Quantum gravitational corrections to the functional Schrödinger equation

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We derive corrections to the Schrödinger equation which arise from the quantization of the gravitational field. This is achieved through an expansion of the full functional Wheeler-DeWitt equation with respect to powers of the gravitational constant. The correction terms fall into two classes: One describes the breakdown of the classical background picture while the other corresponds to quantum gravitational corrections for the matter fields themselves. The latter are independent of the factor ordering which is chosen for the gravitational kinetic term. If the total state evolves adiabatically, the only correction term that survives contains the square of the matter Hamiltonian. In the general case there are also smaller terms which describe a gravitationally induced violation of unitarity. The corrections are numerically extremely tiny except near the big bang and the final stages of a black hole. They are also of principle significance for quantum field theories near the Planck scale.

I. INTRODUCTION

One of the many approaches towards a quantum theory of gravity is the application of canonical quantization procedures to general relativity. In the Dirac scheme, the four constraints which are present in the classical theory are implemented in the quantum theory through four conditions on wave functionals. The traditional, geometrodynamical, choice of variables leads to the concept of superspace—the configuration space of all (spacelike) three-geometries and matter fields. While three of the quantum constraints only express the invariance of the wave functional with respect to diffeomorphisms on three-space, the fourth one, the Wheeler-DeWitt equation, is responsible for the dynamics. It reads explicitly

$$\left(-\frac{16\pi G\hbar^2}{c^2}G_{ijkl}\frac{\delta^2}{\delta h_{ij}\delta h_{kl}}-\frac{c^4}{16\pi G}\sqrt{h}\,{}^{(3)}R+H_m(h_{ij}(\mathbf{x}),\Phi(\mathbf{x}))\right)\Psi[h_{ij}(\mathbf{x}),\Phi(\mathbf{x})]=0. \quad (1)$$

Here $h_{ij}(\mathbf{x})$ denotes the metric on three-space, h its determinant, $\Phi(\mathbf{x})$ symbolically stands for all matter fields, and ${}^{(3)}R$ is the Ricci scalar on three-space (a cosmological constant term has been neglected).

The Wheeler-DeWitt equation (1) does not yield any unification of gravity and matter. One would thus expect that it describes an effective theory which is valid below some unification scale (e.g., of string theory), in the same way as, because of the triviality of the ϕ^4 theory, the standard electroweak theory is considered to be an effective theory which is valid below a certain cutoff given by the Higgs-boson mass. It is thus one of the premises of the canonical approach that (1) is valid at a certain scale between the domain of the "theory of everything" and the domain where classical general relativity is applicable. Moreover, (1) can still correspond to a meaningful theory of "quantum gravity."

Solutions to the Wheeler-DeWitt equation in its full functional form are rare. In the geometrodynamical version (1), this is only possible in the limit of $G\rightarrow\infty$, the strong gravity limit, where the term containing the Ricci scalar is absent [1]. The situation improves if one performs a canonical transformation at the classical level, leading to the description with Ashtekar's variables [2]. Then explicit solutions to the quantum constraints can be given [3]. In contrast with the strong gravity limit, where different space points decouple, the wave functionals now have support on one-dimensional loops. This at least demonstrates that a sensible meaning *can* be attributed to quantum general relativity at a nonperturbative level, although the theory is perturbatively nonrenormalizable. It is, however, difficult to interpret the results in this "loop-space representation" in terms of the old, more familiar, geometrodynamical language.

In view of this situation, most work has dealt with minisuperspace versions of (1), where all degrees of freedom, except very few such as the three scale factors in a Bianchi model, are frozen out. In this context, the main concern has been to study the implementation of certain boundary conditions (see, e.g., [4] and [5]), the construction of a viable Hilbert-space structure, and more conceptual issues such as the role of time in quantum gravity (see, e.g., [6–9]).

One of the important goals in the canonical quantum theory of gravity is of course the establishment of a connection to known physics. The first thing to try is to derive from (1), through a certain approximation scheme, the limit of quantum field theory in a *fixed* classical gravitational background. This has been first investigated in [10] and then studied from various aspects by various authors (see, e.g., [11–15]). Basically, what one does is to perform an expansion of (1) with respect to the Planck mass, through which one finds the functional Schrödinger equation for matter fields propagating on a classical gravitational background. (Of course, while quantum field theory is recovered here in its Schrödinger picture form, it is assumed that this form is equivalent to doing quantum field theory in the Heisenberg picture, in a fixed classical background.)

From this result one may conclude that among the two key ingredients of ordinary quantum field theory, commutation relations and equation of motion, the former is more fundamental. The latter holds true only in the approximation that gravity is classical, and is otherwise to be replaced by the Wheeler-DeWitt equation. The above derivation of quantum field theory from quantum gravity also solves, at least at the mathematical level, the puzzle raised by Smolin [16] regarding the relation between "quantum and gravitational phenomena." In the stochastic interpretation of quantum mechanics [17] one assumes the particle's quantum-mechanical motion to be a special kind of Brownian motion. The Brownian diffusion constant D is assumed to be proportional to Planck's constant, so that $\hbar = Dm_q$. The constant m_q has dimensions of mass and can vary from particle to particle. Smolin emphasizes the coincidence that m_q is "found experimentally to be equal to the particle's inertial mass, to at least 2 parts in 10^{12}." If we accept that nonrelativistic quantum mechanics is an approximation to quantum field theory, and that both general relativity and the functional Schrödinger equation are approximations to the Wheeler-DeWitt equation, this coincidence can be understood. The inertial mass (=gravitational mass) and the quantum mass m_q then both have the same origin: namely, the matter stress-energy operator in the Wheeler-DeWitt equation.

If the Schrödinger equation can be *derived* from the Wheeler-DeWitt equation, a natural question to ask is how quantum gravitational corrections to the Schrödinger equation may look. A first step in this direction has been taken in [18] within the context of a two-dimensional minisuperspace model. Here we present such a derivation of these correction terms for the *full* functional equation (1). Although these corrections prove, of course, to be extremely tiny in the laboratory, they show how, at least in principle, effects of quantum gravity show up through, e.g., a shift in atomic spectral lines.

The paper is organized as follows. In Sec. II, we present a simple but helpful analogy—an expansion of the Klein-Gordon equation with respect to the speed of light which is formally similar to the case of interest here. In Sec. III we define our approximation scheme and derive a functional Schrödinger equation for matter fields on a fixed background. Section IV comprises the main part of our paper. Going one order further in our approximation scheme, we derive corrections to this functional Schrödinger equation. Furthermore, we apply this scheme to the momentum constraints. We then demonstrate how the corrections show up in the spectrum of hydrogen-type atoms. Finally, Sec. V contains a brief summary and a critical discussion of the obtained results.

II. A SIMPLE ANALOGY: RELATIVISTIC CORRECTIONS TO THE SCHRÖDINGER EQUATION FROM THE KLEIN-GORDON EQUATION

In this section we perform an expansion of the Klein-Gordon equation for a first-quantized wave function $\varphi(\mathbf{x},t)$ with respect to powers of the speed of light. In this way we will recover the nonrelativistic Schrödinger equation and can thus give a probabilistic interpretation for the wave function. It has to be emphasized that to that purpose we have to restrict ourselves to the "one-particle sector" of the theory. This is conceptually different from the case of the Wheeler-DeWitt equation which already corresponds to a "second-quantized" theory. The Klein-Gordon equation reads

$$\left(\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial t^2} - \hbar^2\nabla^2 + m^2c^2\right)\varphi(\mathbf{x},t) = 0. \tag{2}$$

If one compares this with the Wheeler-DeWitt equation (1), one recognizes that, formally, there is a correspondence of c^2 in (2) with $c^2/16\pi G$ in (1). The gravitational degrees of freedom (three-metric) in (1) correspond to Minkowski time in (2), while the matter degrees of freedom in (1) correspond to Minkowski three-space in (2). In the following, the nonrelativistic approximation to (2) will be discussed through a Born-Oppenheimer-type approach with c^2 as the parameter. This makes sense, if the relevant velocities are much smaller than the speed of light, as is the case for, e.g., atomic electrons. In this way we will obtain the well-known relativistic corrections to the Schrödinger equation. While our purpose here is to provide an analogy to the discussion of the Wheeler-DeWitt equation, we emphasize that this kind of approximation scheme is mathematically different from the one discussed in the literature, where a Foldy-Wouthysen transformation is applied (see, e.g., [19]).

To make the discussion more general, we insert into (2) a minimally coupled electromagnetic potential A^μ through the usual substitution $p_\mu \to p_\mu - (e/c)A_\mu$, but keep only its zero component $A^0 \equiv \phi$. One then has, instead of (2),

$$\left(\frac{\hbar^2}{c^2}\frac{\partial^2}{\partial t^2} - \hbar^2\nabla^2 + m^2c^2 + \frac{2ie\hbar}{c^2}\phi\frac{\partial}{\partial t} - \frac{e^2\phi^2}{c^2} + \frac{ie\hbar}{c^2}\frac{\partial\phi}{\partial t}\right) \times\varphi(\mathbf{x},t) = 0. \tag{3}$$

We write

$$\varphi(\mathbf{x},t) = e^{iS(\mathbf{x},t)/\hbar} \tag{4}$$

and make the expansion

$$S = c^2S_0 + S_1 + c^{-2}S_2 + \cdots . \tag{5}$$

We insert this into (3) and compare equal powers of the expansion parameter c^2. To order c^4 we find

$$(\nabla S_0)^2 = 0. \tag{6}$$

Thus S_0 is a function of t only (if S_0 is assumed to be real).

The next order (c^2) yields

$$-\left(\frac{\partial S_0}{\partial t}\right)^2 + m^2 = 0. \tag{7}$$

This is a Hamilton–Jacobi-type equation which leads to real solutions for S_0, if $m^2 \geq 0$ ("no tachyons"). It can, of course, be immediately solved,

$$S_0 = \pm mt + \text{const}, \tag{8}$$

so that the wave function up to this order reads

$$\varphi \propto e^{\pm imc^2 t/\hbar}. \tag{9}$$

These are the usual wave functions for a particle of positive (lower sign) and negative (upper sign) energy at rest. Note that, in spite of the real nature of (2), these solutions are intrinsically complex. In the following, we will restrict ourselves to the positive-energy case (lower sign). Of course, it is implicitly assumed throughout that positive and negative energies can be treated separately, i.e., that particle production, etc., does not occur.

The next order (c^0) in (3) then yields

$$2m\dot{S}_1 + (\nabla S_1)^2 - i\hbar\nabla^2 S_1 + 2em\phi = 0, \tag{10}$$

which upon introducing $f \equiv e^{iS_1/\hbar}$ can be written as (for $m \neq 0$)

$$i\hbar\dot{f} = -\frac{\hbar^2}{2m}\nabla^2 f + e\phi f. \tag{11}$$

Thus we have recovered nothing but the Schrödinger equation with an external electrostatic potential. The next order in our expansion will therefore yield the first relativistic corrections.

To order c^{-2} we find

$$i\hbar\ddot{S}_1 - i\hbar\nabla^2 S_2 - \dot{S}_1{}^2 + 2m\dot{S}_2 + 2\nabla S_1\nabla S_2 + ie\hbar\dot{\phi} - e^2\phi^2 - 2e\phi\dot{S}_1 = 0. \tag{12}$$

In this equation we rewrite S_1 in terms of f using the definition given above. Next, we eliminate S_2 by defining $\chi \equiv f e^{iS_2/\hbar c^2}$. Equation (12) can now be interpreted as the Schrödinger equation for the modified wave function χ, and after using (11) for f, (12) can be written as

$$\begin{aligned} i\hbar\dot{\chi} = &\left(-\frac{\hbar^2}{2m}\nabla^2 + e\phi\right)\chi \\ &+\left(-\frac{\hbar^4}{8m^3c^2}\nabla^2(\nabla^2)\right. \\ &\left.+\frac{e\hbar^2}{4m^2c^2}\nabla^2\phi + \frac{e\hbar^2}{2m^2c^2}\nabla\phi\nabla\right)\chi \end{aligned} \tag{13}$$

In this derivation, terms with powers higher than c^{-2} have been neglected for consistency. The result (13) is independent of the value of $\dot{\phi}$.

The terms in the second and third lines of (13) require some explanation. The first term of the second line can be understood to arise from expanding the relativistic expression $\sqrt{p^2c^2 + m^2c^4}$ for the energy in powers of p/mc up to order p^4. The first term of the third line has the form of a Darwin term (which describes the zitterbewegung), while the second term in the third line would correspond, in the case of the Dirac equation, to spin-orbit coupling. Here, however, these terms are artifacts of the kind of approximation scheme we have used. First, the expectation value of these terms with respect to any stationary state vanishes. This can be seen as follows. Let $|\psi\rangle$ be a stationary state. Because the Hamiltonian is invariant under time reversal, it can be chosen to be real without loss of generality. The two last terms in (13) are proportional to $(\nabla^2\phi + 2\nabla\phi\nabla)\chi \equiv R$. Then it follows in the position representation that

$$\begin{aligned} \langle\psi|R|\psi\rangle &= \int d^3x\,\psi(\nabla^2\phi)\psi + 2\int d^3x\,\psi\nabla\phi\nabla\psi \\ &= \int d^3x\psi(\nabla^2\phi)\psi - 2\int d^3x(\nabla\psi)(\nabla\phi)\psi - 2\int d^3x\psi(\nabla^2\phi)\psi \\ &= -\int d^3x\psi(\nabla^2\phi)\psi - 2\int d^3x\psi(\nabla\phi)(\nabla\psi) = -\langle\psi|R|\psi\rangle. \end{aligned}$$

Thus the expectation value has to vanish. Second, the two terms under consideration may be absorbed in this order of approximation through a renormalization of the wave function according to

$$\chi \to \tilde{\chi} \equiv \chi e^{e\phi/mc^2}.$$

The renormalized wave function $\tilde{\chi}$ is the wave function which one obtains by applying a Foldy-Wouthysen transformation (see, e.g., [19], where it is shown that the first "real" Darwin terms in the Klein-Gordon case arise at order c^{-4}). It obeys the corrected Schrödinger equation with only the term of the second line of (13).

In hydrogen-type atoms (with a potential $\phi = -Ze/r$), the first correction term in (13) yields an energy shift (fine structure) according to

$$\Delta E_{\rm rel} = -\int d^3x\, \psi^*_{nlm} \left(\frac{\hbar^4}{8m^3c^2}\nabla^2\nabla^2\right)\psi_{nlm} = -\frac{mc^2}{2}(Z\alpha)^4\left(\frac{1}{n^3(l+\frac{1}{2})} - \frac{3}{4n^4}\right). \quad (14)$$

Here ψ_{nlm} denote the unperturbed wave functions with quantum numbers n, l, and m, and α is the fine-structure constant. The Klein-Gordon equation (3) can also be solved exactly for this potential (see, e.g., [20]), leading to (14) through an expansion of the exact energy eigenvalues. There is, of course, the usual problem of how to recover the reduced mass in (14) instead of the electron mass, but this can be satisfactorily dealt with (see again [20]). The energy shift (14) is exact for pionic atoms but gives of course incorrect values for the experimentally observed fine structure in ordinary atoms [this was the reason for Schrödinger to reject (3) as a candidate for a quantum-mechanical wave equation] where one has to solve the Dirac equation, taking into account the spin of the electron. This aspect, however, is not important for our analogy. We will see in the next sections how a similar formal expansion of the Wheeler-DeWitt equation yields quantum gravitational corrections to the Schrödinger equation.

III. DERIVATION OF THE SCHRÖDINGER EQUATION FROM QUANTUM GRAVITY

Our starting point is the full functional Wheeler-DeWitt equation (1), where we perform an expansion with respect to the parameter $M \equiv c^2/32\pi G$. This has a dimension of mass per length, so that we can expect this expansion to be sensible if, for a particle, its rest mass divided by its Compton wavelength is much smaller than M. This is satisfied for masses which are much smaller than the Planck mass.

In contrast with the case of the previous section, the Wheeler-DeWitt equation already describes a "second-quantized" theory. The restriction to the one-particle sector which we had to make in the Klein-Gordon case corresponds here to the limit where effects of a "third quantization" (which turns the Wheeler-DeWitt wave functional into an operator) can be neglected. Such a third quantization has been discussed extensively in the literature, but there is no general agreement whether it is necessary to perform such a step at all.

In analogy to the Klein-Gordon case we write the wave functional $\Psi[h_{ij}(\mathbf{x}), \phi(\mathbf{x})]$ as

$$\Psi = e^{iS/\hbar} \quad (15)$$

and expand S in the form

$$S = MS_0 + S_1 + M^{-1}S_2 + \cdots. \quad (16)$$

In the following we use a condensed notation, labeling three-metric components h_{ij} by h_a and components of the DeWitt-metric G_{ijkl} by G_{ab}. This is possible because indices will appear only in this combination. Then the Wheeler-DeWitt equation reads

$$\left[-\frac{\hbar^2}{2M}\left(G_{ab}\frac{\delta^2}{\delta h_a \delta h_b} + g_a\frac{\delta}{\delta h_a}\right) + MV(h_{ab}) + H_m(h_{ab},\phi)\right]\Psi = 0. \quad (17)$$

Here V stands for $-2c^2\sqrt{h}^{(3)}R$ (the cosmological constant has been neglected) and H_m stands for the Hamiltonian of matter fields. We will assume in the following the presence of minimally coupled scalar fields with Hamiltonian

$$H_m = -\frac{\hbar^2}{2\sqrt{h}}\frac{\delta^2}{\delta\phi^2} + u(h_{ab}, \phi, \phi_{,a}), \quad (18)$$

but the results will be independent of any special form. The linear derivative term in (17) describes some of the ambiguity in the factor ordering of the kinetic term. One could also include in (17) a term proportional to the curvature scalar in configuration space (see, e.g., [21]), but this would not have any effect on the results discussed below. If one were to demand general covariance in configuration space, one would have to choose the covariant Laplace-Beltrami operator in (17). This requires some care in regularizing products of distributions at the same point (see, e.g., [22] and [23] for a discussion of this point). In the following we do not care about that and treat all functional derivatives in a formal sense, as if we were dealing with ordinary derivatives. Surprisingly, it will turn out that, at least formally, the important part of the corrections is independent of the factor-ordering ambiguity in (17).

We now insert the expansion defined by (15) and (16) into (17) and compare expressions with the same order in M. The highest order (M^2) yields

$$\left(\frac{\delta S_0}{\delta\phi}\right)^2 = 0. \quad (19)$$

If many matter fields were present (which is the realistic case), the term in (19) would have to be replaced by a sum of analogous terms. Thus S_0 depends *only* on the three-metric, provided that all matter fields which are present in (17) have positive-definite kinetic terms so that one can conclude that every single term in (19) must vanish. Implicit in this reasoning is, of course, also the assumption that S_0 is chosen to be real. This, however, is necessary, because the gravitational wave function should not correspond to a classically forbidden region (see the following).

The next order (M^1) yields the Hamilton-Jacobi equation for gravity alone:

$$\frac{1}{2}G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_0}{\delta h_b} + V(h_{ab}) = 0. \quad (20)$$

In a realistic model, there should also be a matter source on the right-hand side of this equation. This is easy to achieve if other, "macroscopic," fields are present for which one can perform a semiclassical ($\hbar$) expansion. Here, however, we are interested in the behavior of quantized matter fields on a given background and thus restrict ourselves to the case (20) without loss of generality. It is well known that (20) is, together with the principle of constructive interference, equivalent to all ten (vacuum) Einstein field equations [24]. Once S_0 is given, every three-geometry can be integrated to give a full four-dimensional solution of the field equations.

The next order (M^0) yields

$$G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_1}{\delta h_b} - \frac{i\hbar}{2}\left(G_{ab}\frac{\delta^2 S_0}{\delta h_a \delta h_b} + g_a\frac{\delta S_0}{\delta h_a}\right) + \frac{1}{2\sqrt{h}}\left(\frac{\delta S_1}{\delta\phi}\right)^2 - \frac{i\hbar}{2\sqrt{h}}\frac{\delta^2 S_1}{\delta\phi^2} + u(h_a,\phi,\phi,\phi_{,a}) = 0. \tag{21}$$

We now define a functional f according to

$$f \equiv D(h)e^{iS_1/\hbar} \tag{22}$$

and, using a condition on D, will derive an equation for f. From (22) we have

$$i\hbar G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta f}{\delta h_b} = \frac{i\hbar}{D}\frac{\delta D}{\delta h_b}G_{ab}\frac{\delta S_0}{\delta h_a}f - G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_1}{\delta h_b}f. \tag{23}$$

From (21) we find

$$H_m f = \frac{i\hbar}{2}\left(G_{ab}\frac{\delta^2 S_0}{\delta h_a \delta h_b} + g_a\frac{\delta S_0}{\delta h_a}\right)f - G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_1}{\delta h_b}f. \tag{24}$$

We choose $D(h_{ab})$ to satisfy (compare [11])

$$G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta D}{\delta h_b} - \frac{1}{2}\left(G_{ab}\frac{\delta^2 S_0}{\delta h_a \delta h_b} + g_a\frac{\delta S_0}{\delta h_a}\right)D = 0. \tag{25}$$

Thus, D plays the role of a Van Vleck determinant. It depends explicitly on the factor ordering in (17). For a minisuperspace model with one degree of freedom Q and $g = 0$ one has [18]

$$D = \sqrt{\frac{dS_0}{dQ}}.$$

From (23) and (24) it is then easy to see that f satisfies

$$i\hbar G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta f}{\delta h_b} \equiv i\hbar\frac{\delta f}{\delta\tau} = H_m f. \tag{26}$$

This is the functional Schrödinger equation for matter fields (the *Tomonaga-Schwinger* equation) propagating on a *fixed* curved background given by (20). As we remarked in the introduction, such an equation has been derived by various authors using various methods. The time τ in (26) (which is a "many-fingered time") labels the "trajectories" in superspace which run orthogonal to hypersurfaces $S_0 = constant$. It is usually called WKB time [25] and plays a prominent role in semiclassical gravity. To this order one can also discuss the "back reaction" of the matter fields on the background given by (20) [26]. Basically, this is obtained if one defines the geometrodynamical momentum with the help of the phase $MS_0 + S_1$. Only under very special circumstances, however, is this term equal to the expectation value of the matter Hamiltonian—for example, in the case when the matter wave function f is in a quasistationary state.

To this order of approximation, the wave functional of the system is

$$\Psi = \frac{1}{D}e^{iMS_0/\hbar}f. \tag{27}$$

By computing the wave functional to the next order, we can find corrections to the Schrödinger equation (26).

We want to conclude this section with one remark concerning the derivation of the Schrödinger equation (26). In its derivation, the gravitational field has been assumed to be in a WKB state. Some authors argue that WKB states are a very special, restricted class of states (see, e.g., [27] and [28]). While we agree that one has to consider an additional mechanism to explain the emergence of classical properties (for example decoherence [14], [29]), the WKB method is the simplest mathematical procedure to establish the quantum to classical correspondence. This remark is reinforced by the results of the present work.

IV. CORRECTIONS TO THE SCHRÖDINGER EQUATION FROM QUANTUM GRAVITY

The next order in our expansion (16), namely, $O(M^{-1})$, yields the following equation for S_2:

$$G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_2}{\delta h_b} + \frac{1}{2}G_{ab}\frac{\delta S_1}{\delta h_a}\frac{\delta S_1}{\delta h_b} - \frac{i\hbar}{2}\left(G_{ab}\frac{\delta^2 S_1}{\delta h_a \delta h_b} + g_a\frac{\delta S_1}{\delta h_a}\right) + \frac{1}{\sqrt{h}}\frac{\delta S_1}{\delta\phi}\frac{\delta S_2}{\delta\phi} - \frac{i\hbar}{2\sqrt{h}}\frac{\delta^2 S_2}{\delta\phi^2} = 0. \tag{28}$$

Proceeding as in the Klein-Gordon case, we rewrite S_1 in terms of f, using the definition (22). Equation (28) then becomes

$$G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta S_2}{\delta h_b} - \frac{\hbar^2}{D^2}G_{ab}\frac{\delta D}{\delta h_a}\frac{\delta D}{\delta h_b} + \frac{\hbar^2}{2D}\left(G_{ab}\frac{\delta^2 D}{\delta h_a \delta h_b} + g_a\frac{\delta D}{\delta h_a}\right) = \frac{\hbar^2}{2f}\left(-\frac{2}{D}G_{ab}\frac{\delta f}{\delta h_a}\frac{\delta D}{\delta h_b} + G_{ab}\frac{\delta^2 f}{\delta h_a \delta h_b} + g_a\frac{\delta f}{\delta h_a}\right) + \frac{i\hbar}{\sqrt{h}f}\frac{\delta S_2}{\delta\phi}\frac{\delta f}{\delta\phi} + \frac{i\hbar}{2\sqrt{h}}\frac{\delta^2 S_2}{\delta\phi^2}. \tag{29}$$

Next we write S_2 as $S_2 = \sigma_2(h_a) + \eta(\phi, h_a)$, and by inspecting the left-hand side of (29), we choose σ_2 to be the solution of the equation

$$G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta \sigma_2}{\delta h_b} - \frac{\hbar^2}{D^2}G_{ab}\frac{\delta D}{\delta h_a}\frac{\delta D}{\delta h_b} + \frac{\hbar^2}{2D}\left(G_{ab}\frac{\delta^2 D}{\delta h_a \delta h_b} + g_a\frac{\delta D}{\delta h_a}\right) = 0. \quad (30)$$

The physical interpretation for this choice is that $\sigma_2[h_{ab}]$ should correspond to the second WKB order for the gravitational part of the wave functional. For a one-dimensional minisuperspace model the equation for σ_2 reads (with $p \equiv dS_0/dQ \equiv S_0')$

$$\sigma_2' = -\frac{\hbar^2}{4p^2}p'' + \frac{3\hbar^2}{8}\frac{p'^2}{p^3},$$

and thus is in full analogy to the second-order WKB corrections for quantum-mechanical wave functions (see, e.g., [30]).

Using (29) and Eq. (30) for σ_2, it is easy to write down the equation satisfied by the functional η:

$$G_{ab}\frac{\delta S_0}{\delta h_a}\frac{\delta \eta}{\delta h_b} = \frac{\hbar^2}{2f}\left(-\frac{2}{D}G_{ab}\frac{\delta f}{\delta h_a}\frac{\delta D}{\delta h_b} + G_{ab}\frac{\delta^2 f}{\delta h_a \delta h_b} + g_a\frac{\delta f}{\delta h_a}\right) + \frac{i\hbar}{\sqrt{h} f}\frac{\delta \eta}{\delta \phi}\frac{\delta f}{\delta \phi} + \frac{i\hbar}{2\sqrt{h}}\frac{\delta^2 \eta}{\delta \phi^2}. \quad (31)$$

The correct wave functional to this order is

$$\Psi(h_a, \phi) = \Psi^{(2)}_{\rm WKB}(h_a) f e^{i\eta/M\hbar}, \quad (32)$$

where

$$\Psi^{(2)}_{\rm WKB} = \frac{1}{D}e^{iMS_0/\hbar}e^{i\sigma_2/M\hbar}. \quad (33)$$

As before we define $\chi = fe^{i\eta/M\hbar}$. This will be the modified Schrödinger wave functional. By using (26) for f and Eq. (31) for η we find that χ satisfies the corrected Schrödinger equation

$$i\hbar\frac{\delta \chi}{\delta \tau} = H_m\chi + \frac{\hbar^2}{2Mf}\left(\frac{2}{D}G_{ab}\frac{\delta f}{\delta h_a}\frac{\delta D}{\delta h_b} - G_{ab}\frac{\delta^2 f}{\delta h_a \delta h_b} - g_a\frac{\delta f}{\delta h_a}\right)\chi. \quad (34)$$

This equation is the gravitational analog of (13). To improve the analogy we now proceed to put (34) in a more transparent form. For this purpose we decompose the derivatives of f with respect to h_a into components normal and tangential to hypersurfaces S_0 =const in superspace. We write

$$G_{ab}\frac{\delta f}{\delta h_a} = -\frac{i}{\hbar}G_{ab}A^a H_m f + G_{cd}\frac{\delta f}{\delta h_c}l^d l_b. \quad (35)$$

The first term on the right-hand side is the component *normal* to S_0 =const. A^a is explicitly given by

$$A^a = \frac{\delta S_0}{\delta h_a}\left(G_{cd}\frac{\delta S_0}{\delta h_c}\frac{\delta S_0}{\delta h_d}\right)^{-1} = -\frac{1}{2V}\frac{\delta S_0}{\delta h_a}, \quad (36)$$

and use has been made of the Schrödinger equation (26) for f. In (36), we have used the Hamilton-Jacobi equation (20). This decomposition breaks down if the three-dimensional Ricci scalar vanishes because then $\delta S_0/\delta h_a$ is a null vector [see (20)] and the classical trajectory "lies within" the hypersurface S_0 =const. This can be the case because of the indefinite nature of the DeWitt metric G_{ab}.

The second term on the right-hand side of (35) is the *tangential* component and l_a denotes a unit vector tangential to S_0 =const, obeying $l^a A_a = 0$, $l^a l_a = \pm 1$, the sign depending on whether the hypersurface is timelike or spacelike. The tangential component is of course not determined by (26). In the following, we will abbreviate this component by a_a.

To decompose the second metric derivatives in (34) in this way, we first differentiate (35) with respect to h_b and then use (35) to eliminate the first derivatives. This yields

$$G_{ab}\frac{\delta^2 f}{\delta h_a \delta h_b} = -\frac{i}{\hbar}G_{ab}\frac{\delta A^a}{\delta h_b}H_m f - \frac{A_a A^a}{\hbar^2}H_m^2 f - \frac{\delta G_{ab}}{\delta h_b}a^a + \frac{\delta a_b}{\delta h_b}. \quad (37)$$

From (36) one infers that

$$\frac{\delta A^a}{\delta h_b} = -\frac{1}{2V}\frac{\delta^2 S_0}{\delta h_a \delta h_b} + \frac{1}{2V^2}\frac{\delta S_0}{\delta h_a}\frac{\delta V}{\delta h_b}. \quad (38)$$

Using (35)–(38) and the equation for the Van Vleck determinant (25), one finds for the correction terms of (34) the expression

$$\frac{\hbar^2}{2Mf}\left(-G_{ab}\frac{\delta^2 f}{\delta h_a \delta h_b} + \frac{2}{D}G_{ab}\frac{\delta f}{\delta h_a}\frac{\delta D}{\delta h_b} - g_a\frac{\delta f}{\delta h_a}\right)\chi \equiv B_n + B_t.$$

The "normal" part B_n of the correction reads

$$B_n = -\frac{1}{4MVf}\left[H_m^2 f - i\hbar G_{ab}\frac{\delta S_0}{\delta h_b}\left(-f\frac{\delta H_m}{\delta h_a} + \frac{\delta V}{\delta h_a}H_m f\right)\right]\chi = -\frac{1}{4MVf}\left[H_m^2 f - i\hbar\left(-f\frac{\delta H_m}{\delta \tau} + \frac{\delta V}{V\delta \tau}H_m f\right)\right]\chi. \quad (39)$$

Because of the use of (25) in this derivation, *all* factor ordering ambiguities have been cancelled in this component.

The "tangential" part B_t reads

$$B_t = -\frac{\hbar^2}{4MVf}\left[\frac{2}{D}\frac{\delta D}{\delta h_b}\left(G_{cd}\frac{\delta f}{\delta h_c}l^d\right)l_b + \frac{\delta G_{ab}}{\delta h_b}\left(G_{cd}\frac{\delta f}{\delta h_c}l^d\right)l^a - \frac{\delta}{\delta h_b}\left(G_{cd}\frac{\delta f}{\delta h_c}l^d\right)l_b - g_a G_{cd}\frac{\delta f}{\delta h_c}l^d l^a\right]\chi. \quad (40)$$

Note that

$$\frac{\delta\chi}{\delta h_a} = \frac{1}{f}\frac{\delta f}{\delta h_a}\chi + O\left(\frac{1}{M}\right), \quad \text{etc.,} \tag{41}$$

so that all f derivatives can be replaced by χ derivatives in this order of approximation.

It would be worthwhile to comment on the nature of the tangential components in some detail. Because the Schrödinger equation (26) determines only the metric derivative of f along a classical trajectory, these components are not determined by the previous order equations themselves but only by the special solution which has been chosen. The presence of these tangential components reflects the breakdown of the classical background picture—they "probe" the superspace environment near a classical solution to Einstein's equations. For the important case that the matter Hamiltonian in (26) can be assumed to depend only adiabatically on the three-metric, f depends on h_a only through τ and the tangential components vanish.

The final result for the corrected Schrödinger equation reads, taking into account only the normal components which are determined by the previous order equations:

$$i\hbar\frac{\delta\chi}{\delta\tau} = H_m\chi + \frac{4\pi G}{c^4\sqrt{h}^{(3)}R}\left[H_m^2 + i\hbar\left(\frac{\delta H_m}{\delta\tau} - \frac{1}{\sqrt{h}^{(3)}R}\frac{\delta(\sqrt{h}^{(3)}R)}{\delta\tau}H_m\right)\right]\chi. \tag{42}$$

This equation is the main result of our paper. We emphasize again that the correction term in (42) is *independent* of the factor ordering which was chosen for the gravitational part of the Wheeler-DeWitt equation—a satisfactory feature. Note also that the correction terms vanish in the nonrelativistic limit $c \to \infty$.

The purpose of discussing the Klein-Gordon example in this paper should now become clear upon comparison of (13) and (42). In both cases one obtains a well-known limit at a certain order, and similar corrections at the next order of approximation. The correction term proportional to H_m^2 appears in both cases, and perhaps the term proportional to H_m in (42) is a "zitterbewegung-like" effect.

The second and third terms in the large parentheses of (42) are imaginary and describe a gravitationally induced violation of unitarity. The presence of such terms is not totally unexpected because (42) is an effective equation for the matter fields *alone*. These terms are, however, in general even much smaller than the first correction term which contains the square of the matter Hamiltonian. This can easily be estimated for the special case of a Friedmann background described by a scale factor a. The ratio of the second to the first correction term is then given by

$$\frac{\hbar\delta H_m/\delta\tau}{H_m^2} \approx \frac{\hbar\dot{a}dH_m/da}{H_m^2} \approx \frac{\hbar H}{E},$$

where E denotes a typical energy for the matter field, and H is the Hubble parameter. For $E \approx 200$ GeV and the present estimates of H, this is about 10^{-43}. The same holds for the ratio of the third to the first correction term. Thus, these unitarity-violating terms are totally negligible for the whole course of the classical evolution of the Universe. Because these terms express the change of the matter Hamiltonian and the gravitational potential with respect to the background, they vanish in an adiabatic approximation. The emergence of such unitarity violating terms can also be understood if one recalls that the full Wheeler-DeWitt equation leads to the conservation of a Klein-Gordon-like current but *not* to a Schrödinger like current. An expansion of this conservation law up to the present order leads to the conservation law for the Schrödinger current *modified* by small corrections proportional to the gravitational constant.

It is interesting to recognize that, analogously to the Klein-Gordon case, the term with the square of the matter Hamiltonian can formally be obtained through an expansion of an appropriate square root: namely,

$$-\left(\frac{c^4\sqrt{h}^{(3)}R}{4\pi G}\right)^{1/2}\left(H_m - \frac{c^4\sqrt{h}^{(3)}R}{16\pi G}\right)^{1/2}$$

$$\approx -\frac{c^4\sqrt{h}^{(3)}R}{8\pi G} + H_m + \frac{4\pi G}{c^4\sqrt{h}^{(3)}R}H_m^2 + \cdots .$$

The "rest energy density" in this expression corresponds to the rest mass mc^2 in the Klein-Gordon case and may indicate the need for a third quantization (see, e.g., [31]).

In the previous section we have briefly remarked that one can under very *special* conditions find a back-reaction-modified Hamilton-Jacobi equation for gravity. For that purpose it is necessary that the WKB time τ is defined with the help of the *full* phase of the wave function up to the present order of approximation. This would also lead, due to the different definition of τ, to an additional term on the right-hand side of (42). Because the back-reaction equation does not follow generically from the formalism, we will, however, keep our definition of τ in accordance with the one made for the uncorrected Schrödinger equation (26). An interesting open problem is the establishment of the connection to an operational definition of time in this context.

In canonical quantum gravity, the Wheeler-DeWitt equation (1) has to be supplemented by the momentum constraints. In their general form,

$$\left(\frac{1}{\sqrt{h}}\frac{\delta\Psi}{\delta h_{ab}}\right)_{|b} = \frac{8\pi G}{c^4}\sqrt{h}T^{0a}\Psi \tag{43}$$

they guarantee that the wave functional depends, apart from matter fields, only on the three-geometry; i.e., it is invariant under coordinate transformations on three-space. Performing an expansion as in (15), (16), one can easily see that the effect of (43) is to guarantee that, at *each step* of the expansion, the corresponding S depends only on the three-geometry (apart from matter fields).

The expression (42) for the corrections does not apply when the Ricci scalar on the three-dimensional hypersurface under consideration vanishes, which is the case, e.g., for the standard foliation of Minkowski and Schwarzschild spacetime. In that case one has to directly use the expression for the corrections in (34). Two different situations may occur. If the solution to (20) is given by S_0 =const, there occurs no dynamics at all and one cannot derive the Schrödinger equation (26). Minkowski spacetime is an example for that situation. This case is in fact against the very essence of geometrodynamics [32], where "the geometry of yesterday cannot be the geometry of today." If S_0 is not a constant, as may occur, e.g., for the case of a Bianchi type-I model, one can derive the Schrödinger equation (26), and the correction terms in (34) are well defined despite the fact that the terms in (42) do formally diverge.

If one takes for example the case of a homogeneous scalar field on a closed Friedmann background with scale factor a, the corrected Schrödinger equation (42) reads (where an integration over three-space has been performed, using $\int d^3x\sqrt{h}{}^{(3)}R = 12\pi^2 a$)

$$i\hbar\frac{\partial\chi}{\partial\tau} = H_m\chi + \frac{G}{3\pi c^4 a}\left[H_m^2 + i\hbar H\left(-\frac{\partial H_m}{a\partial a} + H_m\right)\right]\chi, \tag{44}$$

where H is again the Hubble parameter. The corrections are thus utterly negligible, except for very small values of the scale factor.

Although (42), as it stands, does not hold for, e.g., Schwarzschild spacetime, one might expect heuristically, on purely dimensional grounds, that a length scale analogous to the scale factor plays a prominent role. The term $\sqrt{h}{}^{(3)}R$ in (42) would then have to be replaced by a term proportional to L_c, where L_c is a typical curvature length of the gravitational background. Consider for example a quantum-mechanical Hamiltonian of the form

$$H_m(q,h_a) = -\frac{\hbar^2}{2m}\nabla^2 + u(q,h_a). \tag{45}$$

Although the above corrections have been derived for a functional Schrödinger equation, one might expect that these corrections also show up in quantum mechanics (remember the calculation of the Lamb shift). Then the dominant part of the correction terms in (42) reads

$$H_m^2 = \frac{\hbar^4}{4m^2}\nabla^2\nabla^2 - \frac{\hbar^2}{2m}\nabla^2 u - \frac{\hbar^2}{m}\nabla u\nabla - \frac{\hbar^2}{2m}u\nabla^2 + u^2. \tag{46}$$

The second and third term in (46) are analogous to the "Darwin-like" terms in (13) and do not contribute to stationary states. Let us consider in analogy to the Klein-Gordon case (13) the fourth-order derivative term in (46). When inserted into (42), this yields a correction term of the order

$$\frac{G\hbar^4}{12\pi c^4 m^2 L_c}\nabla^2\nabla^2.$$

This, in principle, would lead to an energy shift of the spectral lines for the hydrogen atom analogous to (14):

$$\Delta E_{\rm QG} = \int d^3x\,\psi^*_{nlm}\frac{G\hbar^4}{12\pi c^4 m^2 L_c}\nabla^2\nabla^2\psi_{nlm} = \frac{Gm^2}{3\pi L_c}(Z\alpha)^4\left(\frac{1}{n^3(l+\frac{1}{2})} - \frac{3}{4n^4}\right). \tag{47}$$

Instead of the rest energy of the electron which occurred in (14), we find here an expression that is proportional to the gravitational self-energy of a mass m distributed over a scale L_c. For an electron in the Schwarzschild metric of a proton ($Z = 1$), the typical curvature length scale at the distance of the Bohr radius is about $L_c \approx 3.5\times 10^{13}$ cm. Thus the energy shift in (47) would be of the order $\Delta E_{\rm QG} \approx 3.3\times 10^{-73}$ eV, which will of course be forever unobservable. This is even much smaller than the corrections to linewidths that would arise through the emission of gravitons in linear quantum gravity [33]. Of course even the correction to the energy shift arising from the classical gravitational interaction between proton and electron is much bigger. Perturbing the potential in (45) by $-Gmm_p/r$, one finds an energy shift

$$\Delta E_G = -\frac{Gm^2 m_p e^2}{\hbar^2 n}$$

which for $n = 1$ is about 1.2×10^{-38} eV. The signature of this energy shift, however, differs from the one in (47). Thus, at least in principle, there is an effect arising from quantum fluctuations of the gravitational field. The importance of these quantum gravitational corrections lies in the conceptual modification they cause to quantum field theory at the Planck scale.

V. DISCUSSION

We have derived in this paper correction terms to the Schrödinger equation which arise from the coupling of quantum gravitational fluctuations to matter fields. This has been achieved through a formal expansion of the Wheeler-DeWitt equation with respect to powers of the Planck mass. The corrected Schrödinger equation is again a linear equation, though in [18] it was wrongly claimed that the corrected equation is nonlinear in the wave function. We could demonstrate that the main part of these correction terms is actually independent of the choice of factor ordering for the kinetic term of the gravitational part. We have also discussed how, in principle, these corrections alter the spectral lines of hydrogen-type atoms. As expected, the actual line shift turns out to be extremely tiny and unobservable forever. This is not surprising because atoms are bound by electromagnetic forces, where even the effect of classical gravity is smaller by 39 orders of magnitude. The effect of quantum gravity calculated in this paper is another 34 orders of magnitude below that. The only known quantum mechanical system where the influence of classical gravity has been successfully tested is that of neutron beams in the gravitational field of the Earth where interference effects are being induced [34]. But even in that case quantum gravitational effects are suppressed by some 34 orders of magnitude. Thus the situation is hopeless, as far as laboratory experiments are concerned.

The only imaginable situations where these corrections could become important are those of the early Universe and the final fate of a black hole. For example, our Eq. (44) directly yields corrections to the Schrödinger equation for higher multipoles on a Friedmann background [12] which physically represent density fluctuations. While in the cosmological context the interpretation of (42) is more or less clear, this is not true for the black-hole case where even the role of the Wheeler-DeWitt equation has not been clarified up to now.

We now discuss the theoretical aspects of (42) and start by comparing these corrections with those in the Klein-Gordon case. Note that even though the Klein-Gordon equation is real, we must choose the leading-order solution to be one of the two complex plane waves, to have a sensible one-particle interpretation. For a similar reason, (see, e.g., [15]) we should choose the leading-order gravitational wave function to be a complex WKB wave functional, even though the Wheeler-DeWitt equation is real. Such a choice is necessary if we are to recover the picture of field propagation in a classical, rather than in a superposition of classical universes. To explain the unobservability of such superpositions, one has to invoke an additional mechanism such as decoherence [14, 29].

The relativistic corrections found in (13) assume a fixed classical electromagnetic field. They have a straightforward physical interpretation of being due to the relativistic mass increase and the smeared Coulomb potential seen by the relativistic particle. An additional correction (the Lamb shift) arises if quantum fluctuations of the electromagnetic field are taken into account. How does one physically interpret the corrections arising in the Wheeler-DeWitt case? Note that unlike the electromagnetic field in the Klein-Gordon case, now the metric is quantized, and this is expressed in the second-order gravitational WKB fluctuations in Eq. (32). It then appears reasonable to think that the corrections in (42) are, in analogy to the Klein-Gordon case, a "gravity-induced mass increase" and a "gravitational zitterbewegung," being caused by a process we do not yet properly understand. One may think that, instead of the Klein-Gordon equation, a better analogy to the Wheeler-DeWitt case would be provided by the functional Schrödinger equation for a quantized scalar field coupled to a quantized electromagnetic field. However, it is not clear how to choose a natural expansion parameter in the latter case.

Because, for the gravitational part of the total wave functional, our expansion is equivalent to a WKB expansion (and thus to a loop expansion), the WKB(2) fluctuations in (32) should correspond to pure graviton graphs of second order around a classical gravitational background. This is not the case for the χ part of the wave functional which should contain loops of gravitons and "matter particles" to any order (although no "particles" are defined in this context). For this reason it is not possible to interpret these corrections straightforwardly as a "Lamb-shift-like" effect. One might also ask what is the effect of averaging these WKB(2) fluctuations in expectation values of a matter observable with respect to χ, but this is not attempted here.

The presence of the H_m^2 term in (42) may have a fundamental significance for quantum field theory. One can no longer expand the wave functional of a free theory into a set of harmonic oscillators as is necessary to relate the functional Schrödinger picture to the more commonly used Fock space representation (see, e.g., [35]). Essentially, the nonlinearity of H_m^2 prevents the separation of the wave functional χ into a product of individual oscillator eigenfunctions. This has drastic consequences for the particle concept. In the approximation of quantum field theory in a fixed background, particles can be defined, but the definition is, in general, not unique. If one takes into account the correction terms derived in this paper, the concept of a particle cannot even be defined.

One of the motivations for the present work is to find a gravity-induced smoothing of divergences in flat space quantum field theory. In principle, this effect should already be contained in (42) and the associated averaging implicit in (32). These two equations together should also imply a lower bound to physical length at the Planck scale. We hope to return to these unresolved issues in a future publication.

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