Particle creation and non-adiabatic transitions in quantum cosmology

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abstract

The aim of this paper is to compute transitions amplitudes in quantum cosmology, and in particular pair creation amplitudes and radiative transitions. To this end, we apply a double adiabatic development to the solutions of the Wheeler-DeWitt equation restricted to mini-superspace wherein gravity is described by the scale factor $a$. The first development consists in working with instantaneous eigenstates, in $a$, of the matter Hamiltonian. The second development is applied to the gravitational part of the wave function and generalizes the usual WKB approximation. We then obtain an exact equation which replaces the Wheeler-DeWitt equation and determines the evolution, i.e. the dependence in $a$, of the coefficients of this double expansion. When working in the gravitational adiabatic approximation, the simplified equation delivers the unitary evolution of transition amplitudes occurring among instantaneous eigenstates. Upon abandoning this approximation, one finds that there is an additional coupling among matter states living in expanding and contracting universes. Moreover one has to face also the Klein paradox, i.e. the generation of backward waves from an initially forward wave. The interpretation and the consequences of these unusual features are only sketched in the present paper. Finally, the examples of pair creation and radiative transitions are analyzed in detail to establish when and how the above mentioned unitary evolution coincides with the Schrödinger evolution.
1 Introduction

In General Relativity, one loses the usual Hamiltonian structure in which time parameterizes the evolution since the theory is invariant under arbitrary changes of coordinates. In order to understand the consequences of this loss in quantum cosmology, one must begin by reexamining the status of time in quantum mechanics and quantum field theory. In particular, we draw the attention to the distinction between the adiabatic deformation of the states and non-adiabatic transitions amongst states. This distinction will be very useful upon addressing the question of the evolution in quantum cosmology.

For simplicity, we first consider the case in which the Hamiltonian is time independent. Then, its eigenstates are stationary and, in the absence of interactions, the probability amplitudes to find the system in each eigenstate are constant. When a time independent interaction Hamiltonian is added, its sole role is to displace the energy levels from their values defined by the free Hamiltonian to their dressed values defined by the (stationary) eigenstates of the full Hamiltonian.

When the Hamiltonian is time dependent, it has a double role. First, it modifies adiabatically the energy levels defined by its instantaneous eigenstates. In the limit of slowly varying situations, one recovers the former case in which the amplitudes stay constant. Secondly, it induces non adiabatic transitions between instantaneous eigenstates, a truly time dependent phenomenon since it characterizes quantum jumps. The importance of these transitions is controlled by $\frac{\partial_t \Delta E}{\Delta E^2}$ where $\Delta E(t)$ is the energy difference between the instantaneous eigenstates. It goes without saying that as long as the interaction Hamiltonian is hermitian, the existence of these transitions do not require a revision of the interpretation of quantum mechanics since the norm of the state stays constant.

In quantum field theory, time dependent gravitational fields induce both effects, although they are somewhat hidden when one works -as is usually done- in a Heisenberg picture. For instance for a free scalar field one would proceed by computing the solutions of the Klein Gordon equation. Its WKB solutions describe the adiabatic deformation of positive frequency waves and lead to no transitions in Fock space. Instead, backscattering between positive and negative frequency waves correspond to non-adiabatic transitions between states, i.e. pair creation from vacuum. What plays the role of $\Delta E(t)$ in quantum mechanics is $2\omega(t)$, the energy of a pair. Note that the existence of the backscattering amplitude leads to the “Klein paradox”, namely the increase of the current carried by the forward wave when some backward wave is generated (since the total current is conserved). This imposes that one abandon a first quantized framework, since no conserved positive local quantity can be built from these solutions.

In the first part of this article we review the notions of adiabatic evolution and adiabatic transitions in a cosmological context in which the evolution of the scale factor $a(t)$ is given from the outset. We show that $a$ itself can replace time and be used as the parameter which controls both the adiabatic deformations of the states and their non adiabatic transitions, although time still appears in the relative phase accumulated by neighboring states. This prepares for the analysis in quantum cosmology where $a$ is a dynamical variable.
We illustrate this formalism by two examples. The first is the recovery of the Golden Rule, i.e. that transition probabilities grow linearly with proper time lapses. We show how the residual time dependence mentioned above guarantees that the transition rate is constant. (Thus a collection of such systems can be viewed as a simple realization of a “clock”.) The second example, taken from field theory, is the process of pair creation in cosmology. We show that pair creation acts are described, in the Schrödinger picture, by non adiabatic transitions between states having different instantaneous particle number. Moreover, this second example introduces useful tools to handle the gravitational part of the solutions of the Wheeler-DeWitt equation.

In the second part this article, we work in quantum cosmology. In that framework, the physical states are solutions of the Wheeler-DeWitt (WDW) equation. Indeed, instead of having as before a Hamiltonian framework in which processes are parameterized in time, one has a constraint that expresses the invariance of the theory under arbitrary changes of time (of time only since our analysis is restricted to mini-superspace). Therefore, to make contact with the conventional analysis, one must understand how to define adiabatic deformations of matter states and how to compute non adiabatic transition amplitudes without having a physical time parameter at our disposal.

The first point is easily addressed. Indeed, since the Wheeler-DeWitt equation is the sum of a kinetic term for gravity, a potential term coming from the curvature of space, and the matter Hamiltonian, \( H_M(a) \), the adiabatic matter states are simply the instantaneous –in \( a \)– eigenstates \( H_M(a) \). Therefore they coincide with the instantaneous eigenstates –in \( t \)– defined in the Schrödinger framework, since in cosmology, the whole dependence in \( t \) of \( H_M \) comes through \( a(t) \) only.

To address the second point, it is necessary to carry out a second adiabatic expansion applied to the gravitational part of the wave function. This generalizes the usual WKB expansion which has been used in \[1\]–\[3\] to extract a time parameter which governs the Schrödinger equation in the mean geometry. The central result of this paper is the (exact) equation satisfied by the coefficients of this double adiabatic expansion for both matter and gravity.

When one works in the adiabatic approximation for gravity, this equation has a very simple structure: it is a linear, first order equation in \( \partial_a \) and bears a simple interpretation. Indeed, the identification of what replaces the probability amplitudes in Schrödinger equation is straightforward. It describes therefore the non adiabatic transitions amplitudes of matter parametrised by \( a \) rather than \( t \). In this, we generalize \[4\]–\[8\] which were based on time dependent perturbation theory. Indeed, in the adiabatic treatment, the dressing energy of matter states is automatically included in the wave functions describing gravity and non-adiabatic transitions are evaluated from gravitational wave functions wherein this back-reaction effect is fully taken into account. Thus we no longer meet the problem\[4\]–\[8\] of defining transitions amplitudes that are non linear in the coupling constant. These advantages are illustrated in the last part of this article when we return to the examples of radiative transitions and particle creation now treated in quantum cosmology. We explicitly show when and how one recovers the background field result. Mathematically this requires to legitimize a first order expansion in the energy difference \( \Delta E(a) \) that characterizes the transition upon investigation.
Physically it means that the universe be macroscopic, i.e. that the matter sources driving gravity be macroscopic.

When one abandons the adiabatic treatment for gravity, one meets new effects which have no counterpart in quantum mechanics. These arise because one must consider superpositions of solutions describing contracting and expanding universes. In this one inevitably encounters the “Klein paradox”, i.e. the generation of backscattered solutions describing contracting universes when the wave was initially purely forward. As in QFT, these backscattered solutions lead to an increase of the current carried by the forward wave describing expanding universes. Our dynamical equation takes exactly into account the contribution of these backscattered solutions. It can thus be exploited to analyze both conceptually and quantitatively their consequences. One must face indeed a double problem. First, one must adopt a framework in which the generation of backscattered waves can be interpreted. In this respect, one must probably proceed to a “third” quantization. Secondly, there is also the more pragmatic problem which consists in determining their consequences onto the matter propagation restricted to the expanding sector, i.e. onto matter belonging to “our” universe.

From our exact dynamical equation, the much debated question of the unitarity of the evolution can now be phrased in precise mathematical terms. One should indeed first identify what mathematically corresponds to the probability amplitude to find a given adiabatic state at a certain moment. Only then can one hope to settle the question of the unitarity of their evolution. In this article we shall only sketch these problems. We hope to return to them in a future publication.

We conclude by noting that the analysis of the Wheeler-De Witt equation presented here possesses illuminating analogues in other physical systems. Indeed the basic problem, which is not specific to quantum cosmology, is to enlarge the dynamics so that a degree of freedom which was treated classically (the radius of the universe $a(t)$) is treated quantum mechanically. Some of the conceptual issues raised by this enlargement will of course be specific to each problem.

The first analogue is a uniformly accelerated detector which can make non adiabatic transitions from its ground state to its excited state, and vice versa. (The description of these events as non adiabatic transitions can be found in the literature on the Golden Rule). These transitions are characterized by a temperature, in similar fashion that the pair creation events in cosmology which we study in this article are characterized by a temperature. In these works the accelerated system follows a given classical trajectory. However, in order to take into account recoil effects one must go beyond this background field approximation, and describe the accelerated system by WKB wave functions or even by second quantized fields. Then not only is the trajectory treated quantum mechanically, but one can also produce pairs of accelerated systems, which is strongly reminiscent of third quantisation in cosmology. In both cases what should be interpreted as the probability amplitudes to find a given adiabatic state in the forward sector do not obey a closed equation. In other words, “our” expanding universe is not isolated. The accelerated detector system also exhibits a remarkable thermodynamic consistency between the radiative transitions of the detector and the pair production events. In quantum
cosmology we will also find an intimate connection between the dynamics of transitions in the universe and the backscattering of universes. We have however only exhibited this connection in this paper, and have not investigated in detail its consequences.

The second analogue is the description of electronic non elasticity, i.e. transitions between electronic states, during atomic or molecular collisions\[13]\[14\]. The simplest treatment is a background field approximation wherein the nuclear trajectories are given classical functions $R(t)$. The electrons then evolve according to the time dependent Hamiltonian $H_{el}(R(t))$. (This corresponds of course, in our case, to QFT in a given space time.) However one can go beyond this approximation and treat the nuclei quantum mechanically (although in first quantization)\[15]\[16\]. To this end one carries out a double adiabatic development in the electronic adiabatic states and the nuclear WKB wave functions. The equation for the coefficients of this double expansion describe the non adiabatic transitions of the electrons, parametrised by the nuclear coordinates in exactly the same way that the equation for non adiabatic transitions of matter is recovered in quantum cosmology. This equation can be used to investigate the validity of the background field approximation. In particular one can investigate in this context to what extent the notion of a (temporal) succession of electronic transitions depends on the nuclei being in a tight wave packet. The analogy with quantum cosmology obtains therefore both at the formal and at the conceptual level (save for the interpretation of the backscattered waves). Hopefully these systems could be used to investigate experimentally some of the conceptual problems of quantum cosmology.

As a final comment, we wish to acknowledge the fact that many people already appeal to the use of adiabaticity to investigate matter dynamics in quantum cosmology. Suprisingly, to our knowledge the full power of the adiabatic treatment (by opposition to the adiabatic approximation) has not been exploited previously. However, after concluding this work, we became aware of refs.\[17]\[18\] wherein the full treatment is used, although the motivations of these authors and the chosen exemples differ significantly from those of the present paper. Indeed they have restricted their analysis to the “Hawking model” wherein matter consists only of a massless scalar field (because of its possible relevance to inflation), whereas we insist on its generality and applicability to all matter processes. Furthermore they have not used this formalism to analyse the origin of time in quantum cosmology and the related conceptual issues which is the main focus of the present paper.

2 The adiabatic treatment in quantum mechanics

2.1 Instantaneous eigenstates and non adiabatic transitions

In this section we recall the basic features of the adiabatic approximation applied to quantum mechanics. We also review how to compute non-adiabatic transitions. To illustrate the usefulness of this formalism in a cosmological setting, we apply it in sub-sections 2.2 and 2.3 to matter transitions and pair creation amplitudes. We put special emphasis in the role played by the expansion of the universe described by $a = a(t)$ since, in cosmology, the expansion is the cause of non adiabatic transitions. Indeed, in
the absence of expansion, the matter would be described by stationary (un-interfering) eigenstates. This sets the stage for Section 4 where the same transitions will be described in quantum cosmology, wherein gravity is described by wave functions, solutions of the Wheeler-De Witt equation.

The Schrödinger equation that governs the evolution of the state $|\psi(t)\rangle$ is

$$i\partial_t |\psi(t)\rangle = H(t)|\psi(t)\rangle \quad (1)$$

We expand $|\psi(t)\rangle$ in terms of the instantaneous eigenstates of the time dependent Hamiltonian $H(t)$:

$$|\psi(t)\rangle = \sum_n \tilde{c}_n(t)|\psi_n(t)\rangle \quad (2)$$

where

$$H(t)|\psi_n(t)\rangle = E_n(t)|\psi_n(t)\rangle$$

$$\langle \psi_n(t)|\psi_m(t)\rangle = \delta_{n,m} \quad (3)$$

Since $H(t)$ is hermitian, the eigen-energies $E_n(t)$ are real. Inserting the decomposition eq. (2) into eq. (1) yields the equation for the $\tilde{c}_n(t)$

$$i\partial_t \tilde{c}_n(t) = E_n(t) \tilde{c}_n(t) + i \sum_m \langle \partial_t \psi_m(t)|\psi_n(t)\rangle \tilde{c}_m(t) = \sum_m H_{nm}^{\text{eff}}(t) \tilde{c}_m(t) \quad (4)$$

where we have introduced, for later convenience, the effective Hamiltonian $H_{nm}^{\text{eff}}(t)$. Note that the antisymmetry of $\langle \partial_t \psi_m(t)|\psi_n(t)\rangle = -\langle \psi_m(t)|\partial_t \psi_n(t)\rangle$ and the reality of $E_n(t)$ ensure that $H_{nm}^{\text{eff}}(t)$ is hermitian. Therefore the conservation of probability $\sum_n |\tilde{c}_n(t)|^2 = 1$ is guaranteed.

Since the states $|\psi_n(t)\rangle$ are defined up to an arbitrary phase, we may use this freedom to require

$$\langle \psi_n(t)|\partial_t \psi_n(t)\rangle = 0 \quad (5)$$

Note however that if $|\psi_n(t)\rangle$ evolves cyclically during the interval $t_0, t_1$, then the state at $t_1$ will in general differ from state at time $t_0$ by a phase, known as the Berry phase$^{[11]}$. Berry’s phase will not be of concern to us in the present paper since in mini-superspace the matter states depend only on one parameter, the scale factor $a$. In this case Berry’s phase vanishes, since all paths can be mapped one onto another by a reparameterisation. However if one goes beyond mini super space, one should take the Berry phase into account.

Upon absorbing, as in time dependent perturbation theory, the diagonal part of $H_{nm}^{\text{eff}}(t)$ into the definition of new coefficients $c_n(t) = \tilde{c}_n(t) e^{i \int t \, dE_n(t)}$, one obtains

$$\partial_t c_n = \sum_{m \neq n} \langle \partial_t \psi_m(t)|\psi_n(t)\rangle e^{-i \int t \, dE_m(t') - E_n(t')} c_m(t) \quad (6)$$

At this point, it is important to notice that this equation is “almost” reparametrisation invariant. The only term that does not satisfy this invariance is the phase containing the change in energy $E_m(t') - E_n(t')$. As we shall show in section 2.2, it is this factor that
Thus the time dependence of $H$ and eigenvalues$^{[20,21]}$. Secondly, they induce transitions among eigenstates$^{[22]}$. These have two physical consequences. First they modify the instantaneous eigenstates $c$.

The evolution of the new coefficients $\tilde{c}_n(a)$ in terms of the Hamiltonian. Indeed differentiating eq. (3) and taking the scalar product with $\langle \psi_m \vert \psi_n \rangle$ gives directly in terms of the Hamiltonian. Indeed differentiating eq. (3) and taking the scalar product with $\langle \psi_m \vert \psi_n \rangle$.

We shall see in Section 3 that it is in that guise, i.e. wherein $H^{\text{eff}}$ appears only as a factor of $E_m(a) - E_n(a)$ and in the form $dt/da$, that the evolution of the $c_n$ will be delivered in quantum cosmology.

To proceed we must evaluate $\langle \psi_n(t) \vert \partial_t \psi_n(t) \rangle (n \neq m)$. If $H$ is non degenerate this is given directly in terms of the Hamiltonian. Indeed differentiating eq. (3)

$$\partial_t H \vert \psi_n \rangle + H \vert \partial_t \psi_n \rangle = \partial_t E_n \vert \psi_n \rangle + E_n(t) \vert \partial_t \psi_n \rangle$$

and taking the scalar product with $\langle \psi_m \vert$ yields

$$\langle \psi_m \vert \partial_t \psi_n \rangle = \frac{\langle \psi_m \vert \partial_t H \vert \psi_n \rangle}{E_n - E_m}, \quad n \neq m$$

Thus the time dependence of $H(t)$ leads to non-vanishing off diagonal elements in $H^{\text{eff}}$. These have two physical consequences. First they modify the instantaneous eigenstates and eigenvalues$^{[20,21]}$. Secondly, they induce transitions among eigenstates$^{[22]}$.

The first effect is described by carrying out an instantaneous diagonalisation of $H^{\text{eff}}(t)$ to obtain new eigenstates and eigenvalues: $H^{\text{eff}}(t) \vert \psi_n^{(1)}(t) \rangle = E_n^{(1)}(t) \vert \psi_n^{(1)}(t) \rangle$. After having diagonalised $H^{\text{eff}}(t)$, one can decompose $\vert \psi \rangle$ as $\vert \psi(t) \rangle = \sum_n \tilde{c}_n^{(1)}(t) \vert \psi_n^{(1)}(t) \rangle$. The evolution of the new coefficients $\tilde{c}_n^{(1)}(t)$ is given by a new effective Hamiltonian $H^{\text{eff}(1)}(t)$. One can then iterate the procedure and diagonalise $H^{\text{eff}(1)}(t)$. This generates an asymptotic series for the state $\vert \psi(t) \rangle$. The series starts diverging when the difference between successive terms becomes comparable to the amplitude for non adiabatic transition.

To work in the adiabatic approximation consists in neglecting the second effect, namely non adiabatic transitions between instantaneous eigenstates. In general, to compute the amplitude of these transitions, it is sufficient to consider only a couple of states, say $\vert \psi_1 \rangle$ and $\vert \psi_2 \rangle$. Then eq. (3) reduces to

$$\begin{align*}
\partial_t c_1 &= \langle \partial_t \psi_2 \vert \psi_1 \rangle \ e^{-i \int^t dt (E_2 - E_1)} \ c_2 \\
\partial_t c_2 &= \langle \partial_t \psi_1 \vert \psi_2 \rangle \ e^{-i \int^t dt (E_1 - E_2)} \ c_1
\end{align*}$$

Let us further assume that at $t = -\infty$ the system is in the state $\psi_1$, i.e. $c_1(-\infty) = 1$, $c_2(-\infty) = 0$. Then the transition amplitude is given by $c_2(+\infty)$. To evaluate it, we proceed exactly like in perturbation theory by taking $c_1 = 1$ in eq. (10) to obtain

$$c_2(+\infty) \simeq \int_{-\infty}^{+\infty} dt \langle \psi_2 \vert \partial_t \psi_1 \rangle \ e^{-i \int^t dt (E_1(t') - E_2(t'))}$$

(11)
We consider only the case in which the resonance condition $E_1(t) - E_2(t) = 0$ has no real solution. This is generally the case in physical problems, because if there is an interaction between the two energy levels the degeneracy is lifted to give rise to an avoided crossing. Then, when the transition amplitude is small, it can be correctly evaluated by a saddle point treatment, exactly like in other cases of classically forbidden transitions such as tunneling processes. The saddle is located at the complex value of $t^*$, solution of $E_1(t^*) - E_2(t^*) = 0$. The result is thus

$$c_2(\pm \infty) \simeq C e^{-i \int_{-\infty}^{t^*} dt'(E_1 - E_2)}$$

(12)

A rigorous analysis shows that $C$ tends to 1 in the adiabatic limit, $\partial_t(E_1 - E_2)/(E_1 - E_2)^2 \to 0$, see [23]. If the problem cannot be reduced to that of two coupled states, then the analysis is more complicated because the non adiabatic transitions can occur by “hopping” from one energy eigenstate to the other, see [24].

### 2.2 The Golden Rule and non-adiabatic transitions

In this section we apply the adiabatic formalism to radiative transitions in cosmology in order to display the crucial role played by the classical expansion $a = a(t)$. The particular problem we consider is the disintegration of a heavy state of mass $M$ into a light state of mass $m$ and a conformally coupled scalar quantum $\phi$. In the language of Unruh, $M$ and $m$ represent the excited and ground state of a particle detector of the $\phi$ field. As in the Unruh analysis, the recoil of the heavy system is neglected. Because this transition takes place in an expanding universe, the energy of the emitted quantum (measured in proper time) is $k/a(t)$ where $k^2$ is the conserved eigenvalue of the three Laplacian. The free initial and final energies are thus $E_{\text{initial}}^0 = M$ and $E_{\text{final}}^0 = m + k/a$. They coincide when the Doppler red shifted energy of the photon is equal to $M - m$, i.e. when

$$a(t_0) = a_0 = \frac{k}{\Delta M}$$

(13)

Thus, in time dependent perturbation theory based on free states, the transition will occur around that value of $a$ wherein the energy of the photon resonates with $\Delta M [7]$. In what follows, we shall see that non adiabatic transitions will also occur in the vicinity of $t_0$ even though the meaning of “to make a transition” will change.

The unperturbed states are coupled by an interaction Hamiltonian

$$H_{\text{int}}(a) = g \left( |M> <m|\hat{\phi} + h.c. \right) = g \left( |M> <m| \sum_k \frac{1}{ak^{1/2}} (b_k + b_k^\dagger) + h.c. \right)$$

(14)

Thus the full Hamiltonian is

$$H(a) = \begin{pmatrix} M & g/ak^{1/2} \\ g/ak^{1/2} & m + k/a \end{pmatrix}$$

(15)

As pointed after eq. (6), the time dependence comes only through $a = a(t)$. Therefore, one can directly work with $a$ as relevant parameter. Because of the non-diagonal elements...
induced by $H_{\text{int}}$, the degeneracy of the free states at $a_0$ is lifted to give an “avoided crossing”\cite{22} when one considers the instantaneous eigenstates, $|\psi_+\rangle$ and $|\psi_-\rangle$, which diagonalize $H(a)$. Indeed, their corresponding eigenvalues are

$$E_\pm(a) = \frac{M + m + k/a}{2} \pm \sqrt{(M - m - k/a)^2 / 4 + g^2 / a^2 k}$$  \hspace{1cm} (16)$$

They coincide only for the complex values

$$a^* \pm = a_0 \pm \frac{i2g}{\Delta M k^{1/2}} = a_0 \pm i\Delta a_i$$  \hspace{1cm} (17)$$

The principle effect of this avoided crossing (for real values of $a$) is that the instantaneous eigenstate $|\psi_+\rangle$ ($|\psi_-\rangle$) which for $a \ll a_0$ coincides with the free initial (final) state $|\psi_{\text{initial}}\rangle$ ($|\psi_{\text{final}}\rangle$) tends to the free state $|\psi_{\text{final}}\rangle$ ($|\psi_{\text{initial}}\rangle$) for $a \gg a_0$. Thus what corresponds to the transition amplitude in terms of free states is given by the amplitude to stay in the same instantaneous eigenstate, whereas the amplitude to stay in the same free state is given by the amplitude to make a non-adiabatic transition from $|\psi_+\rangle$ to $|\psi_-\rangle$.

By writing the probability to make a non-adiabatic transition, that is to stay in the excited state $M$ as

$$P_{\text{no transition}}(k) = e^{-2\mathcal{I}_k}$$  \hspace{1cm} (18)$$

using eqs. (6, 12), we have,

$$\mathcal{I}_k = \text{Im} \int_{a_0}^{a^*} da \frac{dt}{da}(a) [E_+(a) - E_-(a)]$$  \hspace{1cm} (19)$$

since only the integral for imaginary (positive) values of $a$ contributes to $\mathcal{I}_k$. To evaluate this integral, we assume that $g$ be small enough so as to justify the following approximation

$$\mathcal{I}_k \approx \frac{1}{a_0} \frac{dt}{da}(a_0) \text{Im} \int_{a_0}^{a^*} da \sqrt{(\Delta Ma - k)^2 + 4g^2 / k} = \frac{\pi g^2}{k^2} \frac{dt}{da}(a_0)$$  \hspace{1cm} (20)$$

Within this quadratic approximation, the probability for no transition is given exactly by eq. (18), see [14]. This exact result plays an important role here since it guarantees that the probability not to decay decreases exponentially in (proper) time, see eq. (22). This probability is given by

$$P_{\text{no transition}}(a) = \prod_{k(a)} P_{\text{no transition}}(k) = e^{-2\int^{k(a)} \frac{d^3k}{(2\pi)^3} \mathcal{I}_k}$$  \hspace{1cm} (21)$$

To carry out the integral over $k$ in the exponent, we first use the isotropy of the space-time to write $d^3k = 4\pi k^2 dk$ (for simplicity, we work with flat three-geometries). Furthermore, by using the resonance condition eq. (13), we can write $dk$ as $\Delta Ma_0$ and thus relate the final value of $a$ to a maximum value of $k$, see [23] for a more detailed treatment.
concerning the relationships between the integration over momenta and an integration over time (or \(a\)). Using that relation and eq. (20), one gets

\[
P_{\text{no transition}}(a) = e^{-\frac{g^2 \Delta M}{\pi} \int a_0^a \frac{da}{da}} = e^{-\frac{g^2 \Delta M}{\pi} \int t(a) dt}
\] (22)
corresponding to an exponential decay probability in proper time. It agrees with the probability evaluated using more traditional techniques[7].

It is interesting that in the present formalism the role of time and energy seem to be reversed compared to usual treatment of the Golden Rule. Namely if the particle does not decay it seems to be propagating in complex time, see eq. (17), whereas one usually ascribes a complex energy to unstable states. And the time \(T = \int dt\) which multiplies the decay rate in eq. (22) arises from an integral over \(k\), whereas it is usually obtained by letting the excited states interact with the field through \(H_{\text{int}}\) for a finite time \(T\).

The treatment presented here can be enlarged to include the effects of momentum recoils. This gives rise, as discussed in [7], to the concept of spatial displacement.

2.3 Particle creation as a non adiabatic process

In this section we apply the adiabatic formalism to particle creation in the universe. This particle production[26, 27] is a generic feature of quantum field theory which is due to the expansion law \(a = a(t)\).

When the cosmological expansion is described by a classical law, the equation for free matter fields is linear in the dynamical variables. Therefore, it is particularly useful to work in the Heisenberg picture since probability amplitudes to create pairs can be directly evaluated from the sole knowledge of the Bogoliubov coefficients. However, upon abandoning the background field approximation for gravity by working in quantum cosmology, one looses the linearity of the field equation since \(a\) is now a dynamical variable coupled to matter at a quantum level. As noted in [3], this loss of linearity imposes to work in a Schrödinger picture since every transition amplitude should be computed separately. Therefore, in what follows, as a preparation for the analysis in quantum cosmology, we study pair creation amplitudes in the Schrödinger picture. In this picture, they correspond to non-adiabatic transitions among instantaneous eigenstates.

We shall work in a closed Robertson-Walker universe

\[
ds^2 = -dt^2 + a^2(t) \sum_{i,j} h_{ij} dx^i dx^j
\] (23)
where

\[
h_{ij} = \frac{dr^2}{1 - r^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2
\] (24)
The action for a massive hermitian field is

\[
L = \frac{1}{2} \int dt \int d^3 x \sqrt{h} a^3 \left[ \partial_i \phi \partial_i \phi - a^{-2} h^{ij} \partial_i \phi \partial_j \phi - m^2 \phi^2 \right]
\] (25)
The symmetry of the space allows $\phi$ to be decomposed as

$$\phi(t, x) = \sum_k Y_k(x) \phi_k(t)$$  \hspace{1cm} (26)

where $Y_k$ are normalized eigenfunctions of the spatial Laplacian. Using eq. (26), the action reads

$$L = \sum_k \int dt a^3(t) \left[ \partial_t \phi_k \partial_t \phi_{-k} - \Omega_k^2(t) \phi_k \phi_{-k} \right]$$  \hspace{1cm} (27)

where $\Omega_k(a) = (m^2 + k^2 a^{-2})^{1/2}$ is the time dependent frequency at fixed $k$.

The momentum conjugate to $\phi_k$ is $\Pi_k = a^3 \partial_t \phi_{-k}$, and the Hamiltonian is

$$H(a) = \sum_k \left[ a^{-3} \Pi_k \Pi_{-k} + a^3 \Omega_k^2(a) \phi_k \phi_{-k} \right] = \sum_k H_k(a)$$  \hspace{1cm} (28)

We now carry out the instantaneous diagonalisation of $H_k(a)$. To this end we express the Schrödinger operators $\phi_k$ and $\Pi_k$ in terms of the $a$-dependent creation and destruction operators $b_k(a)$

$$\phi_k = \frac{1}{\sqrt{2(a^3 \Omega_k)^{1/2}}} (b_k + b_{-k}^\dagger)$$
$$\Pi_k = \frac{1}{\sqrt{2}} i(a^3 \Omega_k)^{1/2} (b_{-k} - b_k^\dagger)$$  \hspace{1cm} (29)

Inserting eq. (29) into eq. (28) yields

$$H_k(a) = \Omega_k(a)(b_k^\dagger b_k + b_{-k}^\dagger b_{-k})$$  \hspace{1cm} (30)

where we have subtracted the ground state energy by normal ordering with respect to the instantaneous operators $b_k$. The instantaneous eigenstates are therefore those of definite particle number

$$|\psi_{\{n_k\}}(a)\rangle = \prod_k \frac{(b_k^\dagger)^{n_k}}{\sqrt{n_k!}} |0_a\rangle$$
$$E_{\{n_k\}}(a) = \sum_k \Omega_k(a) n_k$$  \hspace{1cm} (31)

where $\{n_k\}$ denotes the collection of occupation numbers and $|0_a\rangle$ the instantaneous vacuum state.

The equation governing non adiabatic transitions is

$$\partial_a c_{\{n_k\}} = \sum_{\{n_{k'}\}} \langle \partial_a \psi_{\{n_{k'}\}} | \psi_{\{n_k\}} \rangle e^{-i \int^{t(a)} dt' (E_{\{n_{k'}\}} - E_{\{n_k\}})} c_{\{n_{k'}\}}$$  \hspace{1cm} (32)

where the state of the $\phi$ field has been decomposed as

$$|\psi(a)\rangle = \sum_{\{n_k\}} c_{\{n_k\}}(a) |\psi_{\{n_k\}}(a)\rangle$$  \hspace{1cm} (33)
To obtain an expression for \( \langle \psi_{\{n_k\}} | \partial_a \psi_{\{n'_k\}} \rangle \), we must calculate \( \partial_a H_k \), see eq. (9),

\[
\partial_a H_k = \partial_a \Omega_k \left( b_k^\dagger b_k + b_{-k}^\dagger b_{-k} \right) + \Omega_k(a) \frac{\partial_a (a^3 \Omega_k)}{a^3 \Omega_k} \left( b_k^\dagger b_{-k}^\dagger + b_k b_{-k} \right)
\]

\( \partial_a H_k \) contains two terms. The first is diagonal in the basis of instantaneous eigenstates and is due to the adiabatic deformation of the eigen-energy through \( \Omega_k(a) \). The second term is due to the time dependence of the operators \( b_k(a), b_k^\dagger(a) \). It couples states which differ by a pair of particles of opposite momentum and engenders non adiabatic transitions. Thus the corresponding physical processes are pair creation (or destruction) of particles with opposite momentum.

We now consider the process of creation of a pair from vacuum. Thus we seek the amplitude for the non adiabatic transition from the ground state \( |0_a\rangle \) to the two particle state \( b_k^\dagger b_{-k}^\dagger |0_a\rangle = |1_k, 1_{-k}\rangle \). We assume that the creation process be small enough so as to legitimate a description restricted to these two states. In that case, the equations are, see eq. (10),

\[
\begin{align*}
\partial_a c_0 &= \frac{1}{2} \frac{\partial_a (a^3 \Omega_k)}{a^3 \Omega_k} e^{-2i \int_{t_0}^{t} \Omega_k c_{k,-k} dt'} \\
\partial_a c_{k,-k} &= \frac{1}{2} \frac{\partial_a (a^3 \Omega_k)}{a^3 \Omega_k} e^{2i \int_{t_0}^{t} \Omega_k c_{0} dt'}
\end{align*}
\]

Thus, for rare creation acts, the probability to produce a pair is, see eqs. (12),

\[
|A_{\text{pair}}|^2 = e^{-Im \left[ \frac{1}{4} \int_{-\infty}^{t(a^*)} \sqrt{m^2 + k^2/a^2} dt \right]}
\]

where \( a^* \) is the complex saddle point defined by \( \Omega_k(a^*) = 0 \) in the positive imaginary half plane.

To illustrate the above formalism, we apply it to de Sitter space. In that case, the expansion is given by

\[
a(t) = \frac{1}{\sqrt{\Lambda}} \cosh \sqrt{\Lambda} t
\]

Thus the complex saddle point of eq. (36) is

\[
\begin{align*}
a^*_\pm &= \pm ik/m \\
t^*_\pm &= t_0 \pm i\Delta t = \frac{1}{\sqrt{\Lambda}} \arcsinh \frac{m}{k\sqrt{\Lambda}} \pm i\pi/2\sqrt{\Lambda}
\end{align*}
\]

It lies in the vicinity of the real time \( t_0 \) at which \( k/a \approx m \), i.e. where the particle ceases to be relativistic. When \( m > \sqrt{\Lambda} \), the probability to produce a pair is small and eq. (36) can be used. The integral is most easily evaluated in the limit of large \( k \), i.e. for \( |a^*| \gg 1/m \). Indeed, in that limit, as in eq. (20), the integrant is quadratic in \( a \)

\[
\text{Im} \left[ 4 \int_{-\infty}^{t_{\text{a}}} \sqrt{m^2 + k^2/a^2} dt \right] = \text{Im} \left[ 4 \int_{a_0}^{a_{\text{a}}} \frac{da}{a} \sqrt{m^2 a^2 + k^2} \right] \approx \text{Im} \left[ \frac{1}{a_0^2 \sqrt{\Lambda}} \int_{a_0}^{a_{\text{a}}} da \sqrt{m^2 a^2 + k^2} \right] = \pi m/\sqrt{\Lambda}
\]
where we have used \( da/dt = a\sqrt{\Lambda} \) valid for large \( a \), and replaced \( a_0 = a(t_0) = k/m \). Thus we have
\[
|A_{\text{pair}}|^2 \simeq e^{-\pi m/\sqrt{\Lambda}}.
\] (40)
This corresponds to the Boltzmannian tail of a thermal distribution at the de Sitter temperature \( T = \sqrt{\Lambda}/\pi \). This is as it should be since the use of the saddle point calculation and neglect of multi pair states cannot reproduce the full Bose Einstein distribution\([27]\).

Before considering how to recover these transitions in quantum cosmology, we shall first relate the present analysis to the more conventional analysis of pair creation based on the solutions of the Klein Gordon equation. The main motivation for this study is that it introduces tools that will be extremely usefull upon studying the solutions of the WDW equation.

### 2.4 The WKB approximation and pair creation

The aim of this section is to phrase in adiabatic terms the standard results concerning the WKB approximation and the backscattering amplitude above a barrier. This will clarify the relationship between pair creation probabilities as calculated above and backscattering. The necessity of normalizing properly the Wronskian of the WKB solutions will be stressed. This will also prepare for the analysis of the solutions of the WDW equation for which a correct normalisation will also be essential.

Consider a one dimensional harmonic oscillator whose frequency depends on time
\[
\left[ \partial_t^2 + \omega^2(t) \right] \varphi(t) = 0 \quad (41)
\]
The WKB solution of unit Wronskian is
\[
\chi(t) = \frac{e^{-i \int_{-\infty}^t d\omega(t)}}{\sqrt{2\omega(t)}} \quad (42)
\]
One can then expand the exact solution in terms of \( \chi(t) \) and \( \chi(t)^* \) as
\[
\varphi(t) = c(t)\chi(t) + d(t)\chi^*(t) \quad (43)
\]
We determine completely the coefficients \( c \) and \( d \) by requiring that
\[
i\partial_t \varphi(t) = \omega(t) \left[ c(t)\chi(t) - d(t)\chi^*(t) \right] \quad (44)
\]
This guarantees that \( c \) and \( d \) are constant in the WKB limit, i.e. in the adiabatic limit \( \partial_t \omega(t)/\omega(t)^2 \to 0 \). Moreover, the conserved current (or Wronskian) takes the simple form
\[
\varphi^*i\partial_t \varphi = |c(t)|^2 - |d(t)|^2 = \text{constant} \quad (45)
\]
This equation replaces the unitary relation governing the coefficients \( c_n(t) \), solutions of the Schrödinger equation, see 2.1. To obtain \( c \) and \( d \), one differentiates eq. (43) and compares the result with eq. (45), so as to obtain
\[
\chi \partial_t c + \chi^* \partial_t d - \frac{1}{2} \frac{\partial_t \omega}{\omega} (\chi c + \chi^* d) = 0 \quad (46)
\]
Now differentiating eq. (44), inserting the result into eq. (41), and using eq. (46) to eliminate either $\partial_t c$ or $\partial_t d$ yields the coupled first order equations

$$
\partial_t c = \frac{1}{2} \frac{\partial_\omega}{\omega} e^{-2it} \int_{-\infty}^{t} dt' \omega d
$$

$$
\partial_t d = \frac{1}{2} \frac{\partial_\omega}{\omega} e^{+2it} \int_{-\infty}^{t} dt' \omega c
$$

(47)

These equations are equivalent to the original equation for $\varphi$, eq. (41). This has been discussed in detail in [28]. They constitute a convenient starting point for the evaluation of the non-adiabatic transitions, which in the present case correspond to backscattering. As in Section 2.1 they are given by the value of value of $d$ at late times, given that $c = 1, d = 0$ at early times. Using the same type of analysis as in section 2.1, one obtains

$$
d(+\infty) \simeq \int_{-\infty}^{+\infty} dt \frac{\partial_\omega}{2\omega} e^{-2it} \int_{-\infty}^{t} d\omega' \omega(dt')
$$

(48)

As before, the saddle point is at the complex value $t^*$ such that $\omega(t^*) = 0$. The norm of $d$ is thus

$$
|d(+\infty)|^2 \simeq C e^{-4Im \int_{-\infty}^{t^*} \omega(dt')}
$$

(49)

A rigorous analysis shows that $C$ tends to 1 in the adiabatic limit [29].

To obtain the relation between this norm and the probability to produce a pair of quanta as calculated in section 2.3, we must first determine the frequency $\omega(t)$ that corresponds to $\Omega_k(a)$ which characterizes the instantaneous energy of a particle of momentum $k$. A standart calculation yields

$$
\omega(t) = \Omega_k(a(t)) - \left( \frac{3}{4} \frac{\partial_i a^2}{a^2} + \frac{3}{2} \frac{\partial^2 a}{a} \right)
$$

(50)

The additional terms arise from the factor of $a^{3/2}$ which relates the amplitude of $\phi_k(t)$ appearing in eq. (28) to $\varphi(t)$. It is important to note that the backscattering amplitude and the pair creation amplitude are related by $|d(+\infty)|^2 = |A_{\text{pair}}|^2$ only if the Wronskians of the WKB waves that multiply $c$ and $d$ are chosen in conformity with the second quantized framework, i.e. are equal to one. In the present case of a single linear equation, only the relative normalisation plays a role, however upon introducing coupling among many oscillators, the normalisation is completely fixed, see [3, 4, 5, 6, 7].

We wish to emphasize this last point since it will play a crucial role in quantum cosmology. The question of the choice of the Wronskians can be considered from two different perspectives. The usual approach is based on the second quantized framework. In that case, the choice of unit Wronskian is directly dictated by the particle interpretation of the Heisenberg creation and destruction operators. However, there is another point of view which is more related to our present understanding of quantum gravity. It is based on the semi-classical behaviour of some dynamical variable (say $a$). In physical circumstances in which $a$ behaves “almost” classically, two different schemes can be used to describe quantum processes occuring to the other variables. First, one can work in the background field approximation for $a$ (in which case, one has quantum fields in a given
gravitational background). Secondly, we can work in an extended quantum framework and use WKB waves for describing a. Then, in order for the two versions of transition amplitudes to coincide, the Wronskians of the WKB waves are univoquely fixed. Therefore, in the next sections, the gravitational waves shall have unit Wronskians, since we must recover the Schrödinger equation in the limit in which a can be described at the background field approximation.

3 The adiabatic treatment in quantum cosmology

3.1 When matter energy is a conserved quantity

As a warming up, we first analyse the WDW equation in the simple case when the matter energy is a constant of motion (which is a stronger condition than being adiabatically conserved). This implies that states with different matter energy are completely decorrelated. In the next sections we shall drop this assumption and see how the coupling to gravity introduces the notion of evolution through interferences among neighbouring matter states characterized by adiabatically conserved energy.

We work in a closed Robertson-Walker universe whose metric is given in eq. (23). Then, only one constraint survives corresponding to the reparametrisation invariance \( t = t(t') \). Classically, this constraint is

\[
H = \frac{-G^2 \pi_a^2 - a^2 + \Lambda a^4}{2Ga} + H_M(\phi, \Pi, a) = 0
\]  

(51)

where \( a \) is the scale factor now promoted to a dynamical variable, \( \pi_a \) its conjugate momentum, \( H_M \) is the matter hamiltonian, with \( \phi \) and \( \Pi \) canonically conjugate matter degrees of freedom. \( \Lambda \) is the cosmological constant. It shall play no other role than to participate to the determination of \( \pi_a \) in terms of \( a \) and \( H_M \).

For the matter energy to be a conserved quantity \( H_M \) must have the form

\[
H_M(\phi, \Pi, a) = a^p h_M(\phi, \Pi)
\]

(52)

(or a sum of such terms). The simple example we consider a very massive field at rest (i.e. \( k = 0 \)). Then \( H_M = h_M = (\Pi^2 + M^2 \phi^2)/2 \) where \( M \) is the mass of the particles, see [3]. Here \( \Pi \) and \( \phi \) are rescaled by a factor \( a^{3/2} \) with respect to the fields defined in section 2.3. This rescalling replaces the adiabatically invariant states characterized by instantaneous occupation numbers given in eq. (33), by truly invariant states characterized by fixed occupation number.

In quantum cosmology, the physical states \( \Xi(a, \phi) \) are solutions of the WDW constraint

\[
\mathcal{H} \Xi(a, \phi) = \left[ G^2 \partial_a^2 - a^2 + \Lambda a^4 + 2GaH_M(\phi, i\partial_\phi, a) \right] \Xi(a, \phi) = 0
\]

(53)

(We neglect any ambiguity due to ordering problems. These would add terms proportional to \( G^2/a^2 \) which could easily be taken into account.) When, \( H_M \) is of the form eq.
(52), \( h_M \) is independent of \( a \) and commutes with \( \mathcal{H} \). We can thus work in a basis of eigenstates of \( h_M \)

\[
\begin{align*}
  h_M |\psi_n\rangle &= E_n |\psi_n\rangle \\
  \langle \psi_m | \psi_n \rangle &= \delta_{m,n}
\end{align*}
\]

(54)

Notice that these eigenstates coincide with the stationary eigenstates of the Schrödinger equation \( i\partial_t |\psi(t)\rangle = h_M |\psi(t)\rangle \), see section 2.1. Using these states, we can decompose \( \Xi \) as

\[
\Xi(a, \phi) = \sum_n C_n \Psi_n(a) \langle \phi | \psi_n \rangle
\]

(55)

Thus, since \( \partial_a |\psi_n\rangle = 0 \), the different terms in eq. (55) are completely uncorrelated. The \( n \)-th wave function \( \Psi_n(a) \), entangled to the matter state \( |\psi_n\rangle \), obeys

\[
\left( -G^2 \partial_a^2 - a^2 + \Lambda a^4 + 2 GaE_n \right) \Psi_n(a) = 0
\]

(56)

It corresponds to the equation for an oscillator whose time (= \( a \)) dependent frequency is given by

\[
\omega^2(a) = \left( -a^2 + \Lambda a^4 + 2 GaE_n \right) / G
\]

(57)

The solutions of this equation have been discussed in section 2.4.

To make contact with former works\[3\][4][30], we recall how a time parameter can be extracted from wave packets made out WKB solutions of eq. (56). Following\[7, 8\], we shall then recall why interactions leading to transitions must be added in order to give physical substance to the expressions.

The WKB solution of eq. (56) with positive unit wronskian is

\[
\chi_n(a) = e^{-i \int^a da p_n(a)}
\]

(58)

where the momentum \( p_n(a) \) is the solution of eq. (57) with \( H_M = E_n \), hence given by

\[
p(a, E_n) = p_n(a) = \frac{1}{G} \sqrt{-a^2 + \Lambda a^4 + 2 GaE_n}
\]

(59)

These WKB solutions correspond to expanding universes. Their complex conjugate describe contracting universes.

Consider now a superposition, eq. (55), made out of WKB solutions with positive Wronskian only. Let’s further assume that the coefficients \( C_n \) form a well peaked enveloppe centered around the mean value \( \bar{n} \) such that the phase shifts appearing in the sum can be evaluated to first order in \( n - \bar{n} \) only and that the dependance in \( n - \bar{n} \) of the prefactors \( p_n(a)^{-1/2} \) be neglected, see subsection 3.3 for more details. Then eq. (55) can be factorized as

\[
\Xi(a, \phi) = e^{-i \int^a da p_n(a)} \left[ \sum_n C_n e^{-i(E_n-E_{\bar{n}}) \int^a da E_n} \langle \phi | \psi_n \rangle \right]
\]

(60)
The factor of \(E_n - E_{\bar{n}}\)

\[
\partial_E \int^a da \, p(a, E)|_{E=E_{\bar{n}}} = t_{\bar{n}}(a)
\]

(61)

is the lapse of proper time evaluated in the classical geometry driven by the mean matter energy \(E_{\bar{n}}\), in virtue of Hamilton-Jacobi equations.

Thus, well peaked wave packets in quantum cosmology factorize into a gravitational piece characterized by the mean matter energy and and a linear superposition of matter states multiplied by the conventional phase factors parametrised by the mean time \(t_{\bar{n}}(a)\). However, in this model characterized by constants of motion, this quantum superposition is physically empty since there is nothing to probe the evolution, i.e. to give physical meaning to the phase factors which arise precisely from the comparison of neighbouring gravitational waves entangled to the corresponding matter states. Therefore, neither a physical interpretation can be given to the coefficients \(C_n\) nor can a principle be invoqued to normalise them.

On the contrary when the matter hamiltonian no longer commutes with the WDW constraint (i.e. which now depends on \(a\)) the interactions among matter states gives a precise physical meaning to both the phase \(\Delta E \int da \partial_E p(a, E) = \Delta Et\) and to the coefficients \(C_n\) whose normalisation will be univoquely fixed. Indeed, \(\Delta Et\) is the phase which accumulates between successive transitions and therefore which governs their rate. And the coefficients \(C_n\) obey a Schrödinger equation only if the Wronskians of the corresponding gravitational waves \(\chi_n(a)\) are all the same, see the end of section 2.4.

### 3.2 Non adiabatic transitions in quantum cosmology

In this subsection, the matter hamiltonian depends explicitly on \(a\). Examples of such Hamiltonians where analysed in section 2.2 and 2.3. They will be further discussed in section 4. The coefficients \(C_n\) then depend on \(a\). To obtain the equation which govern their evolution, we must extend the usual adiabatic procedure given in section 2.1. Indeed, because of the second order character of the WDW equation, a double adiabatic development is now required to obtain a linear equation in \(\partial_a\) for the \(C_n\). First, as in section 2.1, we diagonalise instantaneously the matter hamiltonian and secondly, we apply an adiabatic decomposition of the type given in eq. (43) to the gravitational wave functions entangled to the instantaneous matter eigenstates. Moreover, in order to determine univoquely the coefficients \(C_n\), an additional mathematical condition must still be supplied. We proceed formaly by imposing that \(\Xi(a, \phi)\) satisfies an equation that generalyses eq. (44). The resulting equation for the \(C_n\) describes both non-adiabatic transitions between matter eigenstates and the backscattering from expanding universes into contracting ones. The physical meaning of this equation will be analyzed in the next sections.

Thus, first, we carry out an instantaneous diagonalisation, i.e. at fixed \(a\), of \(H_M\):

\[
H_M(a)|\psi_n(a)\rangle = E_n(a)|\psi_n(a)\rangle
\]

\[
\langle \psi_m(a)|\psi_n(a)\rangle = \delta(m, n)
\]

(62)
We emphasize once more that this diagonalisation does not require the “existence” of a Schrödinger equation, although the eigenstates \( \psi_n(a) \) and the eigenvalues \( E_n(a) \) coincide with ones that one would have obtained if one had started, as in section 2.1, from the Schrödinger equation whose r.h.s. contains the hamiltonian given by \( H_M(a(t)) \).

Using these instantaneous eigenstates, \( \Xi(a, \phi) \), solution of the Wheeler-DeWitt equation (53) can be decomposed, as in eq. (55) but without any lost of generality, as

\[
\langle \phi | \Xi(a) \rangle = \Xi(a, \phi) = \sum_n \varphi_n(a) \langle \phi | \psi_n(a) \rangle.
\]

(63)

The difference with eq. (55) is that the waves \( \varphi_n(a) \) are no longer decorrelated since the instantaneous eigenstates \( |\psi_n(a)\rangle \) do now depend on \( a \). In section 3.4, the correlations among the \( \varphi_n(a) \) will be related to the non-diagonal matrix elements of \( \partial_a \pi_a^2 \), the kinetical term of gravity viewed as an operator acting in the matter Fock states.

Up to now, no difference exists between the present development and the adiabatic treatment of section 2.1. The difference arise from the fact that the WDW constraint is second order in \( \partial_a \). Therefore, to obtain a first order equation for the coefficients \( C_n \), we must proceed to a second adiabatic development. To this end, we express each \( \varphi_n(a) \) in terms of the WKB waves \( \chi_n(a) \), eqs. (58, 59) with \( E_n \) replaced by \( E_n(a) \):

\[
\varphi_n(a) = C_n(a) \chi_n(a) + D_n(a) \chi_n^*(a)
\]

(64)

In the limit where both the adiabatic approximation for the matter states and the WKB approximation for gravity are valid, the coefficients \( C_n \) and \( D_n \) are constants. In that case, we recover the situation presented in section 3.1 wherein there is no correlations among the coefficients \( C_n \) and \( D_n \).

To describe these correlations in the general case, we first need to complete the definition of \( C_n \) and \( D_n \). We proceed mathematically. Notice however that this mathematical choice has deep physical consequences since we shall attribute a physical interpretation to the \( C_n \). We generalise eq. (44) and require

\[
\langle \psi_n(a) | i \partial_a | \Xi(a) \rangle = p_n(a) [ C_n(a) \chi_n(a) - D_n(a) \chi_n^*(a) ]
\]

(65)

The reason for this choice is that it ensures that the total current carried by \( \Xi(a, \phi) \) contains no terms proportional to \( \partial_a C_n(a) \) or \( \partial_a D_n(a) \). Indeed, one has

\[
\langle \Xi(a) | i \partial_a | \Xi(a) \rangle = \int d\phi \, \Xi^*(a, \phi) i \partial_a \Xi(a, \phi) = \sum_n |C_n(a)|^2 - |D_n(a)|^2 = C
\]

(66)

Notice that the absence of relative factors in the above sum directly follows from our choice of identical (unit) Wronskians. The same remark also applies to the next two equations. We are now in position to determine the \( a \)-dependance of \( C_n \) and \( D_n \). Taking the derivative of eq. (63) and using eq. (65) yields

\[
\partial_a C_n \chi_n + \partial_a D_n \chi_n^* - \frac{\partial_a p_n}{2 p_n} (C_n \chi_n + D_n \chi_n^*) + \sum_m \langle \psi_n | \partial_a \psi_m^{\ast} \rangle (C_m \chi_m + D_m \chi_m^{\ast}) = 0
\]

(67)
Then taking the derivative of eq. (65), inserting it in the WDW equation, and using eq. (67) to eliminate either \( \partial_a C_n \) or \( \partial_a D_n \) yields

\[
\partial_a C_n = \sum_{m \neq n} \langle \partial_a \psi_m | \psi_n \rangle \frac{p_n + p_m}{2 \sqrt{p_n p_m}} e^{-i \int^a (p_n - p_m) da} C_m + \sum_m \langle \partial_a \psi_m | \psi_n \rangle \frac{p_n - p_m}{2 \sqrt{p_n p_m}} e^{-i \int^a (p_n + p_m) da} D_m + \frac{\partial_a p_n}{2p_n} e^{-2i \int^a p_n da} D_n
\]

(68)

and the same equation with \( C_n \leftrightarrow D_n, \ i \leftrightarrow -i \).

This is our central equation. We emphasize that it is equivalent to the original WDW equation (51). Its physical meaning is investigated in the next sections.

### 3.3 Time evolution and unitary evolution

To begin the analysis of eq. (68), we assume in this section that the coupling between expanding and contracting universes may be neglected. In the next section, we shall take this unusual quantum coupling into account.

Thus, we drop the second and third term on the r.h.s. of eq. (68). This yields

\[
\partial_a C_n = \sum_{m \neq n} \langle \partial_a \psi_m | \psi_n \rangle \frac{p_n + p_m}{2 \sqrt{p_n p_m}} e^{-i \int^a (p_n - p_m) da} C_m e^{-i \int^a (E_n - E_m) dt} C_m
\]

(69)

In what follows, we shall proceed to the interpretation of this equation in three steps by progressively relaxing restrictions imposed on the coefficients \( C_n \).

When comparing eq. (69) to eq. (7), we see that the main difference is that, in eq. (69), there are additional dependances in the matter states through the momentum of gravity \( p_n(a) \). Therefore, in a first step, we assume that the \( C_n \) form a well peaked wave packet centered around \( C_n \) such that a first order expansion in \( \bar{n} - \bar{n} \) is a valid approximation. Then, using eq. (61), we obtain

\[
\partial_a C_n = \sum_{m \neq n} \langle \partial_a \psi_m | \psi_n \rangle e^{-i \int^a t_n(a) (E_n - E_m) dt} C_m
\]

(70)

This equation is identical to eq. (7). More precisely, through \( t_n(a) \), the proper time evaluated in the mean universe, we recover the Schrodinger equation governing non adiabatic transitions among instantaneous matter states if one identifies the coefficients \( C_n \) with the probability amplitudes \( c_n \) to find the matter states at \( t_n(a) \). We emphasize the a posteriori character of this identification. Indeed, it is based on the comparison of eq. (7) with the resulting simplified equation governing the \( C_n \). We recall that the definition of the coefficients \( C_n \) required three equations, namely eqs. (63, 64, 65). Had we made other choices, we would not have obtained this straightforward identification. Moreover, two approximations were also necessary: first that the coupling between expanding and contracting universes be neglected and secondly that the \( C_n \) form a well peaked distribution. For this later condition to be met, we recall that the universe be macroscopic,
see [3, 4, 7]. The generic character of the recovery of eq. (7) from eq. (68) through these approximations should be re-emphasized. This whole scenario arises whenever one considers how to reach the background field approximation from a more quantized framework, see the end of section 2.4 and [11, 12].

As in the cases treated in these references, eq. (69) contains higher order terms in \( n - \bar{n} \) which define the deviations from the Schrödinger equation when the \( C_n \) form a well defined wave packet. This condition must be met in order to have physically meaningful expansions around mean values. Eq. (69) differs from eq. (70) through both the complex phase and the prefactors. Both give rise to gravitational corrections since the differences arise from the quantum backreaction expressed here by the dependence in \( n \) of \( p_n(a) \).

To analyse these corrections we define new coefficients \( \tilde{C}_n = C_n e^{-i \int^a_0 p_n da} \) which allow to rewrite eq. (69) as

\[
i \partial_a \tilde{C}_n = \sum_{m} \left( \delta_{mn} p_n + i \langle \partial_a \psi_m | \psi_n \rangle \frac{p_n + p_m}{2 \sqrt{p_n p_m}} \right) \tilde{C}_m = \sum_{m} H_{nm}^{\text{eff}}(a) \tilde{C}_m \quad (71)
\]

where we have defined, as in eq. (4), an effective hamiltonian giving the evolution of \( \tilde{C}_n \). We now expand the \( p_n(a) \) around the mean energy \( \bar{E}(a) \) to obtain

\[
H_{nm}^{\text{eff}}(a) = \delta_{mn} p_n(a) + \delta_{mn} (E_n - \bar{E}) \partial_E p_n + i \langle \partial_a \psi_m | \psi_n \rangle \\
\quad + \delta_{mn} \frac{1}{2} (E_n - \bar{E})^2 \partial_E^2 p_n + i \langle \partial_a \psi_m | \psi_n \rangle \frac{(\partial_E p_n)^2}{8 p_n^2} (E_n - E_m)^2 \\
\quad + O(\Delta E^3)
\quad (72)
\]

The first line determines the overall phase of the \( \tilde{C}_n \) and encodes no physics. The second line contains the linear deviation in energy and gives the Schrödinger equation in the mean geometry, eq. (70). The third line contains quadratic terms which furnish the gravitational corrections to the energy levels and the instantaneous eigenstates. It consists of two terms. The first term arises because the energy of matter modifies the propagation of gravity, and hence the phase accumulated by the wavefunction. It can be expressed as a shift of the energy levels

\[
\Delta^{\text{Grav}}(E_n) = \frac{1}{2} \frac{\partial_{\bar{E}}^2 p}{\partial_E p} (E_n - \bar{E})^2 \simeq -\frac{\Delta E^2}{4E}
\quad (73)
\]

where in the second equality we have evaluated the correction for a matter dominated universe in which \( p_E \simeq \sqrt{a \bar{E}/G} \). (Notice that \( \partial_{\bar{E}} p \) plays a role similar to the specific heat of a large system, see App. B of [3].) The second term of the third line in eq. (72), is the first gravitational correction to the non adiabatic coupling. By diagonalising \( H_{nm}^{\text{eff}} \) one can calculate how it modifies the energy levels. This shift will be much smaller than \( \Delta^{\text{Grav}}(E_n) \) of eq. (73) because it carries an additional factor \( 1/p \).

Because of these corrections, there will be a maximum time \( t_{\text{max}} = O(\bar{E}^2/(E_n - \bar{E})^2) \) after which errors in the phases of the \( C_n(a) \) are of order 1. Then the evolution of the \( C_n(a) \) determined by the WDW equation no longer coincides with the one of the \( c_n(t) \),
solutions of the Schrödinger equation. The shift in the energy levels will also modify the non adiabatic transition amplitudes through the modification of the saddle point amplitude. At this point, it is to be emphasized that the calculation of these effects in specific cases is best carried out directly through the effective Hamiltonian eq. (71), or with eq. (72). Indeed the expansion eq. (72) depends explicitly on the mean energy $\bar{E}$ determining the background, whereas the transition amplitudes are independent of $\bar{E}$. Therefore quantum cosmology tells us that the (traditional) understanding of physics as describing matter processes in a given gravitational background should be considered as a convenient approximation with no dynamical justification. This point will be illustrated in section 4 by some examples and further clarified in what follows.

We note indeed that the validity of eq. (69) puts no restriction on the $C_n$ since it requires only the decoupling between expanding and contracting universes. This is sufficient to guarantee that $\sum_n |C_n(a)|^2 = constant$. Therefore one must still interpretate $C_n(a)$ as the amplitude of probability to find matter in the n-th state at $a$, even if they do not form a well defined wave packet\cite{8}. In this case of arbitrary distribution of $C_n$, it is completely meaningless to insist in using a mean background as a reference to parametrize transitions. Thus this raises the interesting question of whether one should require at all that the $C_n$ form a well peaked wave packet in order to recover the notion of a temporal evolution. To this end we note that if one assumes that the matter hamiltonian is described by a field theory with a cutoff (at the Planck energy), non adiabatic transitions never occurs between states whose energy differs by more than one Planck mass. Thus components of $\Xi$ with very different matter energies will essentially never interact. This offers the possibility that various components of the total waves decohere and evolve with their own time. We will not attempt further discussion of this issue here. Note however that this problem possesses an analogue in the emergence of a temporal description of electronic transitions in atomic collisions in which the atoms are described by broad wave packets, see the introduction.

3.4 Backscattering effects

We now turn to the coupling between expanding and contracting universes, that is the coupling between the coefficients $C_n$ and $D_n$ in eq. (68). This coupling is inevitable because the WDW equation is second order in $\partial_a$. It also occurs in the simple harmonic oscillator problem discussed in section 2.4. However in the present case the situation is more complicated because there are backscatterings which keep the matter state unchanged, i.e. the third term in eq. (68), and backscatterings which change the matter state, i.e. the second term in eq. (68). All of these couplings however have the same origin: they can all be expressed in terms of matrix elements of

$$\pi^2 a(a; \phi, \Pi) = (\Lambda a^4 - a^2)I + 2aH_M(a; \phi, \Pi)$$

viewed as an operator parametrised by $a$ and acting on matter states (here $I$ is the identity operator on these states). Indeed, using eq. (9), eq. (68) can be written as

$$i\partial_a C_n = \sum_{m \neq n} i\langle \psi_m | \partial_a \pi^2 a | \psi_n \rangle \frac{1}{2(p_n - p_m)\sqrt{p_n p_m}} C_m$$

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\[ + \sum_m i \langle \psi_m | \partial_a \pi_a^2 | \psi_n \rangle \frac{1}{2(p_n + p_m)\sqrt{p_n p_m}} D_m \]  

(75)

The first term in this equation corresponds to the first term in eq. (68), and the second term regroups the two last terms of eq. (68). Therefore, the operator \( \partial_a \pi_a^2 \) generalises the operator \( \partial H(t) \) in the Schrödinger case, see eq. (1), in that it allows this very simple rewriting of the WDW equation.

The coupling between forward and backward propagating universes described by eq. (75) gives rise to new effects. First it predicts the generation of backward propagating waves, i.e. \( D_n \neq 0 \), from initially purely forward waves and the simultaneous increase the norm of the “forward” coefficients \( C_n \) so as to ensure conservation of the Wronskian eq. (66). This is strictly the analogue of the Klein paradox in relativistic quantum field theory. Indeed, no positive local conserved quantity can be either constructed from the solutions of the Wheeler-DeWitt, contrary to the situation in quantum mechanics. It is possible that the resolution of this problem requires that one proceeds to third quantization wherein \( \Xi(a) \) is interpreted as an Heisenberg operator acting on universe Fock states.

Secondly, eq. (75) stipulates that there are quantum interferences among matter states associated with the expanding and contracting solutions. This means that the knowledge of the coefficients \( D_n(a) \) is required to determine the evolution of the \( C_n(a) \) at other values of \( a \). Thus the set composed of the \( C_n \) only form an open system.

In a future publication we hope to return to these aspects of quantum cosmology.

4 Applications of the formalism

In this section we return to the examples of non adiabatic transitions of section 2. We shall now treat them in the context of quantum cosmology when gravity is described in the adiabatic approximation hence with the amplitudes of matter transitions described by eq. (69). The essential difference is that whereas in section 2 it was merely convenient to parametrise the evolution by \( a \), see eqs. (1, 2), here it is mandatory to do so. This is particularly clear when calculating gravitational corrections to the transition amplitudes, since these corrections depend only on the structure of the energy levels \( E_n(a) \), and are independent of the mean energy \( \bar{E} \) and the mean time \( \bar{t} \) defining the reference background.

However before starting we must address the following problem. In the examples treated in section 2, the particles have non vanishing momentum which will backreact onto gravity and break the symmetry of minisuperspace. The way around this difficulty is to note (32, 7) that if the momentum of the particles is small, then one can treat the corresponding metric fluctuations perturbatively. Thus one expands both of the spatial metric \( h_{ij} \) and the lapse and shift in a fourier series, and keeps in the Einstein-Hilbert-
matter action only quadratic terms with \( k \neq 0 \). The Hamiltonian then becomes
\[
\int d^3x N^\mu H_\mu = N^0(k = 0)H_0(k = 0) + \sum_{k \neq 0} N^\mu(k)H_\mu(-k) \tag{76}
\]

All the new constraints \( H_\mu(k) \) which are multiplied by \( N^\mu(k \neq 0) \) are linear in the gravitational perturbation \( h_{ij}(k) \) and simply serve to eliminate the non propagating parts of \( h_{ij} \). The only non trivial constraint is \( H_0(k = 0) \). Thus to this order, one has recovered a minisuperspace model, but which contains matter and linearised gravitons with non vanishing momenta. Since they are not coupled, one can treat them separately. We shall for simplicity only consider the matter part of the Hamiltonian.

We first consider the recovery of the Golden Rule in quantum cosmology. The instantaneous eigenstates \( |\psi_\pm\rangle \) and eigenenergies \( E_\pm \) where already obtained in section 2.2. Therefore the effective hamiltonian eq. (71) for the coefficients \( \tilde{C}_\pm \) multiplying \( |\psi_\pm\rangle \) is
\[
H^{\text{eff}}(a) = \begin{pmatrix}
p_+(a) & i\langle \partial_a \psi_-|\psi_+ \rangle \frac{p_+ + p_-}{2\sqrt{p_+ p_-}} \\
-i\langle \partial_a \psi_-|\psi_+ \rangle & p_-(a)
\end{pmatrix} \approx \begin{pmatrix}
p_+(a) & i\langle \partial_a \psi_-|\psi_+ \rangle \\
-i\langle \partial_a \psi_-|\psi_+ \rangle & p_-(a)
\end{pmatrix} \tag{77}
\]

where in the second equality we have neglected the gravitational corrections to the non adiabatic couplings. Here the momenta of gravity \( p_\pm \) characterizing the gravitational waves entangled to the matter states \( |\psi_\pm\rangle \) are
\[
p_\pm = \sqrt{2Ga(E_T + E_\pm(a))} = \sqrt{2Ga(E_T + \frac{M + m + k/a}{2} \pm \sqrt{(M - m - k/a)^2/4 + g^2/a^2k}} \tag{78}
\]

We have chosen to work in a flat matter dominated universe with conserved matter energy \( E_T \). Since eq. (77) has exactly the same structure as eq. (4), we can calculate the non adiabatic transition amplitude as in section 2. We recall that the probability to make a non adiabatic transition is the probability for the excited atom not to decay. In the saddle point method it is given by
\[
P_{\text{no transition}}(k) = \text{e}^{-2Im \int^{a^*} da [p_+(a) - p_-(a)]} \tag{79}
\]

where \( a^* \) is the complex value of \( a \) where the momenta of the universe are equal
\[
p_+(a^*) - p_-(a^*) = 0 \tag{80}
\]

This gravitational resonance condition leads back to the background field resonance condition \( E_+(a^*) - E_-(a^*) = 0 \), since \( p_\pm(a) = p(a, E_\pm) \), see eq. (78). Thus \( a^* \) is unaffected by the dynamical character of gravitons and still given by eq. (17).

The integral which yields the transition probability is simply
\[
I_k = \text{Im} \int_{a_0}^{a_+} da [p_+(a) - p_-(a)] \tag{81}
\]
In order to estimate this integral, we first expand the integrant around the average total energy \( \bar{E} = E_T + (E_+ + E_-)/2 \). The important word in the previous sentence is “total”. This is why this expansion is physically meaningful: the mass-energy of the matter content of the universe which is not involved in the process determines the “inertia” of gravity. Indeed, we obtain

\[
I_k = \text{Im} \int_{a_0}^{a^*} da \partial_{E p}(a, E)|_{E=\bar{E}} \left[ E_+(a) - E_-(a) \right] + O \left( \frac{(E_+ - E_-)^3}{E_T^3} \right)
\]

Note that this is still not strictly equivalent to the background field approximation since the “time” parameter \( \bar{t} \) determined by

\[
\partial_{E p}(a, E)|_{E=\bar{E}} = \frac{d\bar{t}}{da}
\]

depends both on the initial state of energy \( E_T + M \) and on the final state of energy \( E_T + m + k/a \). Thus successive transitions, corresponding to successive \( k \), are described by (slightly) different time parameters. A single classical time parameter could be chosen to consist of the atom in its excited state of energy \( M \), call it \( \bar{t}(a) \). This is particularly appropriate in the present case because we are considering the probability for the atom to stay in its excited state. Then eq. (82) becomes

\[
I_k = \text{Im} \int_{a_0}^{a^*} da \frac{d\bar{t}}{da}(a) \left[ E_+(a) - E_-(a) \right] \left( 1 - \frac{\Delta M}{2(E_T + M)} \frac{(a - a_0)}{a_0} + O((a - a_0)^2) \right) + O \left( \frac{(E_+ - E_-)^3}{E_T^3} \right) \quad (84)
\]

The first term corresponds to eq. (13) evaluated in the background driven by \( E_T + M \). The second term is the first gravitational correction to the decay probability. It leads to a modification of the decay rate of the order of \( \Delta M/E_T \). Note that the correction decreases with increasing \( a_0 = k/\Delta M \). Indeed as the universe expands it is larger and larger and the background approximation becomes better and better.

We now apply the same techniques to the calculation of pair creation amplitudes in quantum cosmology. As in section 2.3 we consider only the transition from the vacuum state to the state containing one pair of momentum \( k, -k \). The only relevant quantities are the momenta of gravity associated with these two states. They are given by

\[
p_0(a) = \sqrt{\Lambda a^4 - a^2} \\
p_{k,-k}(a) = \sqrt{\Lambda a^4 - a^2 + 4Ga\sqrt{m^2 + k^2/a^2}} \quad (85)
\]

Then, in the saddle point calculation, the amplitude to produce a pair is simply given by

\[
|A_{\text{pair}}|^2 = e^{-2Im \int a^* da \left[ p_0(a) - p_{k,-k}(a) \right]} \quad (86)
\]
The saddle point $a^*$ of eq. (86) is again determined by the equality of the two gravitational momenta: $p_0(a^*) - p_{k,-k}(a^*) = 0$. Thus $a^*$ is still given by $a^* = ik/m$, which is the result obtained in the background field approximation eq. (38).

To estimate the integral of eq. (86) one can expand the integrand around empty de Sitter space, by exploiting the inertial delivered by the cosmological constant. However, it is more interesting to note that this expansion around a background is neither physically intrinsic nor mathematically necessary. Indeed, the integral of eq. (86) is easily evaluated by deforming the integration over $a$: by first integrating along the real axis to $a = +\infty$, then along the circle at infinity from $a = +\infty$ to $a = +\infty e^{i\pi/2}$ and finally along the imaginary axis from $a = i\infty$ to $a = a^* = ik/m$. The first piece of the integral, being real, does not contribute to the pair production probability, the second piece yields the background field result, eq. (36), and the third piece yields the gravitational corrections to the pair production probability. One finds that for large $k$, corresponding to productions occurring far from the classical turning point $a = 1/\sqrt{\Lambda}$, the probability is

$$|A_{pair}|^2 \simeq e^{-\frac{2\pi m}{\Lambda} + O(Gm^5/k^3 \Lambda^{3/2})}$$

Thus in minisuperspace, the gravitational corrections to pair creation decrease as the time (which is related to $k$ by the real part of eq. (38)) of production increases. This is natural since at late times the inertia delivered by the cosmological constant is huge, and thus, accordingly, the background field approximation better and better. It should however be noted that there probably are local gravitational corrections to pair creation which survive even at late times. In particular in de Sitter space these should be related to changes of the area of the horizon[33]. Similar corrections should also obtain for the radiative transitions discussed in the previous paragraph.

5 Conclusion

In this article we have developed a formalism for analysing the Wheeler-DeWitt equation based on a double adiabatic development. The matter part of the wave function was expanded in terms of the adiabatic matter states and the gravitational part in terms of the adiabatic (WKB) waves. The equation for the coefficients of this development is the main result of this paper. Because of its generality this formalism is useful to study conceptual problems such as the recovery of a temporal evolution for matter, and the identification of the probability amplitude to be in a given matter state. We have applied it to two examples: radiative transitions and particle creation, and we have compared how these processes are described in the background field approximation and in quantum cosmology.

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