PHYSICAL REVIEW D, VOLUME 59, 123519

Unitary and nonunitary evolution in quantum cosmology

S. Massar
Service de Physique Théorique, Université Libre de Bruxelles, Code Postal 225, Boulevard du Triomphe, B1050 Brussels, Belgium

R. Parentani
Laboratoire de Mathématiques et Physique Théorique, CNRS UPRES A 6083, Faculté des Sciences, Université de Tours, 37200 Tours, France

(Received 14 December 1998; published 17 May 1999)

We analyze when and why unitarity violations might occur in quantum cosmology restricted to minisuperspace. To this end we discuss in detail backscattering transitions between expanding and contracting solutions of the Wheeler-DeWitt equation. We first show that upon neglecting only backscattering, one obtains an intermediate regime in which matter evolves unitarily but which does not correspond to any Schrödinger equation in a given geometry since gravitational back reaction effects are taken into account at the quantum level. We then show that backscattering amplitudes are exponentially smaller than matter transition amplitudes. Both results follow from an adiabatic treatment valid for macroscopic universes. To understand how backscattering and the intermediate regime should be interpreted, we review the problem of electronic transitions induced by nuclear motion since it is mathematically very similar. In this problem, transition amplitudes are obtained from the conserved current. The same applies to quantum cosmology and indicates that probability amplitudes should be based on the current when backscattering is neglected. We then review why, in a relativistic context, backscattering is interpreted as pair production whereas it is not in the nonrelativistic case. In each example the correct interpretation is obtained by coupling the system to an external quantum device. From the absence of such external systems in cosmology, we conclude that backscattering does not have a unique consistent interpretation in quantum cosmology. [S0556-2821(99)03312-3]

PACS number(s): 98.80.Hw

I. INTRODUCTION

Quantum gravity suggests the possibility of nonunitary evolution. In particular singularities and regions of strong curvature, such as black holes and the big bang, are natural places where such effects could occur. However, in these cases, the lack of the comprehension of Planck scale physics precludes us from reaching any definitive conclusions.

More surprisingly, when the universe is macroscopic and the curvature is small, the possibility of nonunitarity remains. Moreover, in this long wavelength regime, it seems unavoidable that quantum gravity implies the Wheeler-DeWitt (WDW) equation [1,2] (truncated to a finite set of modes so as to eliminate ultraviolet problems) since this constraint expresses and guarantees reparametrization invariance.

Thus the theoretical basis for investigating unitarity violation in quantum cosmology seems well established. Nevertheless, no definite analysis has been carried out, even in minisuperspace. Indeed, in the literature one finds either prudent discourses which avoid the problem or claims ranging from ''there are no unitary violations'' [3] to ''there are finite violations of unitarity'' [4].

In order to understand the origin of the difficulties which have hindered previous work on this question, it is necessary to recall how the usual unitary evolution of quantum matter in a given four-geometry is recovered from the WDW equation. This has already been thoroughly investigated [3–14] and it is now well understood that *if* the wave function is in a tight wave packet, i.e. if the spread of matter energy is small, and *if* gravity can be treated semiclassically, i.e. if it can be described by a WKB wave function, then one should factor out this WKB wave and interpret the remainder as the wave function of matter which evolves according to the Schrödinger equation.

Therefore, when investigating the problem of unitary violations, two problems must be confronted. The first one is technical and concerns the precise mathematical characterization of the corrections to the Schrödinger equation which are due to the abandonment of the two restrictions. In this respect, it should be mentioned that most approaches have kept as starting point (i.e. as an ansatz) that the total wave function can be factorized into a gravitational wave characterizing the background and the rest which is still interpreted as the matter wave function. It is then very difficult to distinguish the intrinsic corrections from the those due to this factorization ansatz.

The second aspect is more fundamental and has to do with the interpretation of the wave function of the universe $\Psi(a,\phi)$, solution of the WDW equation (a designates the scale factor and ϕ matter variables in a minisuperspace context). In particular, in order to address the question of possible violations of unitarity, one must know how to extract the wave function of matter when matter is not in a tight wave packet. Several proposals have been made in the literature; see [8] for a review. Two of the most specific are the conditional probability interpretation wherein the probability to find ϕ at a is given by $|\Psi(a,\phi)|^2/\int d\phi|\Psi(a,\phi)|^2$ and the Vilenkin [4] interpretation which is based on the current carried by $\Psi(a,\phi)$.

In this paper, by exploiting the generalized adiabatic treatment of [14], we circumvent the difficulties which have hindered previous work. The major advantage of this treatment is to organize the WDW equation in such a way that the corrections to the two approximations can be separately and systematically analyzed before adopting any interpretation scheme. We then focus on the possibility of unitary violations in the light of the mathematical properties of these corrections. Our analysis will be restricted to minisuperspace models. In a subsequent paper, we intend to extend it to cosmologies characterized by many variables.

The first important conclusion of this work (which generalizes that of [13]) is that when matter is not in a tight wave packet but in the absence of backscattering between waves with positive and negative gravitational momentum (which correspond to contracting and expanding universes), the only consistent interpretation is that based on the current. From our analysis, it will also be clear why when matter is in a tight wave packet, i.e. when both approximations mentioned before are exact, different interpretations, such as the probability or the current interpretations, become equivalent.

The second point of this article is to analyze the importance of the effects induced by backscattering of gravitational waves. We show that because of destructive interference, the amplitude for a forward wave to backscatter is proportional to $\exp(-\partial_a p/p^2)$ where p is the momentum of a. This is much smaller than previous estimates that suggested that the amplitudes were proportional to the quantity $\partial_a p/p^2$ itself.

The third main conclusion concerns the consequences for matter evolution of the couplings induced by backscattering. We show that even though these transition amplitudes can be precisely evaluated, it is impossible to deduce what are exactly their physical consequences. That is, quantum cosmology is an incomplete theory that does not carry its own interpretation. Happily this incompleteness only manifests itself at the level of backscattering and therefore concerns exponentially small effects.

To reach these conclusions we address successively the mathematical and interpretational aspects. In the first part of the article (Secs. II–V), we carry out an analysis of the WDW equation which does not make the ansatz that matter should be in a tight wave packet. Dropping this ansatz has already been advocated in [10–13]. Here we shall follow the treatment of [14] (see also the earlier work of [15]) which does not require the validity of the WKB approximation. Thus it can be used to obtain quantitative estimates for both amplitudes to backscatter and effects of widely spread wave functions. From this treatment one unambiguously establishes the following:

(i) When backscattering amplitudes can be neglected and matter is in a tight wave packet, matter obeys the Schrödinger equation in the background defined by the center of the wave packet, thereby recovering the situation of Refs. [6,4,3].

(ii) When matter is no longer in a tight wave packet, but backscattering amplitudes are still neglected, matter obeys a Schrödinger-like equation wherein evolution is parametrized by a and wherein gravitational back reaction effects are included at the quantum level, i.e. not only in the mean. Unitarity follows from the ordered nature of the WKB propagation of a.

(iii) When backscattering amplitudes are not neglected, matter evolution is drastically modified in the sense that matter states associated with forward and backward propagating universes interact. This directly follows from the second order character of the WDW equation in ∂_a.

These results follow from the separation of the length scales which govern the dynamics in quantum cosmology when the universe is macroscopic. The Compton wavelength of a, $1/p$, is much smaller than both the Compton wavelength of a typical matter degree of freedom and than the time over which the geometry changes $(\partial_a p/p)^{-1}$.

In the second part of this article (Secs. VI–XI) we address the problem of interpretation. As basis for the discussion, we consider two physical examples whose mathematical description is similar to the WDW equation. These examples are electronic nonadiabatic transitions during atomic collisions and pair creation in an external potential. The manner in which the wave functions should be interpreted in these examples is standard textbook material. Nevertheless, it is very instructive to delve in detail into the mathematical and physical bases of these interpretations in order to see if they apply to quantum cosmology.

In both cases the conserved current serves as a basis for extracting predictions from the theory. The basic mathematical reason is that this is the only quantity which is conserved by virtue of the equations of motion. In cosmology, in the absence of backscattering, this procedure leads unambiguously to the current interpretation. In this derivation, the existence of well-separated length scales plays also a crucial role: It provides the possibility of asking questions concerning light degrees of freedom under the condition that the heavy one is propagating forward and located in a small neighborhood.

The other important point is that when backscattering between the forward and backward propagating waves occurs, an *additional* principle is required in order to interpret backscattering amplitudes. Moreover, this principle differs for the two examples. In each case, it is dictated by the possibility of coupling the system to a quantum external device which can act as a measuring device. In quantum cosmology, no such external quantum device can be introduced, and it is therefore impossible to decide which of these two interpretations, or possibly a completely different third one, applies to the WDW equation. Hopefully the resolution of this problem can ultimately be obtained from a deeper understanding of the inner (i.e. ultraviolet) structure of quantum gravity.

II. BACKSCATTERING

In view of the importance of backscattering effects in the problem of unitarity violation in quantum cosmology, it is appropriate to understand clearly why backscattering occurs and how to compute backscattering amplitudes. To this end, we first consider the simple problem of a universe in which matter stays in a given eigenstate $|n\rangle$ of constant energy E_n. This enables us to study the corrections to the WKB approximation unencumbered by the details of matter evolution.

This analysis will serve as a guide to the next section wherein the matter Hamiltonian no longer commutes with the WDW equation.

With this mathematical simplification, the WDW equation in minisuperspace reduces to one degree of freedom moving in a potential

$$H_T\Psi=[G^2\partial_a^2+V(a)+2aGE_n]\Psi=0 \tag{1}$$

where G is Newton's constant. The gravitational potential $V(a)$ comes from the curvature of space (for instance, $V=-a^2+\Lambda a^4$ in a closed universe with a cosmological constant Λ).

The WKB solutions to Eq. (1) with unit Wronskian are

$$\chi_n(a)=\frac{\exp\left[-i\int^a da'p_n(a')\right]}{\sqrt{2p_n}} \tag{2}$$

and its complex conjugate, where $p_n(a)=(1/G)\sqrt{V(a)+2aGE_n}$ is the classical solution of $H_T=0$ when matter has energy E_n. These solutions correspond to expanding and contracting universes.

This identification relies on a sign convention which we now explain. First one expands (as usual when building wave packets) the phase in Eq. (2) around a reference energy $\bar{E}$ to obtain

$$\chi_n(a)\simeq\frac{\exp\left[-i\int^a da'\bar{p}_n(a')\right]}{\sqrt{2p_n}}\times\exp\left(-i\int^a da'\frac{\partial p}{\partial E}(E_n-\bar{E})\right). \tag{3}$$

Classical mechanics tells us that $\partial p/\partial E|_{E=\bar{E}}=\pm d\bar{t}/da$ where $\bar{t}(a)$ is the proper time obtained from the classical trajectory of a driven by the reference matter energy $\bar{E}$. The $\pm$ sign corresponds to expanding and contracting universes respectively. Thus we obtain

$$\chi_n(a)\simeq\frac{\exp\left[-i\int^a da'\bar{p}_n(a')\right]}{\sqrt{2p_n}}e^{\mp i\bar{t}(a)(E_n-\bar{E})}. \tag{4}$$

If one adopts the usual convention that the phase dependence on energy and time should be e^{-iE_nt}, then one must take the $-$ sign in Eq. (4). Hence χ_n corresponds to an expanding universe and χ_n^* to a contracting universe. Obviously this choice is purely conventional and has nothing intrinsic to it. The problem of defining an intrinsic arrow of time in quantum cosmology is a delicate one, and we shall briefly return to it at the end of this paper.

There are two kinds of corrections to the WKB solutions. The first are corrections to the phase and norm of χ_n and χ_n^* separately. They are obtained by a standard calculation in which one writes $\Psi=Ae^{iS/\hbar}$, inserts this ansatz into Eq. (1) and calculates A and S as series in $\hbar$; see for instance [16]. The second kind of corrections are due to the couplings between the forward and the backward solution. They describe the backscattering amplitudes engendered by the a dependent effective potential $V_n(a)=V(a)+2aGE_n$.

We are interested in the second corrections since, as we shall later see, these are the relevant ones for the problem of unitarity violations. To analyze them we rewrite Ψ as

$$\Psi=\mathcal{C}_n(a)\chi_n(a)+\mathcal{D}_n(a)\chi_n^*(a), \tag{5}$$

$$\partial_a\Psi=ip_n(a)[\mathcal{C}_n(a)\chi_n(a)-\mathcal{D}_n(a)\chi_n^*(a)]. \tag{6}$$

The coefficients $\mathcal{C}_n$ and $\mathcal{D}_n$ are uniquely determined by these equations [17] and the conserved current (Wronskian) takes the simple form

$$\Psi^*i\overleftrightarrow{\partial}_a\Psi=|\mathcal{C}_n(a)|^2-|\mathcal{D}_n(a)|^2=\text{const}. \tag{7}$$

Differentiating Eq. (5) and comparing with Eq. (6) yields

$$\partial_a\mathcal{C}_n\chi_n(a)+\partial_a\mathcal{D}_n\chi_n^*(a)-\frac{\partial_a p_n}{2p_n}[\mathcal{C}_n(a)\chi_n(a)+\mathcal{D}_n(a)\chi_n^*(a)]=0. \tag{8}$$

Inserting Eq. (6) into Eq. (1) and using Eq. (8) yields first order coupled equations

$$\partial_a\mathcal{C}_n=\frac{\mathcal{D}_n}{2}\frac{\partial_a p_n}{p_n}\exp\left(-2i\int^a da\,p_n\right),$$

$$\partial_a\mathcal{D}_n=\frac{\mathcal{C}_n}{2}\frac{\partial_a p_n}{p_n}\exp\left(+2i\int^a da\,p_n\right) \tag{9}$$

which are equivalent to the original WDW equation (1).

From Eq. (9) one reads that the instantaneous coupling between the forward and backward propagating waves is proportional to $\partial_a \ln p_n$ times an oscillating phase. Thus, naively, one would think that backscattering effects are of order $\partial_a \ln p_n$. However, when the effective potential $V_n(a)$ is slowly varying (i.e. in the WKB limit $\partial_a p_n/p_n^2\ll 1$) this is incorrect because successively backscattered waves destructively interfere. This destruction is so effective that the backscattering amplitude is exponentially small.

To establish this, suppose that there are two asymptotic regions, $a<a_-$ and $a>a_+$ wherein $V_n=\text{const}$ and hence the WKB approximation is exact. Let us consider the solution which initially contains no backward propagating wave: $\mathcal{D}_n(a<a_-)=0$ and $\mathcal{C}_n(a<a_-)=1$. The backscattering amplitude is then $\mathcal{D}_n(a>a_+)$. It can be calculated perturbatively by taking $\mathcal{C}_n=1$ in Eq. (9) (for a more rigorous justification of this result see [18,16]):

$$B_n=\mathcal{D}_n(\infty)\simeq\int da\frac{1}{2}\frac{\partial_a p_n}{p_n}\exp\left(+2i\int^a da'\,p_n(a')\right)$$
$$\simeq\exp\left(2i\int^{a^*}da'\,p_n(a')\right). \tag{10}$$

The second approximation follows from the fact that in the WKB limit, the integral is dominated by the (complex) saddle point a^* where $p(a^*)=0$. For instance when $V_n(a)$ has a minimum at $a=a_0$: $V_n(a)=v_n+(V_n''/2)(a-a_0)^2+O((a-a_0)^3)$, the saddle is located at $a^*\simeq a_0 \pm i\sqrt{2v_n/V_n''}$ and the backscattering amplitude is $\mathcal{D}_n(+\infty)\simeq e^{-\pi v_n/2G\sqrt{V_n''}}$ upon neglecting cubic and higher order terms in $a-a_0$. The lessons from this exercise are the following:

(i) The naive estimate of the backscattering amplitude is incorrect. A more detailed analysis shows that it is exponentially small.

(ii) If the kinetic energy of gravity ($=V_n(a)/G^2$) has a minimum at a_0, then the backscattering arises from a region of width $\Delta a=[(1/p_n)\partial_a^2 p_n]^{-1/2}$ around the minimum.

However, when the effective potential $V_n(a)$ does not have adequate asymptotic regions, it is impossible to isolate unambiguously a backscattering amplitude. Indeed, since the WKB approximation is no longer asymptotically exact, one needs an additional principle to distinguish backward from forward classical motion. This situation generally arises in cosmology. For instance, for a de Sitter universe, $V(a)=-a^2+\Lambda a^4$ and backscattering around any $a\gg\Lambda^{-1/2}$ far from the turning point results from interference over a distance $\Delta a\simeq a$. So it is impossible to isolate the backscattering around a from the effects due to the turning point at $\Lambda^{-1/2}$. A similar situation obtains for a matter dominated universe $V_n(a)=-a^2+2aGE_n$: one cannot isolate the backscattering around a given a from the contribution of the origin $a=0$ and the turning point $a=2GE_n$. In these cases, effects at the turning points (for instance boundary conditions at $a=0$ or $a=\infty$) might dominate any backscattering which occurs in intermediate regions.

III. WHEELER-DeWITT EQUATION IN MINISUPERSPACE

We now generalize the previous analysis to the case when the matter Hamiltonian is not constant. Our aim is to find the equivalent of Eqs. (9) so as to be able to reveal the interplay between matter transitions and backscattering effects. We thus consider

$$[G^2\partial_a^2+V(a)+2aG\hat{H}_M(\pi,\phi,a)]|\Psi(a)\rangle=0 \qquad (11)$$

where $\hat{H}_M$ is the matter Hamiltonian operator. It depends on the matter coordinates ϕ, and their conjugate momenta π and a. Notice that the wave function $|\Psi(a)\rangle$ is expressed as a ket only for the matter degrees of freedom.

Our analysis of the solutions of Eq. (11) is based on a double hypothesis. First we require that the universe be macroscopic. This condition is satisfied if the radius of the universe is larger then the Planck length and if the total matter energy $\langle H_M\rangle$ is larger than the Planck mass. This condition guarantees that the propagation of a is WKB, i.e. $d\ln p/da \ll p$. Second, we require that no individual matter quantum dominate the kinetic energy of gravity. That is we do not consider the case of an inflaton field whose expectation value $\langle\phi\rangle$ is macroscopic. Instead we are considering usual field configurations such that $\langle\phi\rangle\simeq 0$ but with $\langle H_M\rangle\neq 0$ and macroscopic.

This second condition breaks the otherwise existing symmetry between the radius of the universe a and the matter degrees of freedom. It ensures that a is the heaviest and is therefore singled out to parametrize the *transitions* among neighboring matter states.

We therefore postulate a neat separation of length scales: the Compton wavelength $1/p$ of the universe is much smaller than both distance over which the momentum of gravity changes $(d\ln p/da)^{-1}$ (i.e. approximately the Hubble radius) and $1/(E_n-E_m)$, the time scale associated with a typical matter transition. We emphasize however that our treatment is exact. That is, we do not neglect corrections; we simply postulate that they are small.

Since the matter transitions are the lightest, they should be treated quantum mechanically. This is implemented by making an adiabatic expansion for the matter states, following [14,15]. On the other hand the radius of the universe is the heaviest degree of freedom, and satisfies the WKB condition; hence we shall make a WKB expansion for the gravitational waves. This double expansion is the basic tool we use to analyze Eq. (11).

The adiabatic expansion for matter is realized by making the instantaneous (i.e. at fixed a) diagonalization of the matter Hamiltonian

$$\hat{H}_M(a)|\psi_n(a)\rangle=E_n(a)|\psi_n(a)\rangle,$$
$$\langle\psi_m(a)|\psi_n(a)\rangle=\delta_{m,n}. \qquad (12)$$

We combine this with the WKB expansion in the following way. Let p_n be the classical momentum if matter has energy $E_n(a)$:

$$-G^2p_n^2(a)+V(a)+2aGE_n(a)=0. \qquad (13)$$

Then we generalize Eqs. (5), (6) and decompose $|\Psi\rangle$ as

$$|\Psi(a)\rangle=\sum_n\left[\mathcal{C}_n(a)\frac{\exp\left[-i\int^a p_n(a')da'\right]}{\sqrt{2p_n(a)}}+\mathcal{D}_n(a)\frac{\exp\left[+i\int^a p_n(a')da'\right]}{\sqrt{2p_n(a)}}\right]|\psi_n(a)\rangle, \qquad (14)$$

$$\partial_a|\Psi(a)\rangle=\sum_n -ip_n(a)\left[\mathcal{C}_n(a)\frac{\exp\left[-i\int^a p_n(a')da'\right]}{\sqrt{2p_n(a)}}-\mathcal{D}_n(a)\frac{\exp\left[+i\int^a p_n(a')da'\right]}{\sqrt{2p_n(a)}}\right]|\psi_n(a)\rangle. \qquad (15)$$

These equations univocally define the $\mathcal{C}_n$ and $\mathcal{D}_n$ coefficients and ensure that these coeficients are constant in the limit wherein both the WKB approximation and the adiabatic approximation are exact. Moreover, using these expressions, the conserved current yields the simple expression

$$\langle\Psi|i\overleftrightarrow{\partial}_a|\Psi\rangle=\sum_n |\mathcal{C}_n(a)|^2-|\mathcal{D}_n(a)|^2=\text{const.} \tag{16}$$

Taking the derivative of Eq. (14) and comparing with Eq. (15) yields a relation between $\mathcal{C}_n$, $\mathcal{D}_n$ and their derivatives which generalizes Eq. (8). Then inserting Eq. (15) into the WDW equation (11) and using this relation gives

$$\begin{aligned}\partial_a\mathcal{C}_n=&\sum_{m\neq n}\langle\partial_a\psi_m|\psi_n\rangle\frac{p_n+p_m}{2\sqrt{p_np_m}}\exp\left(i\int^a(p_n-p_m)da'\right)\mathcal{C}_m\\&+\frac{\partial_ap_n}{2p_n}\exp\left(2i\int^a p_n da\right)\mathcal{D}_n\\&+\sum_m\langle\partial_a\psi_m|\psi_n\rangle\frac{p_n-p_m}{2\sqrt{p_np_m}}\exp\left(i\int^a(p_n+p_m)da'\right)\mathcal{D}_m\end{aligned} \tag{17}$$

and the same equation with $\mathcal{C}_n\leftrightarrow\mathcal{D}_n$, $i\leftrightarrow -i$. These equations are *equivalent* to the original WDW equation. The essential advantage of this rewriting is that it neatly separates the backscattering effects encoded in the last two terms from the matter transitions in the forward sector which are described by the first term. As an important consequence, it enables the WKB approximation to be implemented without factorizing, as usually done in former analyses, a gravitational wave common to all matter states, i.e. without being obliged to make the hypothesis that matter is in a tight wave packet in energy.

IV. UNITARY EVOLUTION

When the WKB condition $\partial_a p/p^2\ll 1$ is fulfilled, there is no backscattering and one can correctly neglect the coupling between the forward and backward propagating waves. One thus obtains two uncoupled evolutions for forward and backward propagating universes. The equation governing the forward sector is

$$\partial_a\mathcal{C}_n=\sum_{m\neq n}\langle\partial_a\psi_m|\psi_n\rangle\frac{p_n+p_m}{2\sqrt{p_np_m}}\exp\left(i\int^a(p_n-p_m)da\right)\mathcal{C}_m. \tag{18}$$

This equation has two nice properties [14]. First it describes the unitary evolution[1] of matter as a function of a and second it includes gravitational backreaction effects at the quantum level, i.e. not only in the mean.

Unitarity directly follows from the fact that the right hand side (RHS) of Eq. (18) is antisymmetric. This can also be deduced from Eq. (16) and the fact that the coefficients $\mathcal{C}_n(a)$ and $\mathcal{D}_n(a)$ evolve independently. To see more explicitly how this Schrödinger character is obtained, we define two effective matter wave functions associated respectively with the expanding and contracting sectors:

$$\begin{aligned}|\phi^+_{eff}(a)\rangle=&\sum_n\frac{\exp\left(-i\int^a p_n da'\right)}{\sqrt{2p_n}}|\psi_n\rangle\\&\times\langle\psi_n|\left[\exp\left(i\int^a p_n da'\right)i\overleftrightarrow{\partial}_a|\Psi(a)\rangle\right]\\=&\sum_n\mathcal{C}_n(a)\exp\left(-i\int^a p_n da'\right)|\psi_n(a)\rangle,\\|\phi^-_{eff}(a)\rangle=&\sum_n\mathcal{D}_n(a)\exp\left(+i\int^a p_n da'\right)|\psi_n(a)\rangle.\end{aligned} \tag{19}$$

They obey Schrödinger type equations

$$\pm i\partial_a|\phi^\pm_{eff}\rangle=\hat{H}_{eff}(a)|\phi^\pm_{eff}\rangle \tag{20}$$

where the Hermitian operator $\hat{H}_{eff}$ plays the role of Hamiltonian. It is defined by its instantaneous diagonalization in the basis $|\psi_n(a)\rangle$:

$$\hat{H}_{eff}(a)_{nm}=\delta_{nm}p_n(a)+i\langle\partial_a\psi_m|\psi_n\rangle\frac{(\sqrt{p_n}-\sqrt{p_m})^2}{2\sqrt{p_np_m}}. \tag{21}$$

The peculiar form of the second term arises from the interplay between the RHS of Eq. (18) and the derivatives acting on the $|\psi_n(a)\rangle$ in the left-hand side (LHS) of Eq. (20).[2]

Thus, in the absence of backscattering, $\phi^\pm_{eff}$ have the following properties:

(i) ϕ^+_{eff} is decoupled from ϕ^-_{eff}.

(ii) $\phi^\pm_{eff}$ are local in the sense that they depend only on $|\Psi(a)\rangle$ and $\partial_a|\Psi(a)\rangle$ at a.

(iii) $\phi^\pm_{eff}$ obey a linear equation, since they depend linearly on the original ket $|\Psi(a)\rangle$. Thus they still obey the superposition principle.

(iv) Their norm is constant since $H_{eff}(a)$ is Hermitian:

$$\begin{aligned}\langle\phi^+_{eff}(a)|\phi^+_{eff}(a)\rangle=&\sum_n|\langle\psi_n(a)|\phi^+_{eff}\rangle|^2=\sum_n|\mathcal{C}_n(a)|^2\\=&\text{const.}\end{aligned} \tag{22}$$

[1]Some authors [19] have advocated that the WDW equation should be replaced by a first order equation in ∂_a so as to eliminate backscattering and guarantee unitarity. In our setting, this would correspond to postulating that Eq. (18) is the ''correct'' equation governing quantum cosmology.

[2]Equation (21) corrects an error in [14].

(v) If one works with wave packets tightly centered around a mean energy $\overline{E}$, $\phi^{\pm}_{eff}$ obey the time dependent Schrödinger equation $i\partial_{\overline{t}}\phi^{\pm}_{eff}=\hat{H}_M(\overline{a}_{\pm})\phi^{\pm}_{eff}$ where $H_M(\overline{a}_{\pm}(t))$ is the matter Hamiltonian of Eqs. (11),(12) with $\overline{a}_{\pm}(t)$ describing respectively the classical expansion or contraction of the universe driven by $\overline{E}$. To see this, as in Eqs. (3), (4), it suffices to develop the state dependent functions $p_n(a)$ around the mean value $\overline{p}(a)$. To first order in $E_n-\overline{E}$, the second term of Eq. (21) vanishes and the first one gives

$$\hat{H}_{eff}(a)_{nm}\simeq\delta_{nm}\{(\overline{p}(a)+\partial_E\overline{p}(a)(E_n-\overline{E})\}. \tag{23}$$

Up to a term proportional to the identity $[=\delta_{nm}\{\overline{p}(a)-\partial_E\overline{p}(a)\overline{E}\}]$ which plays no physical role, this diagonal matrix is identical to that defined by the matter Hamiltonian [see Eq. (12)], since the overall factor $\partial_E\overline{p}(a)=\pm d\overline{a}_{\pm}/dt$ is precisely what is needed to convert ∂_a in $\partial_{\overline{t}}$ in Eq. (20).

(vi) When one drops the tight wave packet approximation, H_{eff}, defined in Eq. (21), includes gravitational back reaction effects to the matter propagation which depend on n. These are encoded in the nontrivial dependence of $p_n(a)$ on E_n and in the second term on the right hand side. Then, matter evolution must be parametrized by a since it is meaningless to call upon a mean time parameter.

In conclusion, we claim that $\phi^{\pm}_{eff}$ defined in Eq. (19) are the unique functions of Ψ which have these properties. The only ambiguity lies in the definition of the WKB approximation since one could modify p_n in Eq. (19) by local terms of order $p_n[1+O(d\ln p_n/da)]$ without modifying these properties. This ambiguity reflects the choice of normal ordering of the operator ∂_a^2 in Eq. (11). However, these modifications are negligible in the WKB regime.

Before discussing the role of backscattering effects, we wish to recall that Eq. (18) is a convenient expression when matter evolves quasiadiabatically, that is when the distance scale over which matter makes transitions, given by $[d\ln(E_n-E_m)/da]^{-1}$, is large compared to the wavelength $(E_n-E_m)^{-1}$. In this case one can easily calculate the nonadiabatic transition amplitude $A_{m\to n}$ from $|\psi_m\rangle$ to $|\psi_n\rangle$. Moreover, it proceeds along lines very similar to the computation of the backscattering amplitude $\mathcal{D}_n$ in Eq. (10). Indeed, one first neglects transitions and sets $\mathcal{C}_n=\delta_{mn}$ for all values of a. Then one inserts this zeroth order solution in Eq. (18) and integrates over a to obtain

$$\begin{aligned}A_{m\to n}&=\mathcal{C}_n(a=+\infty)\\&\simeq\int da\langle\partial_a\psi_m|\psi_n\rangle\frac{p_n+p_m}{2\sqrt{p_np_m}}\exp\left(i\int^a(p_n-p_m)da\right)\\&\simeq\exp\left(i\int^{\tilde{a}}da'(p_n(a')-p_m(a')]\right).\end{aligned} \tag{24}$$

In the second line, as in Eq. (10), we have evaluated the integral by saddle point. The saddle is now at the complex value $\tilde{a}$ solution of $p_n(\tilde{a})=p_m(\tilde{a})$.

Since $a(E_n-E_m)$ is much smaller than Gp_n^2 (by virtue of the hierarchy of length scales discussed above), one can expand p_n-p_m in powers of E_n-E_m. Keeping only the first term in this series, one finds that the transition is given by the usual expression controlled by the imaginary time to reach the saddle point times the difference of energy of the matter states; see [14] for further discussion of matter transitions in quantum cosmology.

V. CONSEQUENCES OF BACKSCATTERING

To determine the range of validity of the truncated equation (18), one must compute the importance of the effects induced by backscattering. These effects arise when one abandons the WKB approximation. In this respect, it should be stressed that there are two types of corrections to this approximation: local ones which can be evaluated by expanding the wave function as a series in $\hbar$ [16] and global ones which mix forward and backward waves. Only the latter lead to drastic modifications of matter evolution. Thus, one should differentiate ''in the WKB approximation'' from ''in the absence of backscattering.'' Our computation of backscattering amplitudes shall be based on Eq. (17) and shall proceed as in Eqs. (24) and (10).

Our first conclusion is that these amplitudes are exponentially small, whether or not matter dynamics are neglected. The new feature with respect to Sec. II is that in Eq. (17) there are now coupling terms between $\mathcal{C}_n$ and all $\mathcal{D}_m$. This leads to the fact that the relative amplitude to backscatter into different states is approximately thermal, with the inverse temperature given by the twice the imaginary time needed to reach the saddle point. These backscattering transitions modify in a fundamental way the structure of the evolution of the coeficients $\mathcal{C}_n$ since the evolution no longer closes onto itself. This implies two unusual features: first, an initially purely forward wave packet will inevitably leak out into the backward sector and, second, knowledge of the initial values of the $\mathcal{D}_n$ is necessary to determine the evolution of the $\mathcal{C}_n$.

Let us first analyze the backscattering without a change of the matter state. The second term of Eq. (17) has exactly the same form as the term studied in Sec. II. Thus it can be analyzed in the same way: let us suppose that the effective potential $V_n(a)=V(a)+2aGE_n(a)$ has a minimum at a_n and that we can approximate $G^2p_n^2=V_n(a)\simeq V_n(a_n)+(V_n''/2)(a-a_n)^2$. Then, if the universe is purely forward propagating in state n for $a\ll a_n$, that is $\mathcal{C}_m(a\ll a_n)=\delta_{nm}$ and $\mathcal{D}_m(a\ll a_n)=0$, the amplitude to backscatter into matter state n is $\mathcal{D}_n(a\gg a_n)$. As in Sec. II this amplitude can be perturbatively calculated by the saddle point technique. The saddle is the solution of $p_n(a_n^*)=0$ and it is located at $a_n^*\simeq a_n+i\sqrt{2V_n(a_n)/V_n''}$. Upon neglecting higher order derivatives of $V_n(a)$, the amplitude to backscatter is

$$\begin{aligned}B_{n\to n}=\mathcal{D}_n(a\gg a_n)&\simeq\exp\left(-\frac{\pi V_n(a_n)}{G\sqrt{2V_n''}}\right)\\&=\exp\left(-\frac{\pi}{2}p_n(a_n)\mathrm{Im}(a_n^*)\right).\end{aligned} \tag{25}$$

The quantity which appears exponentiated is the ratio of the distance over which $V_n(a)$ changes $[=\mathrm{Im}(a_n^*)]$ to the wavelength of the universe $(=1/p_n)$. It is the ratio of the longest length scale in the universe to the shortest. Therefore, $p_n(a_n)\mathrm{Im}(a_n^*)\gg[p_n(\tilde{a})-p_m(\tilde{a})]\mathrm{Im}(\tilde{a})$ [cf. Eq. (24)], since the second expression is controlled by the *difference* p_n-p_m. Thus $B_{n\to n}$ is exponentially smaller than $A_{n\to m}$. It is this latter inequality which determines the validity of the first order equation (18).

The backscattering with change of matter state is mediated by the last term in Eq. (17). It can be evaluated in the same way and is given by

$$B_{n\to m}\simeq\int_0^\infty da\langle\partial_a\psi_m|\psi_n\rangle\frac{p_n-p_m}{2\sqrt{p_np_m}}\times\exp\left(+i\int^a da'[p_n(a')+p_m(a')]\right)\simeq\exp\left(i\int^{a^*}da'[p_n(a')+p_m(a')]\right)\qquad(26)$$

where a^* is the saddle point solution of $p_n(a^*)+p_m(a^*)=0$. To evaluate this saddle point integral, we define the mean energy $\overline{E}(a)=(E_n+E_m)/2$ and expand the integrand to first order in $E_n(a)-E_m(a)$: $p_n(a')+p_m(a')=2\overline{p}(a')+(E_n-E_m)\partial_E\overline{p}$. This yields

$$|B_{n\to m}|^2\simeq\exp\left[-4\,\mathrm{Im}\left(\int^{a^*}da'\overline{p}(a')\right)\right]\times\exp\left(-2\int_0^{\mathrm{Im}\,T^*}dt(E_n-E_m)\right)\qquad(27)$$

where $T^*=\int^{a^*}da'\,\partial_E\overline{p}$ is the time to reach the saddle point in the mean geometry. Thus the relative distribution of the backscattered states is approximately thermal with the extremely low temperature given by $(2\,\mathrm{Im}\,T^*)^{-1}$.

In the above we have neglected the fact that backscattering can take place in several steps. For instance one can first backscatter from matter state $\mathcal{C}_m$ to matter state $\mathcal{D}_{n'}$ and then change matter state from $\mathcal{D}_{n'}$ to $\mathcal{D}_n$. Such multistep transitions can compete with the direct transition. Determining which channel is dominant is a difficult task (see for instance [20]). Nevertheless, a rough calculation of these multistep backscatterings shows that the result based on the direct channel gives a correct estimate: the amplitude to backscatter is an exponentially small quantity governed by the total momentum p_n and the backscattered states are approximately thermally distributed.

Note that if the (unusual) sign of the kinetic term of gravity were positive instead of negative, then the opposite would be true and backscattering to states with higher matter energy would be favored. Mathematically this change comes about because $\partial_E p$ would have the opposite sign.

VI. INTERPRETATION: INTRODUCTION

The literature on quantum cosmology abounds with interpretations of the wave function of the universe, Ψ. This reflects contradictory views that are held on what the wave function should describe and what it should predict. However, the question of interpretation is, to a large extent, determined by mathematical and physical consistency.

In order to develop a coherent interpretation we shall first consider simple physical systems—electronic nonadiabaticity in atomic or molecular collisions and particle creation in external fields—whose mathematical formulation is extremely close to the WDW equation in minisuperspace models. For these systems the interpretations, i.e. the procedures that must be used to extract predictions from the theory, are known. They can thus serve as guides to suggest the interpretation in quantum cosmology but also as laboratories to formulate the restricted set of questions that we, living in the universe, can ask in quantum cosmology. We then return to the WDW equation and compare different interpretations of Ψ that have been proposed in the literature.

The first conclusion of this investigation is that, upon neglecting backscattering, the current interpretation of Vilenkin appears to be singled out as the only consistent one. Indeed, it leads to probability amplitudes which satisfy the usual properties of quantum amplitudes: the superposition principle and decoherence of remote configurations are both guaranteed. This is not the case if one adopts the conditional probability interpretation. This interpretation instead does make sense for systems on which localized external devices can interact. Therefore it is inoperative in quantum cosmology since no such external system can be introduced.

The second point concerns the physical interpretation of backscattering for the two examples. In each case, an additional principle, also based on the possibility of coupling the system to an external device, is required to reach the correct interpretation. In cosmology, no such principle is available and therefore the interpretation of backscattering remains ambiguous. For instance whether or not one should ‘‘third quantize’’ and attribute some statistic to Ψ would modify the physical consequences of the backscattering amplitudes.

VII. ELECTRONIC NONADIABATICITY IN ATOMIC COLLISIONS

Let us begin by considering the problem of two colliding atoms. After factoring the center of mass coordinate and the total angular momentum, the residual Hamiltonian looks like

$$H_{atom}=\frac{P^2}{2M}+V(R)+H_{el}(R,q_i,p_i)\qquad(28)$$

where R is the relative distance between the two nuclei, P the momentum conjugate to R, and q_i,p_i the electronic coordinates. If we consider an energy eigenstate of this Hamiltonian,

$$\left[-\frac{\partial_R^2}{2M}+V(R)+\hat{H}_{el}(q_i,p_i,R)\right]|\Psi_E(R)\rangle=E|\Psi_E(R)\rangle,\qquad(29)$$

it has exactly the same structure as the WDW equation in minisuperspace; see Eq. (11). Indeed in both cases there is a heavy degree of freedom (the scale factor a or the nuclear coordinate R) and light degrees of freedom (the matter ϕ or the electrons q_i). Because of this similarity, the same techniques can be applied to both equations.

The simplest approximation consists in treating the coordinate R classically as a given function of time: $R(t)$. Then the residual degrees of freedom, the electrons, propagate according to the time dependent equation $i\partial_t|\psi_{el}\rangle = \hat{H}_{el}(R(t),q,p)|\psi_{el}\rangle$ and the nonadiabatic dynamics are encoded in the transition amplitudes from one instantaneous eigenstate to another one (Landau-Zener effect).

If these transitions are too energetic or the motion of R is governed by a too spread out wave packet, the background field approximation is no longer correct. Then one must solve Eq. (29) and the techniques discussed in Sec. III should be brought to bear [15]. Upon neglecting backscattering effects but taking recoil effects into account, one obtains a second regime in which the dynamics is governed by the equivalent of Eq. (20): Schrödinger like equations for the electrons in terms of the amplitudes $\mathcal{C}_n(R)$ and $\mathcal{D}_n(R)$ associated respectively with forward and backward WKB waves governing the inward and outward motion of R. In these equations, unitarity is respected for the $\mathcal{C}_n$ and $\mathcal{D}_n$ amplitudes separately and the role of time is played by the heavy coordinate R. When backscattering effects in R cannot be neglected, these effective Schrödinger equations are no longer valid and one obtains the third situation wherein one must solve the full equations for coupled $\mathcal{C}_n,\mathcal{D}_n$ system, the equivalent of Eq. (17).

The sole difference between the atomic problem and the WDW equation in minisuperspace is the sign of the kinetic energy of the heavy nuclei which is positive whereas that of a is negative. This difference only plays a role in the third situation wherein it affects the identification of in and out modes and the spectrum of backscattered states; see the remark at the end of Sec. V. As far as the light degrees of freedom are concerned, the second regimes in atomic physics and in cosmology are completely analogous.

For this reason it is very instructive to review the interpretation of the solutions of Eq. (29). Indeed, the aspects which are often glossed over in textbooks are precisely the ones needed for the interpretation of quantum cosmology. In particular, we shall discuss two compatible but nevertheless different schemes of interpretation. In the first, one restricts the analysis to asymptotic amplitudes to find the system in a given state. In the second scheme, it is the wave function itself which is interpreted at all times. Upon investigating the relationship between these schemes, the separation of the length scales governing electrons and nuclei will again play a crucial role.

The first interpretation, proposed by Born [21], concerns scattering amplitudes. In the present case as well, Eq. (29) describes a scattering event and the main question one wants to answer (and to compare to experimental data) is how the amplitude of finding a certain final state depends on the initial state of the atom. Let us therefore suppose that the atoms are initially in their ground state and approaching each other, i.e. $\mathcal{C}_n(R=+\infty)=\delta_{n0}$. According to Born, the probability for the atoms to end up in state n is $|\mathcal{D}_n(R=+\infty)|^2$. The mathematical basis for this identification is the conservation of the Wronskian $\int dq_i \Psi_E^* i\overleftrightarrow{\partial}_R \Psi_E$. Indeed, since the nuclei repel each other, the region $R<0$ is inaccessible and one must impose $\Psi_E(R=0)=0$. Hence the Wronskian vanishes everywhere (since it vanishes at $R=0$). Therefore, if one expands Ψ_E in terms of forward and backward coefficients $\mathcal{C}_n$ and $\mathcal{D}_n$ as in Sec. III, the vanishing of the Wronskian implies that $\Sigma_n|\mathcal{C}_n(R)|^2=\Sigma_n|\mathcal{D}_n(R)|^2$. In particular, if $\Sigma_n|\mathcal{C}_n(R=+\infty)|^2=1$, then $\Sigma_n|\mathcal{D}_n(R=+\infty)|^2=1$ which expresses the conservation of probability during the scattering process.

In order to deal with dynamically induced backscattering (which occurs in quantum cosmology) it is necessary to consider situations in which the wave function is not restricted to vanish at a certain place. For instance one can think of a single atom moving in one dimension in a static but inhomogenous electric field. The Schrödinger equation for the atom has the same form as Eq. (29), but now R is the position of the atom and the R dependence of $V(R)+H_{el}(R,q,p)$ is due to the electric field. Consider an atom incoming from $R=-\infty$ in a given energy eigenstate n_0. This is implemented by requiring that the solution satisfy the following boundary conditions $|\mathcal{C}_{n_0}(R=-\infty)|^2=\delta_{n,n_0}$. Since there is no atom incoming from $R=+\infty$, one should also impose $\mathcal{D}_n(R=+\infty)=0$ for all n. By these boundary conditions one specifies what are the in-modes, i.e. modes which possess a well-defined semi-classical behavior in the remote past. In this determination, there is an identification of the asymptotic waves carrying a unit Wronskian with the corresponding classical trajectories obtained by the stationary phase condition applied to wave packets or by identifying directly the wave length times $\hbar$ with the momentum of the particle.

Upon solving the full (untruncated) Schrödinger equation one obtains both the asymptotic amplitudes for the atom to continue over the potential barrier, $\mathcal{C}_n(R=+\infty)$, as well as those to be reflected by the potential $\mathcal{D}_n(R=-\infty)$. Unitarity is expressed by the equality of the ingoing current to the sum of the outgoing currents:

$$\int dq_i \Psi_E^* i\overleftrightarrow{\partial}_R \Psi_E = 1 = |\mathcal{C}_{n_0}(R=-\infty)|^2$$
$$= \sum_n |\mathcal{D}_n(R=-\infty)|^2 + \sum_n |\mathcal{C}_n(R=+\infty)|^2. \quad (30)$$

We emphasize that in Born's interpretation the identification of the quantities $\mathcal{D}_n,\mathcal{C}_n(R=\pm\infty)$ as scattering amplitudes and, hence, unitarity follow from the internal structure of Eq. (29) and the use of asymptotic waves normalized to unit Wronskian for all n. An external concept was only necessary to identify the asymptotic incoming and outgoing modes (i.e. the left and right movers).

The essential simplification of this interpretation is that one considers only asymptotic states. This leads naturally to the question of whether one can also give an interpretation to the electronic dynamics in the intermediate region. The coefficients $\mathcal{C}_n(R)$ and $\mathcal{D}_n(R)$ are natural candidates for this interpretation since they generalize to finite R the coefficients that were the basis for the asymptotic interpretation. Moreover, this is also supported by the fact that, when backscattering can be neglected, they obey a Schrödinger like equation with a Hamiltonian that tends in the limit of infinitely heavy nuclei to the time dependent electronic Hamiltonian $H_{el}(R(t),q,p)$.

To further investigate this question, we now turn to the second interpretation of the solution of Eq. (29). In this interpretation—which for reasons of simplicity is generally the first one presented in textbooks—$|\Psi_E(R,q)|^2$ is interpreted as the probability for the atom to be at R in electronic configuration q. The basis for this interpretation is twofold. First if one considers time dependent solutions $\Psi(t,R,q)$ of the Schrödinger equation, then there is a conserved current

$$\partial_t|\Psi(t,R,q)|^2+\partial_R J_R+\partial_q J_q=0 \tag{31}$$

where

$$J_R=\Psi^* i\overleftrightarrow{\partial}_R\Psi, \quad J_q=\Psi^* i\overleftrightarrow{\partial}_q\Psi. \tag{32}$$

Hence it is consistent to interpret $|\Psi(t,R,q)|^2$ and therefore $|\Psi_E(R,q)|^2$ as probability densities; see e.g. [22]. The second basis, due to von Neumann [23], is the following: if we couple the atom to an idealized measuring device (initially in the state $X_R=0$, $X_q=0$) through a coupling $\delta(t)|q\rangle|R\rangle P_{X_q}P_{X_R}\langle q|\langle R|$ where P_{X_R} and P_{X_q} are the variables conjugate to X_R and X_q, the measuring device will record outcomes R,q (i.e. $X_R=R$ and $X_q=q$) with probability $|\Psi(t,R,q)|^2$.

An essential point to note about these two arguments is that they both necessitate the introduction of external concepts which are used *in situ* and no longer only asymptotically: in the first case, external time and, in the second, the local measuring device. For this reason the application of this second interpretation will be problematic in quantum cosmology since these external concepts cannot be invoked.

It is now very instructive to show that this interpretation—when used with care—is consistent with the S matrix interpretation. In particular, we shall show when and why the second interpretation also implies that the coefficients $\mathcal{C}_n(R)$ and $\mathcal{D}_n(R)$ should be interpreted as the amplitudes for the electrons to be in state n when the nuclei are propagating forward and backward at (better near) R. In this, the necessity of having well-separated length scales is crucial.

Consider the probability $|\Psi_E(R,q)|^2$ that the atom is at R and the electrons in state q. In terms of the coefficients $\mathcal{C}_n(R)$ and $\mathcal{D}_n(R)$ it takes the form

$$|\Psi_E(R,q)|^2=\sum_n\left|\left(\mathcal{C}_n(R)\frac{\exp\left[i\int^R p_n dR\right]}{\sqrt{2p_n(R)}}+\mathcal{D}_n(R)\frac{\exp\left[-i\int^R p_n dR\right]}{\sqrt{2p_n(R)}}\right)\langle q|\psi_n(R)\rangle\right|^2. \tag{33}$$

This quantity is wildly oscillating because of the interference terms between $\mathcal{C}_n(R)$ and $\mathcal{D}_n(R)$. These interferences arise from the localized measuring device which has interacted strongly with both the electrons and the nuclei. Since we are interested only in the electrons, we would like the measuring device to interact weakly with the nuclei. Thus we consider a measuring device that interacts with the nucleus over a certain range of R, and with a certain momentum sensitivity. That is we consider the probability that the nucleus be in a wave packet $\varphi_{R_0,P_0}=e^{-(R-R_0)^2/\Delta^2}e^{iRP_0}/\sqrt{2\pi\Delta}$ where as an example we have taken a Gaussian packet. If the interval Δ satisfies both $\Delta\gg 1/p_n$ and $\Delta\ll(\partial_R\ln\mathcal{C}_n)^{-1}$, the probability amplitude to find the nuclei in state φ_{R_0,P_0} is approximately

$$\int dR\varphi^*_{R_0,P_0}(R)\Psi_E(R,q)\simeq\sum_n \mathcal{C}_n(R_0)\langle q|\psi_n(R_0)\rangle\times\frac{e^{-[p_n(R_0)-P_0]^2\Delta^2}}{\sqrt{2p_n}} \tag{34}$$

where we have neglected the R dependence of $\mathcal{C}_n(R)\langle q|\psi_n(R)\rangle$ over the interval Δ, and dropped the exponentially small contribution of the $\mathcal{D}_n$ coefficients. Thus only the amplitudes with momentum in the interval $P_0\pm 1/\Delta$ are selected. From this expression it follows that

$$\frac{|\mathcal{C}_n(R_0)|^2}{2p_n(R_0)} \tag{35}$$

is the probability that the electrons are in state n if the nuclei are in the interval $R_0\pm\Delta$. Recalling we are working at fixed total energy E and that $p_n(R_0)$ is proportional to the speed of the nuclei, it follows that what we have calculated is the probability for the electrons to be in state n multiplied by the time they spend in the interval $R_0\pm\Delta$. This confirms the interpretation of $\mathcal{C}_n(R)$ as the probability[3] amplitude for the electrons to be in state n.

In this derivation the identification of $\mathcal{C}_n(R)$ as electronic amplitudes is inevitably approximate. Indeed Eq. (34) followed from the fact that the wavelength of the nucleus and that of the electrons are very different. The same separation of length scales was also the justification for neglecting the

[3]For the same reason in relativistic theory one must remove $1/\sqrt{2\omega}$ from scattering matrix elements in order to get probability amplitudes. This is known as the reduction formula.

coupling between forward and backward propagating modes in Eq. (17), thereby obtaining a Schrödinger equation for the forward propagating coefficients only. Thus, this separation is twice used in order to reach an interpretation of $\mathcal{C}_n(R)$ as the amplitude for the light degrees of freedom to be in state n.

We now turn to the consequences of backscattering. In this case, $\Sigma_n|\mathcal{C}_n(R)|^2$ is no longer constant. How is this interpreted in the context of electronic nonadiabaticity?

To address this question, consider a generic solution of Eq. (29) in the context of the atom propagating in a background field so that the whole real axis $-\infty<R<+\infty$ is accessible. For such a solution, none of the coefficients $\mathcal{C}_n(\pm\infty)$, $\mathcal{D}_n(\pm\infty)$ are zero. Using the equality

$$\sum_n |\mathcal{C}_n(+\infty)|^2+\sum_n |\mathcal{D}_n(-\infty)|^2 =\sum_n |\mathcal{C}_n(-\infty)|^2+\sum_n |\mathcal{D}_n(+\infty)|^2 \tag{36}$$

the probability to be in state n and forward propagating at $R=+\infty$ is

$$P(\mathcal{C}_n(+\infty))=\frac{|\mathcal{C}_n(+\infty)|^2}{\sum_n |\mathcal{C}_n(+\infty)|^2+\sum_n |\mathcal{D}_n(-\infty)|^2} \tag{37}$$

when the WKB approximation is asymptotically exact. This probability is a highly nonlocal concept since it involves the coefficients $\mathcal{C}_n$ and $\mathcal{D}_n$ at + and − infinity respectively. For this reason it is a relevant and useful concept only for an external observer who has access to both the forward and backward waves at $R=\pm\infty$. However, there are many relevant quantities which are local in R. Moreover, these quantities govern the physical outcomes when one is in the second regime wherein backscattering is neglected. In addition light subsystems can presumably only ask questions concerning these quantities. An example of such a local quantity is the relative probability to be forward propagating in state n or state m at $R=+\infty$:

$$\frac{P(\mathcal{C}_n(+\infty))}{P(\mathcal{C}_m(+\infty))}=\frac{|\mathcal{C}_n|^2}{|\mathcal{C}_m|^2}. \tag{38}$$

In such local quantities the absolute normalization involving a mixture of $\mathcal{C}_n$ and $\mathcal{D}_n$ coefficients disappears. However, they do not obey a closed equation since the $\mathcal{C}_n$ are coupled to the $\mathcal{D}_n$. Thus, the effect of the backscattering is to modify the effective Schrödinger equation for the forward propagating coefficients $\mathcal{C}_n(R)$ into a stochastic equation, where the stochasticity is given by the absence of knowledge a forward propagating subsystem has about the backward propagating part of the solution. At the end of the calculation an average must be taken over the unknown coefficients $\mathcal{D}_n$. Happily, when the electronic length scales are well separated from the nuclear length scales, this stochasticity is exponentially small.

VIII. RELATIVISTIC PARTICLE IN AN EXTERNAL FIELD

In order to further investigate the relationships between the conservation of the Wronskian, the identification of the asymptotic solutions and the interpretation of the wave functions, another situation should be considered: the Klein-Gordon (KG) equation governing the propagation of a relativistic particle in an external field. This example has in common with the WDW equation a Lorentzian signature; i.e., the quadratic form determining the kinetic energy term is not positive definite.

This analogy has been emphasized by many authors (see e.g. [24] for a discussion at the classical level) and has been used to advocate the necessity of performing a ''third quantization.'' Indeed, in the case of the relativistic particle, unitarity is implemented by carrying out a ''second quantization.'' The difference with the nonrelativistic case is that the Wronskian is no longer interpreted as a particle current density but as a charge density. This follows from a different identification of the in and out asymptotic modes which in turn dictates the new interpretation.

Let us review these features by considering the propagation of a charged particle in an external electric field. We shall take for simplicity the electric field to be homogeneous and to point in the x direction. We impose that the electric field vanish for $t\to-\infty$ and for $t\to+\infty$ which provides us with asymptotic regions in which the momentum is constant and therefore the modes are exactly WKB. The Klein-Gordon equation in the gauge $A_t=0$, $A_x=f(t)$, $A_y=A_z=0$ takes the form

$$\{\partial_t^2-[\partial_x+ieA_x(t)]-\partial_y^2-\partial_z^2+m^2\}\Psi=0. \tag{39}$$

Writing $\Psi=e^{i(k_x x+k_y y+k_z z)}\phi_k(t)$, one finds that ϕ_k obeys the equation

$$[\partial_t^2+V_k(t)]\phi_k=0 \tag{40}$$

where $V_k(t)=[k_x+eA_x(t)]^2+k_y^2+k_z^2+m^2$.

This equation is identical to that studied in Sec. II and can be analyzed in the same way. To reach an interpretation one first needs to identify the in-mode describing a particle incoming from $t=-\infty$. This is achieved by decomposing ϕ_k as $\mathcal{C}_k(t)\chi_k(t)+\mathcal{D}_k(t)\chi_k^*(t)$, where $\chi_k(t)$ is the WKB solution with unit positive Wronskian of Eq. (40). The in modes are then given by imposing the boundary condition $|\mathcal{C}_k(t=-\infty)|^2=1,\mathcal{D}_k(t=-\infty)=0$. (Notice that the condition on the coefficient $\mathcal{D}_k$ is applied on the same ''side'' of the potential in opposition to what is done in the nonrelativistic case.) As in the nonrelativistic case, the potential $V_k(t)$ induces backscattering effects and both the coefficients $\mathcal{C}_k$ and $\mathcal{D}_k$ are nonvanishing at $t=+\infty$. The conservation of the Wronskian now reads

$$1=\int d^3x\Psi^* i\overleftrightarrow{\partial}_t\Psi=|\mathcal{C}_k(t=-\infty)|^2 =|\mathcal{C}_k(t=+\infty)|^2-|\mathcal{D}_k(t=+\infty)|^2. \quad (41)$$

How should one interpret these coefficients at $t=+\infty$ and, in particular, the fact that $\mathcal{C}_k(t=+\infty)>1$? This is the content of the Klein paradox that was discussed in the early days of relativistic quantum field theory [25].

Probably the simplest way to reach a physical understanding is to proceed as in the nonrelativistic case by building wave packets (in k) and following the classical trajectories they describe. One then finds that the wave packets made of $\mathcal{C}_k\chi_k$ follow, both for early and late times, the trajectories of a positive charged particle. But the part of the wave packets proportional to $\mathcal{D}_k\chi_k^*$ follows trajectories of negatively charged particles. Thus the conservation of the Wronskian expresses charge conservation and the decomposition into $\mathcal{C}_k$ and $\mathcal{D}_k$ is a decomposition into positive and negative charged particles. Hence the extra charge carried by the $\mathcal{C}_k(t=+\infty)$ is compensated by the presence of antiparticles that reach $t=+\infty$: $|\mathcal{D}_k(t=+\infty)|^2>0$. Another more mathematical way to reach this conclusion is to note that Eq. (39) is invariant under gauge transformations, and that the Wronskian is the charge associated with the gauge field A_μ.

Once this is realized one still faces the problem of extracting (probabilistic) predictions from the theory. This is done by second quantizing Ψ: the coefficient $\mathcal{C}_k$ becomes an operator destroying a particle of momentum k. In this framework, one establishes that in addition to the ''elastic'' scattering of initial (anti)particles, one is describing pair creation. Even in the in-vacuum state, pairs of particles are spontaneously created with probability amplitudes governed by the backscattering amplitude $B_k=\mathcal{D}_k(t=+\infty)$ calculated in Eq. (10), which in this context are called Bogoljubov coefficients. If some particle is initially present, one finds that there is also induced emission. By this reasoning the conclusion that the Wronskian is expressing charge conservation relied on an external input, namely that t in Eq. (40) is an external time which was allowed to follow asymptotic motion. Moreover, the prediction that many pairs can be produced can be checked experimentally.

We now discuss how these new effects modify the dynamics of *internal* degrees of freedom. The most natural way to implement internal degrees of freedom is to go back to Eq. (39) and take the momenta along the x,y,z directions to be the additional degrees of freedom. The model becomes nontrivial when the electric field is not homogeneous, so that k_x, k_y, k_z are not constants of motion (they can be replaced by adiabatic constants of motion as in Sec. III). The choice of how the field should be second quantized is dictated by the spin-statistics theorem [26]; i.e. Ψ is either a bosonic or a fermionic field. The important conclusion for us is that these different second quantization procedures are not equivalent, even if one restricts oneself to the dynamics of the internal degrees of freedom.

To second quantize one first selects a complete set of modes with only positive frequency at $t=-\infty$, ϕ_k^{in} to which one associates a particle destruction operator a_k^{in}. To the complex conjugate of these modes one associates an antiparticle destruction operator b_k^{in}. If we neglect backscattering, then the number operators $N_{part}=\Sigma_k a_k^{in\dagger}a_k^{in}$ and $N_{anti-part}=\Sigma_k b_k^{in\dagger}b_k^{in}$ commute with the second quantized Hamiltonian. The Fock space then decomposes into noninteracting sectors. The simplest sector is the vacuum $|0\rangle$. The first nontrivial states are the one particle (or antiparticle) states $\Sigma_k f(k)a_k^{in\dagger}|0\rangle$. These states are exact analogues of the forward propagating modes in the atomic example of the previous section, and should be interpreted in the same way. The next states are the two particle states $\Sigma_{k,k'}f(k,k')a_k^{in\dagger}a_{k'}^{in\dagger}|0\rangle$ where f is symmetric or antisymmetric according to the statistics of the field. Since f does not factorize into a product of a function of k and k', the interpretation of this state cannot reduce to that of one particle states. Moreover, the statistics play a role in the determination of the final amplitudes since the presence of a particular quantum modifies the spectrum of transition amplitudes through either Bose enhancement or Pauli suppression. Whether or not this has an interpretation from the point of view of an internal degree of freedom is unclear.

The situation is worse when one takes backscattering into account. In this case, the number operators no longer commute with the Hamiltonian because of the nonvanishing character of the Bogoliubov coefficients $B_{k\to k'}$ [calculated in Eqs. (25) and (26)] relating in and out modes. This implies that in order to determine the amplitude to find a given state k in the one particle sector, it is necessary to know all the initial amplitudes (in Fock space) to find particles and antiparticles. Thus the amount of initial data needed in order to extract exact predictions from the theory in the one particle sector is (infinitely) larger than in the nonrelativistic case. For this reason third quantization is not a very attractive alternative since it diminishes the predictivity of quantum cosmology. Furthermore, the additional ingredients which imposed second quantization, namely the presence of an absolute time and of a gauge field coupled to Ψ, are not present in quantum cosmology. For these reasons it seems advisable, in the absence of additional strong arguments in favor of it, not to resort to third quantization in quantum cosmology.

IX. CONDITIONAL PROBABILITY INTERPRETATION BASED ON THE NORM OF Ψ

In the light of the previous examples we now return to the interpretation of the WDW equation.

For many authors, conservation of probability is a necessary requisite for quantum cosmology to possess a coherent interpretation. The most widely adopted scheme which implements from the start unitarity and conservation of probability is the conditional probability interpretation [27,3].[4] In this interpretation one identifies

$$\tilde{\phi}_{eff}(a,\phi)=\frac{\Psi(a,\phi)}{\sqrt{\int d\phi\Psi(a,\phi)^*\Psi(a,\phi)}} \tag{42}$$

as the amplitude of probability to find matter in state ϕ at radius a. By construction the norm square of $\tilde{\phi}_{eff}$ is constant, independently of the validity of the WKB approximation or any other condition.

The main problem with this construction is that $\tilde{\phi}_{eff}$, contrarily to $\phi^{\pm}_{eff}$ defined in Eq. (19), does not obey a linear equation (since Ψ does). Therefore it does not satisfy the superposition principle. This can be ignored as long as one considers tight wave packets such that the factorization of a single gravitational wave, common to all matter states, offers a good approximation. However, once the spread in matter energy is large, the probabilities significantly vary even in the total absence of interactions. To see this suppose that the matter Hamiltonian has only two instantaneous eigenstates $|\psi_0\rangle$ and $|\psi_1\rangle$. Then, in the WKB regime, the wave function of the universe is

$$|\Psi(a)\rangle=\mathcal{C}_0\frac{\exp\left[-i\int^a da\,p_0(a)\right]}{\sqrt{2p_0(a)}}|\psi_0\rangle+\mathcal{C}_1\frac{\exp\left[-i\int^a da\,p_1(a)\right]}{\sqrt{2p_1(a)}}|\psi_1\rangle. \tag{43}$$

Let us further suppose that it is impossible to make transitions from state 0 to state 1. Then the instantaneous states are truly stationary, $\partial_a|\psi_0\rangle=\partial_a|\psi_1\rangle=0$, and the coefficients $\mathcal{C}_0$ and $\mathcal{C}_1$ are constant. Using the conditional probability interpretation, one then finds that the probability for finding matter in state $|\psi_0\rangle$ is

$$P(\psi_0|a)=\frac{|\mathcal{C}_0|^2}{|\mathcal{C}_0|^2+[p_0(a)/p_1(a)]|\mathcal{C}_1|^2}. \tag{44}$$

It reduces to the usual expression $P_0(a)=|\mathcal{C}_0|^2$ only when $p_0(a)/p_1(a)=1$, i.e. when $E_0=E_1$. Therefore $P_0(a)$ varies once $E_0\neq E_1$ through the ratio of the two gravitational momenta p_0 and p_1 entangled with the two matter states by the constraint. The more remote these energy are, the bigger the effect since the associated momenta will be more different. Moreover, upon taking into account backscattering effects, the probability receives in addition to the continuous component a rapidly oscillating component with frequency $2p_0$ whose origin is the interference between expanding and contracting solutions.

In our opinion, these two properties are sufficient to reject the conditional probability interpretation. Before explaining our reasons, it is interesting to recall why a similar construction can be meaningful for a nonrelativistic atom. In that case, the probability to find the atom in electronic state ϕ under the condition that it be at R is indeed given by Eq. (42). What does give meaning to this expression is the possibility (and the necessity) of coupling the atom to a localized external device so heavy that its own recoils be negligible. Only then does the factor p_0/p_1 in Eq. (44) take meaning as the relative time each state interacted with the detector, and only then can the forward and backward waves give rise to the interferences at frequency $2p_0$. But if one couples the atom to a measuring device that does not significantly disturb the motion of the nuclei (see Sec. VII), one obtains the current interpretation based on Eq. (38) instead that based on the norm;[5] see Eq. (33).

To present our arguments against Eq. (44) we first recall the following point. In quantum mechanics, from solutions of the linear equation determining evolution (which can be either the Schrödinger or the WDW equation) one obtains that very remote states neither interact nor interfere. From this mathematical property and the conventional interpretation of probability amplitudes, one then gets that the probabilities of such remote states do not influence each other. But this fundamental decorrelation of remote configurations does not obtain in Eq. (44).

From an epistemological point of view, the fact that linearity of the WDW equation does not reflect itself in a simple property of the physical probabilities $|\tilde{\phi}_{eff}|^2$ is disturbing. Indeed, if linearity does not manifest itself in a simple way at the level of observation, why insist that we start with a linear equation? We might as well introduce nonlinearity at the level of the WDW equation directly.

In our opinion, the only way to save this interpretation probably requires to first restrict the applicability of Eq. (42) to neighboring states only. But then its status would be of an

[4]Although [3] does not use the name ''conditional probability interpretation,'' it implicitly adopts it. Indeed in [3] the decomposition of the wave function into a gravitational and a matter wave is uniquely fixed by imposing that the matter wave satisfy $\int d\phi\chi_s^*(a,\phi)\chi_s(a,\phi)=\text{const}$. Hence $\chi_s(a,\phi)$ is identical to $\tilde{\phi}_{eff}(a,\phi)$ defined in Eq. (42).

Another recent paper that claims that matter evolves unitarily in quantum cosmology [28] contains mathematical errors. Indeed $\psi(h_a)$ in Eq. (7) must carry an index n since the equation it obeys depends on n (see [10] for a discussion of this n dependence). But this implies that the second term on the right hand side of Eq. (10) is non Hermitian. Furthermore, the third term proportional to Ω is non Hermitian (it would only be Hermitian if integrated over h_a). Hence the conclusion of [28] that $\Sigma_n|c_n|^2$ is constant is incorrect.

[5]Some authors have proposed to introduce an additional variable η such that the modified WDW equation reads $i\partial_\eta\Psi=H\Psi$, thereby recovering a situation similar to that of an atom in a time dependent state. It is then very tempting to interpret $|\Psi(a,\phi,\eta)|^2$ as the probability to find a and ϕ at η. However, since in cosmology one must restrict oneself to questions such that only little momentum is transferred to a, one recovers the current interpretation of Eq. (38) (see Sec. VII). Thus this latter interpretation naturally arises irrespective of the use of an additional variable as time.

approximate character rather than a starting point from which all solutions of the WDW equations can be interpreted.

X. VILENKIN INTERPRETATION WITHIN THE WKB REGIME

Of the different interpretations of the wave function of the universe which have been proposed, the closest to the physical examples presented above is that of Vilenkin [4], as generalized in [13]. Indeed the essential lesson of these examples is that they give physical substance to the coefficients $\mathcal{C}_n$ and $\mathcal{D}_n$. This is not surprising since these coefficients have the following mathematical properties:

(i) The conserved current is expressed most simply in terms of these coefficients upon working with modes normalized to unit Wronskian.

(ii) They obey a linear first order equation in a.

(iii) If backscattering is neglected, they evolve independently and unitarily. In the absence of backscattering, these properties designate the $\mathcal{C}_n$ and $\mathcal{D}_n$ as the probability amplitudes for matter to be in state n in the forward or backward sector. We invite the reader to compare this reasoning with the original one of Born; see [21].

Very important is also the fact that in this interpretation, decoherence effects arise naturally and obey the usual properties, in contradistinction to what occurs in the conditional probability interpretation. For instance, when two states or two groups of states have only vanishing matrix elements of $H_{eff}(a)$, their evolution is completely independent. It is thus fully legitimate to interpret the wave function composed of their sum as representing two different universes rather than a quantum superposition of states residing in the same universe. This decoherence is the most basic one (when compared to that induced by the environment or measuring devices) since it is solely determined by the nature of the full Hamiltonian, i.e. the WDW constraint. It therefore provides a natural explanation for the fact that one should not consider quantum superpositions of states giving rise to different semi-classical geometries (histories) since these states completely decouple.

The neglection of quantum backscattering effects can also be conceived as a manifestation of decoherence. Indeed, the appropriate character of the decomposition into forward and backward solutions (rather than in sines or cosines) follows from the effective decoupling of these two sets. Thus, there is a hierarchy of decoherence associated with the hierarchy of length scales. Indeed, the decoupling of the forward and backward sectors is the most efficient since backscattering amplitudes are exponentially smaller than matter transition amplitudes. This leads to a clear separation of the solutions into two sets characterized by the sign of $p_n(a)$.

Thus the only aspect which differs from that presented in the physical examples of Secs. VII and VIII is the identification of these sets with forward and backward propagation in time. In the previous examples, it was necessary to use an external time to identify which asymptotic modes correspond to forward motion at $t=-\infty$. (Recall that this identification was different for the nonrelativistic and relativistic examples.) In cosmology, an external time does not exist and thus the eventual determination of forward motion in time, i.e. the arrow of time, should be intrinsic. Presumably, the answer is thermodynamic: if the matter is out of equilibrium, then the arrow of time is determined by the direction in which entropy is increasing. This point of view was recently advocated in the quantum cosmological context in [29]. If this is indeed the case, quantum cosmology is incomplete since it can only be interpreted for macroscopical universes containing enough degrees of freedom so that thermodynamics applies. For such universes, the hierarchy of matter and gravity scales that we twice exploit will be well established. Therefore it appears that only macroscopic universes can be meaningfully investigated and interpreted.

XI. INTERPRETATION IN THE PRESENCE OF BACKSCATTERING

As emphasized by Vilenkin, since the WKB approximation is not exact, *''probability'' and ''unitarity'' are inherently approximate concepts*. Indeed neither the norm of ϕ^+_{eff} nor of ϕ^-_{eff} is separately conserved in the presence of backscattering.

However, this is not an insurmountable problem for the following reason. Any subsystem of the universe, for instance the degrees of freedom within the cosmological horizon, is necessarily an open system and its dynamics is therefore necessarily nonunitary. The coupling between forward and backward propagating universes will appear to this subsystem as an additional coupling to the environment. Furthermore, this coupling gives rise to exponentially small effects, with approximately the ratio of the Hubble radius to the wavelength of the universe appearing in the exponential. Hence it is completely negligible compared to the other couplings to the environment at least for macroscopic universes.

Having said this, one may nevertheless want to know what the possible effects of backscattering could be—however small they are—and how they should be interpreted.

A first point to be noticed is that in most realistic cosmologies, backscattering cannot be dissociated from effects at the origin of the universe, the reason being that the distance $(d \ln p/da)^{-1}$ over which the backscattering occurs is comparable to the distance to the origin of the universe. For this reason backscattering and its interpretation may be intimately linked to the ultraviolet structure of quantum gravity. If this is the case, the interpretation cannot be discussed in the context of a truncated WDW equation.

Nevertheless, one may imagine universes in which asymptotic regions exist. Then backscattering events can be localized and their amplitudes properly evaluated. In this case, one can inquire into their interpretation even in the context of simplified WDW equations. As discussed in Secs. VII and VIII there are at least two consistent interpretations of backscattering. In both cases the choice of interpretation was dictated by reinserting the system into a wider context. In the cosmological context we do not know into what (if any) wider context the WDW equation fits, and thus the precise way backscattering should be interpreted is unclear.

Let us nevertheless briefly discuss the consequences of backscattering. For a subsystem of the universe which is forward propagating, the effect of backscattering is included by averaging over the (unknown) state of the rest of universe. In a first quantized context, the rest of the universe would simply be the backward propagating waves. In the second quantized context it would correspond to all the other sectors of the theory with different ''universe and antiuniverse numbers.'' Thus the averaging and hence, the effect of the averaging are different in both cases.

Moreover, the interpretation of backscattered waves themselves is problematic. For instance what is the physical principle which would determine the arrow of time in the part of the wave function whose origin is backscattering? To be concrete, consider a solution of the WDW equation which for $a \ll a_0$ contains only $\mathcal{C}_n$ coefficients, but for $a \gg a_0$ contains both $\mathcal{C}_n$ and $\mathcal{D}_n$ coefficients (a_0 is the center of the region where the backscattering occurs). From Sec. V we know that the $\mathcal{D}_n(a)$ coefficients will ultimately be more or less thermally distributed with a very low temperature. In which direction does the arrow of time point for the $\mathcal{D}_n$ coefficients? Is $a \simeq a_0$ the origin or the end of the universe?

In conclusion the separation between forward and backward propagating universes, and hence the appearance of an effective Schrödinger equation for matter, appears to be a more robust concept than previously thought. Indeed the corrections to the Schrödinger equation are exponentially smaller than any matter transitions. On the other hand the precise way the backscattering manifests itself does not seem to be constrained by the WDW equation—at least in the simple models we have considered in this paper. Hopefully this interpretational problem can be resolved once we have a deeper understanding of the structure of quantum gravity. The inclusion of anisotropies and inhomogeneities, and more importantly of the ultraviolet sector of the theory, could lead to a unique consistent interpretation.

ACKNOWLEDGMENTS

S.M. is a ''chercheur qualifié du FNRS.'' He would like to thank the Institute of Theoretical Physics at Utrecht University where part of this work was carried out. S.M. also thanks the IISN for financial support.

[1] J. A. Wheeler, in *Battelles Rencontres: 1967 Lectures on Mathematical Physics*, edited by C. DeWitt and J. Wheeler (Benjamin, New York, 1968).
[2] B. DeWitt, Phys. Rev. **160**, 1113 (1967).
[3] C. Bertoni, F. Finelli, and G. Venturi, Class. Quantum Grav. **13**, 2375 (1996).
[4] A. Vilenkin, Phys. Rev. D **39**, 1116 (1989).
[5] T. Banks, Nucl. Phys. **B249**, 332 (1985).
[6] R. Brout and G. Venturi, Phys. Rev. D **39**, 2436 (1989).
[7] J. B. Hartle, in *Gravitation and Cosmology*, edited by B. Carter and J. Hartle (Plenum, New York, 1986).
[8] C. J. Isham, in *Integrable Systems, Quantum Groups and Quantum Field Theories* (Kluwer Academic Publishers, London 1993), gr-qc/9210011.
[9] C. Kiefer, in *Canonical Gravity—from Classical to Quantum*, edited by J. Ehlers and H. Friedrich (Springer, Berlin, 1994).
[10] S. P. Kim, Phys. Rev. D **52**, 3382 (1995).
[11] R. Parentani, Nucl. Phys. **B492**, 475 (1997).
[12] R. Parentani, Nucl. Phys. **B492**, 501 (1997).
[13] R. Parentani, Phys. Rev. D **56**, 4618 (1997).
[14] S. Massar and R. Parentani, Nucl. Phys. **B513**, 375 (1998).
[15] J. B. Delos, W. R. Thorson, and S. K. Knudson, Phys. Rev. A **6**, 709 (1972).
[16] A. D. Migdal, *Qualitative Methods in Quantum Theory* (Benjamin, Reading, MA, 1977).
[17] L. C. Baird, J. Math. Phys. **11**, 2235 (1970).
[18] V. L. Pokrovskii, S. K. Savvinykh, and F. R. Ulinich, Sov. Phys. JETP **7**, 879 (1958); V. L. Pokrovskii and I. M. Khalatnikov, *ibid.* **13**, 1207 (1961).
[19] A. Peres, ''Critique of the Wheeler-DeWitt equation,'' gr-qc/9704061.
[20] J. Hwang and P. Pechukas, J. Chem. Phys. **67**, 4640 (1977).
[21] M. Born, in *Quantum Theory of Measurement*, edited by J. A. Wheeler and W. Zureck (Princeton University Press, Princeton, NJ, 1983).
[22] A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1969).
[23] J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Princeton, 1955).
[24] C. W. Misner, K. S. Thorne, and J. A. Wheeler, *Gravitation* (Freeman, San Fransisco, 1973).
[25] C. Itzykson and J.-B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).
[26] R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics, and All That* (Benjamin, New York, 1964).
[27] D. N. Page and W. K. Wootters, Phys. Rev. D **27**, 2885 (1983).
[28] S. P. Kim, Phys. Rev. D **55**, 7511 (1997).
[29] S. W. Hawking, R. Laflamme, and G. W. Lyons, Phys. Rev. D **47**, 5342 (1993).