; this can be seen from (25) and from Table 1. The σ_j for $j > 1$ are hence only defined up to the addition of an arbitrary τ -independent functional. Such additional terms do not follow from the previous orders, so their form depends solely on the boundary conditions [5].

⁹ This τ should not be confused with the Mead–Berry connection of the last section.

¹⁰ It should be noted that with this definition of the time derivative, (24) leads to $\sigma_0 = -2 \int V d\tau$, which differs from the usual WKB case by having V instead of its square root.

Plugging (2) into (1), we find

$$\frac{\hbar^2}{M} \frac{1}{\chi} G_{ab} \frac{\delta \chi}{\delta h_a} \frac{\delta \psi}{\delta h_b} = H_m \psi + \rho_\chi \psi - \frac{\hbar^2}{2M} \left(G_{ab} \frac{\delta^2 \psi}{\delta h_a \delta h_b} + g_a \frac{\delta \psi}{\delta h_a} \right). \quad (27)$$

With the choice $\rho_\chi = 0$, we can now obtain from (27) with the definition of the time derivative in (26) and the definition of P in (22) an equation for the time evolution of ψ :

$$i\hbar \frac{\delta \psi}{\delta \tau} = H_m \psi - i\hbar G_{ab} \frac{\delta P}{\delta h_a} \frac{\delta \psi}{\delta h_b} - \frac{\hbar^2}{2M} \left(G_{ab} \frac{\delta^2 \psi}{\delta h_a \delta h_b} + g_a \frac{\delta \psi}{\delta h_a} \right). \quad (28)$$

One can proceed further by demanding that the gradient of ψ is proportional to the gradient of σ_0 as suggested in [3], which is some sort of adiabatic approximation in superspace; that is,

$$\frac{\delta \psi}{\delta h_a} = \alpha[h] \frac{\delta \sigma_0}{\delta h_a}, \quad (29)$$

for some functional $\alpha[h]$. Equation (24) then yields $\frac{\delta \psi}{\delta \tau} = -2V\alpha$, and we can express $\frac{\delta \alpha}{\delta \tau}$ in terms of τ -derivatives of ψ and V . We further assume that there is a total (not necessarily Hermitian) Hamiltonian H such that we can write

$$i\hbar \frac{\delta \psi}{\delta \tau} = H\psi. \quad (30)$$

Using this definition together with (25) and expressing the second time-derivatives in (28) with the Hamiltonian by using again (30), Eq. (28) reduces to the following compact expression:

$$i\hbar \frac{\delta \psi}{\delta \tau} = H\psi = H_m \psi - \frac{1}{4MV} \left(H^2 + i\hbar \frac{\delta H}{\delta \tau} - i\hbar KH \right) \psi, \quad (31)$$

where

$$K := \frac{1}{V} \frac{\delta V}{\delta \tau} - \frac{2iM}{\hbar} \sum_{j=2}^{\infty} \left(\frac{\hbar}{iM} \right)^j \frac{\delta \sigma_j}{\delta \tau}. \quad (32)$$

This equation is the full functional Schrödinger equation for ψ including all quantum gravitational corrections within the vacuum gravity ($\rho_\chi = 0$) approximation. Note that the Hamiltonian H appears on both sides of (31), so it is also an implicit equation for the Hamiltonian itself. As we see, it correctly reproduces the limit of quantum field theory in a fixed curved background spacetime at zeroth order in M^{-1} . The equations at any other order in M^{-1} can be found from (31) in a straightforward way by iteration.

We see that this equation is not only an equation for the dynamics of ψ , but can also be used for determining the Hamiltonian H itself. For simple cosmological models one could try to solve (31) for H as a differential equation in time. Within a semiclassical approximation, one could assume that H is a function of H_m alone, which resembles a restriction to the one-particle sector of the theory [3], and further expand H and H_m in M^{-1} . This approach is in fact in the spirit of the traditional Born–Oppenheimer approximation [8]. For instance, the first order correction to (31) is

$$\begin{aligned}
 i\hbar \frac{\delta\psi}{\delta\tau} &= H_m\psi - \frac{1}{4MV} \left(H_m^2 + i\hbar \frac{\delta H_m}{\delta\tau} - \frac{i\hbar}{V} \frac{\delta V}{\delta\tau} H_m \right) \psi + \mathcal{O}(M^{-2}) \\
 &= H_m\psi - \frac{H_m^2}{4MV} \psi - \frac{\hbar}{4M} \frac{\delta}{\delta\tau} \left(\frac{iH_m}{V} \right) \psi + \mathcal{O}(M^{-2}), \quad (33)
 \end{aligned}$$

as presented in [3]. It should be noted that (31) is independent of any factor ordering ambiguities, as the g_a -term has canceled due to (25). It is also interesting to note that the same expression, Eq. (31), is obtained if we assume that all σ_i , V , and ψ only depend on τ such that we consider only the τ and τ - τ components of g_a and G_{ab} and drop all other components from the beginning in Eq. (1). This is at first glance rather surprising, and seems to be a direct consequence of (25), whose form in either case assures that all additional terms are canceled. However, we see that (24) has a solution of the form $\tau = V$ and $\sigma_0 = -\int V^2 d^3x$ (recall that $G_{\tau\tau} = -1/2V$). In this case, σ_0 and V indeed only depend on τ .

3.2 Problems with unitarity

We recognize from (31) that the gauge choice $\rho_\chi = 0$ leads to a non-unitary time evolution for ψ at order M^{-1} and higher. In applications to cosmological models, the unitarity violating terms have often been neglected as they are small compared to the unitary terms [7, 14, 17]. We can see two reasons for the occurrence of non-unitarity directly in this equation. First, the Wheeler–DeWitt equation is a Klein–Gordon type of an equation, whose unitary time evolution (with respect to the usual quantum mechanical inner product) is spoiled due to the second time derivatives, giving rise to the term $i\hbar \frac{\delta H}{\delta\tau}$ in (31); see equation (3.13) in [18]. Secondly, the choice $\rho_\chi = 0$ leads to the term $i\hbar K H$.

The major problem at this stage is then the physical interpretation of ψ with a non-unitary time evolution: is ψ really the physical quantity described by the functional Schrödinger equation plus quantum gravitational corrections? If yes, the gauge choice $\rho_\chi = 0$ has physical meaning above all other physical requirements on our semiclassical limit. Then unitarity violation is physical for ψ . Yet, the only important guiding principles we have is to recover the correct classical limit (Hamilton–Jacobi equation) and the functional Schrödinger equation in a fixed curved background. But the condition $\rho_\chi = 0$ leads to a set of additional equations at each order in M^{-1} , whose interpretation is not clear. In the next section we therefore show how one can, in principle, render the theory unitary by modifying the gauge choice and allowing $\rho_\chi \neq 0$.

4 Unitary functional Schrödinger equation and non-vacuum gravity background ($\rho_\chi \neq 0$)

Following the standard Born–Oppenheimer approximation (see Sect. 2 and [5, 6]), we shall in this section demand unitary time evolution for the matter wave function ψ , where unitarity is defined with respect to the standard Schrödinger inner product.

Since the full wave functional is given as a solution to the Wheeler–DeWitt equation, this will modify both ψ and the gravitational wave function χ compared to the last section. We shall see that this leads to different quantum gravitational corrections at order M^{-1} .

The main procedure is simple: we adjust the matter wave functional such that we get, order by order, a unitary evolution in WKB time. For simplicity, we will assume in this section that V and the σ_i (and thus χ) only depend on the WKB time τ defined in (26), and that $\psi = \psi(\tau, \phi)$, and $H_m = H_m(\tau, \phi)$. This captures the essential point of unitarity restoration; for the general case, one has to include the terms discussed in [5]. In this section, we set $\hbar = 1$ for simplicity. The Wheeler–DeWitt equation then reduces to the following equation:

$$\left[-\frac{1}{2M} \left(G_{\tau\tau} \frac{\delta^2}{\delta\tau^2} + g_\tau \frac{\delta}{\delta\tau} \right) + MV(\tau) + H_m(\tau, \phi) \right] \Psi = 0. \tag{34}$$

This form is obtained by an orthogonal decomposition of the DeWitt metric as presented in [16]. For the total wave functional, we make an ansatz similar to (2),

$$\Psi[\tau, \phi] = \chi[\tau]\psi[\tau, \phi]. \tag{35}$$

We assume Ψ to be of the form

$$\Psi = \exp(iM\sigma_0[\tau]) \psi_0[\tau, \phi] =: \chi_0 \psi_0, \tag{36}$$

and demand that $\rho_{\chi_0} = \mathcal{O}(M^0)$, where now, similar to the last section,

$$\rho_\chi := \frac{1}{\chi} \left[-\frac{1}{2M} \left(G_{\tau\tau} \frac{\delta^2}{\delta\tau^2} + g_\tau \frac{\delta}{\delta\tau} \right) + MV(\tau) \right] \chi.$$

This leads to the Hamilton–Jacobi equation (24) for σ_0 at order M ; it also allows us to keep the definition (26) for τ ; hence, $G_{\tau\tau} = -1/2V$ as before. With this new ρ_{χ_0} , we find instead of (31),

$$i \frac{\delta\psi_0}{\delta\tau} \equiv H\psi_0 = H_m\psi_0 - i \left(\frac{1}{2V} \frac{\delta V}{\delta\tau} - Vg_\tau \right) \psi_0 - \frac{1}{4MV} \left(H^2 + i \frac{\delta H}{\delta\tau} - 2iVg_\tau H \right) \psi_0. \tag{37}$$

At this stage, ψ_0 experiences a non-unitary time evolution as before. In order to remedy this, we could split the Hamiltonian H into Hermitian and anti-Hermitian parts, $H = H_H + H_N$, and redefine the wave functional such that the new one evolves unitarily. In case that the Hamiltonian commutes at different times, this can be achieved by $\psi = \exp(i \int d\tau H_N) \psi_0$, leading to $i\delta\psi/\delta\tau = H_H\psi$. The wave functional ψ can then be interpreted as a physical wave functional. This would, however, only be possible if we knew H , which is in general not the case. We will thus follow here an alternative route and show how (37) can be solved iteratively by demanding unitarity for the matter wave functions *at each order*.

Let us define two functions $E(\tau)$ and $\varepsilon(\tau)$ such that $H\psi_0 = E\psi_0$ and $H_m\psi_0 = \varepsilon\psi_0$; E is in general complex, but ε is always real. The second equation means that we have to solve the matter Schrödinger equation and take ψ_0 as an eigenfunction of H_m . Let us further expand these functions in the spirit of Born and Oppenheimer as

$$E = E^{(0)} + M^{-1}E^{(1)} + M^{-2}E^{(2)} + \dots, \tag{38}$$

and similarly for ε . Inserting these expansions into (37) yields for the first two orders:

$$\begin{aligned} E^{(0)} &= \varepsilon^{(0)} - i \left(\frac{1}{2V} \frac{\delta V}{\delta \tau} - V g_\tau \right) \\ E^{(1)} &= \varepsilon^{(1)} - \frac{1}{4V} \left((E^{(0)})^2 + i \frac{\delta E^{(0)}}{\delta \tau} - 2iV g_\tau E^{(0)} \right); \end{aligned} \tag{39}$$

in the last line, the expression for $E^{(0)}$ should be plugged in to get an expression for $E^{(1)}$ in terms of $\varepsilon^{(0)}$ and $\varepsilon^{(1)}$. Next we define

$$\psi_1 := \exp \left(- \int \Im(E^{(0)}) d\tau \right) \psi_0 = \exp \left(\int \left(\frac{1}{2V} \frac{\delta V}{\delta \tau} - V g_\tau \right) d\tau \right) \psi_0, \tag{40}$$

so that ψ_1 obeys a unitary Schrödinger equation *at order* M^0 , that is, $i \frac{\delta \psi_1}{\delta \tau} = H_m \psi_1 + \mathcal{O}(M^{-1})$. The total wave function thus reads

$$\Psi = \chi_0 \psi_0 = \exp \left(iM\sigma_0 - \int \left(\frac{1}{2V} \frac{\delta V}{\delta \tau} - V g_\tau \right) d\tau \right) \psi_1 =: \chi_1 \psi_1. \tag{41}$$

Note that if $g_\tau = 0$, one can integrate the exponent to yield $\chi_1 = \frac{1}{\sqrt{V}} \exp(iM\sigma_0)$, which is similar to the usual WKB case (except for the difference mentioned in footnote 10). One can now compute ρ_{χ_1} and finds that the zeroth order of ρ_{χ_1} vanishes, $\rho_{\chi_1} = \mathcal{O}(M^{-1})$. Hence, Eq. (25) (with only τ -derivatives) remains unchanged. This could have been anticipated by noting that the unitary violating terms in (31) are of order $\mathcal{O}(M^{-1})$ and higher. If we write, similar to our discussion above, $\chi_1 = \exp(iM\sigma_0 + \sigma_1)$, we can read off (25) directly from the exponent of (41):

$$\frac{\delta \sigma_1}{\delta \tau} = V g_\tau - \frac{1}{2V} \frac{\delta V}{\delta \tau}.$$

In the next order, we define in an analogous way

$$\begin{aligned} \psi_2 &:= \exp \left(- \frac{1}{M} \int \Im(E^{(1)}) d\tau \right) \psi_1 \\ &= \exp \left(\frac{1}{M} \int \left(-\varepsilon^{(0)} \left[\frac{1}{4V^2} \frac{\delta V}{\delta \tau} - \frac{1}{2} g_\tau \right] + \frac{1}{4V} \frac{\delta \varepsilon^{(0)}}{\delta \tau} - \frac{1}{2} g_\tau \varepsilon^{(0)} \right) d\tau \right) \psi_1 \\ &= \exp \left(\frac{1}{4MV} \varepsilon^{(0)}(\tau) \right) \psi_1, \end{aligned} \tag{42}$$

where in the last step we have performed a partial integration and omitted a constant. We see that the g_τ -term has dropped out in this step. We hence get a new expression for the total wave function:

$$\Psi = \exp\left(iM\sigma_0 - \int\left(\frac{1}{2V}\frac{\delta V}{\delta\tau} - Vg_\tau\right)d\tau - \frac{1}{4MV}\varepsilon^{(0)}(\tau)\right)\psi_2 =: \chi_2\psi_2. \quad (43)$$

If we define again $\chi_2 = \exp(iM\sigma_0 + \sigma_1 - iM^{-1}\sigma_2)$, we get for σ_2 the surprisingly simple result:

$$i\sigma_2 = \frac{1}{4V}\varepsilon^{(0)}(\tau), \quad (44)$$

so σ_2 is purely imaginary. This is different from the situation of the last section.

One can easily see that at this order M^{-1} , ρ_{χ_2} does not vanish. Requiring unitary time evolution for ψ_2 leads to the occurrence of a back reaction of the matter part onto the gravitational sector, cf. [5,6]. This is closer in spirit to the traditional Born–Oppenheimer scheme than the approach discussed in the previous section, as we will briefly discuss now.

Let us consider Eq. (34) with $G_{\tau\tau} = -1/2V$ and $\Psi = \chi[\tau]\psi[\tau, \phi]$. The original approach of Born and Oppenheimer was to multiply this equation with ψ^* from the left and integrating over ϕ . We now require unitary time evolution for ψ . We define a real-valued function $\bar{E}(\tau)$ by $i\frac{\delta\psi}{\delta\tau} = \bar{E}\psi$, \bar{E} being real as ψ is assumed to evolve unitarily. This leads to the standard form for the ‘nuclear’ wave function:

$$\left[\frac{1}{4MV}\left(\frac{\delta}{\delta\tau} - i\bar{E}\right)^2 - \frac{1}{2M}g_\tau\left(\frac{\delta}{\delta\tau} - i\bar{E}\right) + \varepsilon + MV\right]\chi = 0. \quad (45)$$

At this stage, the large gauge group $e^{A[\tau]}$ has been reduced to the unitary group, that is, A is purely imaginary. We see that \bar{E} , which is the effective energy of the matter degrees of freedom, assumes the role of the Mead–Berry connection in this approach, which is different from the usual approach in molecular physics.¹¹ Note that, even though in general the Mead–Berry connection can be gauged away by a unitary transformation (by switching to the diabatic picture, see e.g. [11]), this makes no sense here, for we want to determine \bar{E} in this particular frame.

As above, we can now make an ansatz of the form (also compare [6] for such a WKB-like ansatz within the traditional Born–Oppenheimer approach)

$$\chi = \exp\left(iM\eta_0 + \eta_1 + M^{-1}\eta_2 + \dots\right), \quad (46)$$

where $\eta_{0,1} = \sigma_{0,1}$, $\eta_2 = -i\sigma_2$, etc., and all η_i are taken to be real; the phase of ψ is hence influenced at the lowest order only. Expanding \bar{E} in powers of M^{-1} , plugging this ansatz into (45), and matching the real and imaginary parts at each order, we find at order M^1 again the Hamilton–Jacobi equation (24). At the next order M^0 , the real

¹¹ Hence, employing the Born–Oppenheimer approximation, i.e. dropping the Mead–Berry connection, will not help us here.

part of Eq. (45) yields $\bar{E}^{(0)} = \varepsilon^{(0)}$, while the imaginary part yields an equation for the Van Vleck determinant similar to (25),

$$\frac{\delta\eta_1}{\delta\tau} = g_\tau V - \frac{1}{2V} \frac{\delta V}{\delta\tau}. \quad (47)$$

At the next order, we find for the imaginary part Eq. (44), while the real part yields

$$\bar{E}^{(1)} = \varepsilon^{(1)} - \frac{1}{4V} (\varepsilon^{(0)})^2 + \frac{1}{4V} \left(\frac{3}{4V^2} \left(\frac{\delta V}{\delta\tau} \right)^2 - V^2 g_\tau^2 - \frac{1}{2V} \frac{\delta^2 V}{\delta\tau^2} + V \frac{\delta g_\tau}{\delta\tau} + g_\tau \frac{\delta V}{\delta\tau} \right), \quad (48)$$

which we would also get from (39) if we considered only the real part. Hence, as expected, the two methods lead us to the same result if we require unitary time evolution for ψ . At order M^{-1} , the energy ε , introduced above as the eigenvalue corresponding to H_m , is thus shifted by quantum gravitational corrections; this shift is given by (recall that a factor M^{-1} must be added to the terms on the right-hand side in (48) to get the energy)

$$\Delta\varepsilon = \frac{1}{4MV} \left(-\varepsilon^2 + \frac{3}{4V^2} \left(\frac{\delta V}{\delta\tau} \right)^2 - V^2 g_\tau^2 - \frac{1}{2V} \frac{\delta^2 V}{\delta\tau^2} + V \frac{\delta g_\tau}{\delta\tau} + g_\tau \frac{\delta V}{\delta\tau} \right) + \mathcal{O}(M^{-2}). \quad (49)$$

The only relevant term is the contribution proportional to ε^2 , because the other terms are matter-independent. This relevant term is, in fact, the term that was used to calculate the quantum gravitational correction to the power spectrum of the cosmic microwave background (CMB) anisotropies [7, 14, 17]. In these papers, the first method was used and the unitarity-violating terms were neglected by hand. This procedure can be justified by the discussion presented here.

5 Discussion

Let us summarize the main results of our paper. We have investigated semiclassical (Born–Oppenheimer type of) approximation schemes for the Wheeler–DeWitt equation of canonical quantum gravity. The analogous situation in molecular physics was reviewed with an emphasis on the gauge freedom that arises within this framework. Although the total entangled quantum state of electrons and nuclei is always the same, this gauge freedom allows to shift terms between the electronic and nucleonic parts. Requiring unitarity separately for the electronic part, we get a definite expression for the back reaction onto the nuclei; this is the usual Born–Oppenheimer approximation.

The Born–Oppenheimer like ansatz for the total wavefunctional entails a similar gauge freedom for the Wheeler–DeWitt equation. As in molecular physics, a straightforward expansion in terms of the inverse Planck-mass squared without back reaction

of matter on gravity spoils unitarity in the matter sector.¹² We have discussed this scheme and extended it to all orders in the expansion parameter. We then have modified the expansion scheme by using the gauge freedom to guarantee unitary evolution for the matter sector. This is closer in spirit to the standard Born–Oppenheimer scheme and leads to back reaction terms for the gravitational part. This point of view was taken in [4–6]. A concrete normalization of the matter states is not needed—the important thing is the unitary development. We note that the issue of avoiding unitarity violating terms also occurs when performing a non-relativistic expansion for the Klein–Gordon equation in external electromagnetic and gravitational fields [19].

A good understanding of the semiclassical approximation to quantum gravity is of fundamental importance for two main reasons. On the theoretical side, it provides a bridge between full quantum gravity and established physics. One can apply this scheme not only to quantum general relativity with minimally coupled fields, but also to scalar-tensor theories [20], Weyl gravity [21], and others. On the observational side, first tests of quantum gravity will most likely occur from small correction terms that modify the usual limit of quantum field theory in curved spacetime [13, 14]. For this purpose, it is of great importance to develop and compare approximation schemes like the ones discussed here and investigate their empirical consequences.

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¹² One should note, however, that the analogy between these two cases is limited, since we are dealing with two fundamentally different equations—the Schrödinger equation and the Wheeler–DeWitt equation, which is of Klein–Gordon type. The latter obeys a conservation law different from the former [18].

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