Coarse-graining approach to quantum cosmology

Esteban Calzetta, and Mario Castagnino
Instituto de Astronomía y Física del Espacio, Casilla de Correo 67, Sucursal 28, 1428 Buenos Aires, Argentina and Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria, 1428 Buenos Aires, Argentina

Román Scoccimarro
Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria, 1428 Buenos Aires, Argentina
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We consider a Friedmann-Robertson-Walker model with both classical radiation and a massive (conformally coupled) quantum scalar field in the framework of quantum cosmology. We define a density matrix and introduce a notion of "relevance" which splits this density matrix into a "relevant" and an "irrelevant" part. A "generalized coarse-graining method" is used to obtain the evolution (in Robertson-Walker a "time") of the relevant density matrix, taking into account the back reaction of the irrelevant variables. We discuss the physical basis for the choice of a concept of relevance, and the features of cosmic evolution brought forward by the effective dynamics. In the limit of "small universes," the relevant subdynamics is dissipative.

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I. INTRODUCTION AND MOTIVATION

Cosmology is the study of the dynamics and structure of the Universe, based on observational facts. To account for these observations (isotropy and homogeneity of the microwave background, Hubble's law, etc.) the "standard model" has been proposed [1]. This model is based on Friedmann-Robertson-Walker models of cosmic evolution, whose dynamics are characterized by a few relevant parameters. More general dynamical systems describing cosmologies ("minisuperspace models" [2]) are also based on the study of the dynamics of a very restricted set of modes. On the other hand, the configuration space for a general cosmological model (superspace) is infinitely dimensional.

The selection of a few relevant variables which can show the physical essence of a system is similar to the main task of statistical mechanics [3]. However, the minisuperspace "approximation" neglects the influence of the ignored degrees of freedom on the dynamics of the relevant ones. From the point of view of statistical mechanics, this approach is questionable [4] and, in fact, the consideration of the influence of "irrelevant" degrees of freedom in quantum cosmology leads to important results such as the decoherence of the minisuperspace density matrix [5], and the dissipation of anisotropies [6].

Therefore, it is interesting to study the relevant dynamics taking into account the back reaction of the irrelevant degrees of freedom [7]. In cosmology, splitting the whole system into "relevant" and "irrelevant" subsystems may pose some conceptual difficulty since, by definition, the entire Universe is a closed system and therefore has no external environment. However, one is never interested in observing more than a small subset of the potentially measurable observables. This subset of modes evolves according to an effective dynamics in which the "irrelevant" variables act as a "bath." This description leads (under certain conditions [6,8–11]) to dissipative evolution in the relevant variables [9,10,12–14]. The selection of certain degrees of freedom as relevant is motivated by the particular physical situation and by "robustness," in the sense that these variables change adiabatically and are assumed to be almost insensitive to perturbations [10].

In particular, we shall implement the "system-bath" splitting in the context of quantum cosmology [15], for a Friedmann-Robertson-Walker model with both classical radiation and a massive inhomogeneous (conformally coupled) quantum scalar field. Despite its simplicity, this model contains the basic elements to simulate a more realistic treatment.

To follow the effective dynamics of the relevant subsystem, we shall use the "density operator method," thus obtaining a generalized master equation for the relevant density matrix. In this case, to make the distinction between relevant and irrelevant density matrices, one has to specify the basis in which the splitting is going to be made [10]. Here we shall use the "particle number" basis, and adopt the diagonal part of the density matrix in this representation as the relevant density matrix.

This concept of relevance is more "fine-grained" than the usual one when dealing with decoherence (i.e., tracing over *all* the scalar field), and will allow us to get the dissipative behavior associated with the mechanism of particle creation [16], whose dissipative nature has been already demonstrated in the framework of quantum field theory in curved spacetime [17–20].

The specification of a concept of relevance includes the choice of a coarse-graining procedure to average over the irrelevant variables. This procedure is a generalization of the coarse-graining concept developed by Gibbs. Concretely, we shall utilize the projection techniques implemented in statistical mechanics to obtain irreversible master equations from reversible dynamics, based on the application of an idempotent operator which maps the density matrix into its relevant part [9,10,12–14].

These coarse-graining techniques, originally developed in the field of nonequilibrium statistical mechanics, have been widely used in various branches of physics, such as laser optics [13], nuclear physics [14], astrophysics [21], quantum measurement theory [22], quantum tunneling [23], quantum field theory [20,24], inflationary cosmology [25], and semiclassical gravity [11,17,18,19,26]. In quantum cosmology, they have been employed to study the quantum to classical transition [5] and the issue of anisotropy dissipation [6]. In fact, this work can be considered as a quantum extension of previous semiclassical work that deals with the problem of dissipation from particle creation [17–19,20].

To confirm the dissipative evolution of the relevant subsystem, we shall construct a Lyapunov functional (such that it remains constant for reversible evolutions and changes monotonically in Robertson-Walker a "time" for irreversible ones [27]) from the relevant density matrix, related to the mechanism of particle creation.

Let us summarize the organization of this paper. Section II introduces the model and the corresponding Wheeler-DeWitt equation for the wave function of the Universe. In this model, particle creation arises when conformal invariance is broken by the scalar field's mass. This feature allows us to treat the mass as a coupling constant between matter and geometry. When the scalar field's mass is zero, matter and geometry are uncoupled and the Wheeler-DeWitt equation can be solved exactly. Thus, in the massive case, we can follow the evolution of the wave function in the "interaction picture," in which the uncoupled dynamics is already solved and the evolution is due to the coupling between metric and scalar field. This issue is treated in Sec. III.

Section IV deals with the "interaction picture" evolution of the density matrix, which describes a given configuration of the quantum field. In Sec. V we specify our concept of relevance and find the dynamics of the relevant density matrix. This "subdynamics" is very complicated, but it can be shown, through the definition of a Lyapunov functional, that in the limit of "small universes" the evolution is dissipative. This is done in Sec. VI. Finally, we briefly state our conclusions in Sec. VII.

II. THE MODEL: WHEELER-DEWITT EQUATION

Let us consider a simple model, but with enough elements as to allow a physically meaningful separation between relevant and irrelevant variables. For simplicity, we shall use a quantum, conformally coupled, scalar field to represent the matter degrees of freedom. In this case, the action is ($m_{\rm P}$ is the Planck mass)

$$S=\int d^4x(-g)^{1/2}\left[\frac{m_{\rm P}^2}{12}(R-12\rho_c)-\tfrac{1}{2}(g^{\mu\nu}\partial_\mu\Phi\partial_\nu\Phi+\tfrac{1}{6}R\Phi^2)+\tfrac{1}{2}m\Phi^2\right], \tag{2.1}$$

where m stands for the mass of the field's quanta, and ρ_c represents the contribution of classical matter.

We shall incorporate into the action some simplifications. Concretely, we assume that the metric corresponds to that of the closed Friedmann-Robertson-Walker model. Thus, it is not possible to satisfy Einstein's equations unless the quantum scalar field is homogeneous. Recall, however, that we are interested in the identification, within our model, of an irrelevant subsystem (a "bath"). That would not be possible if we have only two degrees of freedom (the scale factor a and the homogeneous mode of Φ). For this reason, we must go beyond the minisuperspace "approximation."

To obtain a consistent model with inhomogeneous matter fields, it would be necessary to introduce metric degrees of freedom (which, in a first approximation, can be described in terms of gravitons). Nevertheless, for our purposes, it will be enough to retain the inhomogeneous scalar field (from which we shall define the irrelevant information) and, in place of introducing gravitons, we shall not impose the momentum constraints, but only the Hamiltonian constraint averaged over each spatial hypersurface. Formally, this will result from the fact that the lapse function N depends exclusively on time.

Thus, the interval takes the form

$$ds^2=-N^2dt^2+a^2(t)g_{ij}dx^idx^j\ , \tag{2.2}$$

where g_{ij} is the metric tensor defined on the spatial hypersurface labeled with time t.

The mass term in the action (2.1) is a key term for our purposes, since particle creation depends strongly upon it. Indeed, when $m=0$ there is conformal invariance and particle creation is suppressed. Therefore, the quantum field mass acts as a coupling constant, whose intensity is a measure of the "interaction" between our subsystem and the "bath" (to be defined below).

At this point it is convenient to introduce the eigenfunctions of the spatial Laplacian, the spherical harmonics on the two-sphere Q^n_{lm}. In terms of these functions, we can write an arbitrary scalar field configuration as

$$\Phi(\mathbf{x},t)=\frac{1}{a}\left[\sum_n Q_n(\mathbf{x})\phi_n(t)\right], \tag{2.3}$$

where n denotes the whole set $\{n,l,m\}$ and we assume that we have chosen the Q_n functions real, so that the amplitudes ϕ_n are real too.

Following the canonical quantization procedure, and choosing the factor ordering so that the term in second derivatives becomes the Laplacian operator in the midisuperspace metric, we obtain the Wheeler-DeWitt equation for this model [28,29]:

$$\left[\frac{1}{2m_{\rm P}^2}\partial_a^2-\frac{m_{\rm P}^2}{2}a^2+m_{\rm P}^2\rho_B+\frac{1}{2}\sum_n[-\partial_{\phi_n}^2+(n^2+m^2a^2)\phi_n^2]\right]\Psi=0\ , \quad (2.4)$$

where we used $\rho_c=\rho_B a^{-4}$ for the classical radiation density.

III. "INTERACTION PICTURE" IN QUANTUM COSMOLOGY

A. Exact solution when the interaction is "turned off"

When studying the dynamics of the relevant subsystem, but taking into account its coupling with the "bath," great simplification is achieved by working in the interaction picture. In this picture, the "trivial" uncoupled dynamics has been previously worked out, and the evolution is solely due to the interaction between relevant and irrelevant degrees of freedom [13]. A comparable simplification can be obtained in the framework of quantum cosmology, reducing the Wheeler-DeWitt equation to a set of two coupled first-order differential equations [6].

To proceed with this reduction technique, we have to solve first the "uncoupled" dynamics. In our model, when the scalar field's mass vanishes, particle creation ceases and the Wheeler-DeWitt equation (2.4) can be solved exactly through separation of variables. For the scalar field modes, we seek solutions which go to zero when $\phi_n\to\pm\infty$; i.e., we want a normalizable scalar field wave function, since in the semiclassical limit we expect to retrieve the usual interpretation of quantum field theory in curved spacetime [30]. For this purpose, we introduce the functions $H_n(\phi_n,p_n)$ satisfying

$$\tfrac{1}{2}(\partial_{\phi_n}^2-n^2\phi_n^2)H_n(\phi_n,p_n)=-(p_n+\tfrac{1}{2})nH_n(\phi_n,p_n)\quad(p_n=0,1,\ldots)\ . \quad (3.1)$$

Now we propose a solution to the Wheeler-DeWitt equation, in the zero-mass case, of the type

$$\Psi^{(m=0)}=\sum_p C(a,p)H(\phi,p)\ , \quad (3.2)$$

where p denotes the set $\{p_n\}$, the sum extends over all the possible sequences of natural numbers (including zero), and $H(\phi,p)\equiv\prod_n H_n(\phi_n,p_n)$. Substituting this ansatz into the Wheeler-DeWitt equation (2.4) we get

$$\left[\tfrac{1}{2}\partial_x^2-\tfrac{1}{2}x^2+\gamma_p\right]C(x,p)=0\ , \quad (3.3)$$

where $x\equiv m_{\rm P}a$, and $\gamma_p\equiv m_{\rm P}^2\rho_B+\sum_n(p_n+\frac{1}{2})n$; thus, the zero-point energy of the field can be absorbed into a renormalization of the classical radiation density (i.e., $m_{\rm P}^2\rho_B+\sum_n\frac{1}{2}n\equiv m_{\rm P}^2\rho_D$). This *ad hoc* renormalization will be sufficient for our purposes. Satisfactory renormalization schemes have been proposed in the literature [31,32]. Putting $C(x,p)=\exp(-x^2/2)F(x,p)$ and substituting in (3.3) we obtain

$$z\frac{d^2F(z,p)}{dz^2}+\left[\frac{1}{2}-z\right]\frac{dF(z,p)}{dz}+\left[\frac{\gamma_p-\frac{1}{2}}{2}\right]F(z,p)=0\ , \quad (3.4)$$

where $z\equiv x^2$. Therefore, $F(z,p)$ satisfies the hypergeometric confluent equation. In this way, one can obtain a solution to the Wheeler-DeWitt equation as

$$\Psi^{(m=0)}=\sum_p e^{-x^2/2}[\alpha_1U(-N_p/2,1/2,x^2)+\alpha_2V(-N_p/2,1/2,x^2)]H(\phi,p)\ , \quad (3.5)$$

where $N_p\equiv\gamma_p-\frac{1}{2}=\sum_n p_n n+m_{\rm P}^2-\frac{1}{2}$, and U and V are the independent solutions to the hypergeometric confluent equation [33].

B. Evolution of Ψ in the interaction picture

Let us see what happens in the case of interest, i.e., when $m\neq0$ and particle creation takes place. The last ("interaction") term in the Wheeler-DeWitt equation (2.4) can be rewritten by means of the relation

$$\phi_n^2H(\phi,p)=\sum_q A_n(p,q)H(\phi,q)\ , \quad (3.6)$$

where

$$A_n(p,q)=A_n(q,p)=\frac{1}{2n}[(2p_n+1)\delta(p_n,q_n)+\sqrt{p_n(p_n-1)}\delta(p_n-2,q_n)+\sqrt{(p_n+1)(p_n+2)}\delta(p_n+2,q_n)]\delta_n(p,q)\ , \quad (3.7)$$

with $\delta_n(p,q)\equiv\prod_{n'\neq n}\delta(p_{n'},q_{n'})$. Notice that $A_n(p,q)$ contains the information about the interaction term, and it connects "states" that differ in their sequences of particle numbers by the creation or destruction of one pair [we shall see later that the first term in (3.7) does not contribute to the evolution equation of the density matrix in the interaction picture]. We now make the ansatz [remember (3.5)]

$$\Psi=\sum_p \alpha_i(x,p)F^i(x,p)H(\phi,p)\ , \quad (3.8)$$

where we use summation convention in the index $i=1,2$ (henceforth, indices i,j,k and l will run from 1 to 2, and summation convention will be used), and

$$F^1(x,r)\equiv2^{-1/2}e^{-x^2/2}U(-N_r/2,1/2,x^2)\ , \quad (3.9)$$

$$F^2(x,r)\equiv 2^{-1/2}(-1)^{-(N_r+1)/2}e^{-x^2/2}V(-N_r/2,1/2,x^2)\ . \tag{3.10}$$

The F^i's are real and satisfy

$$F^i(x,r)\partial_x F^j(x,r)-F^j(x,r)\partial_x F^i(x,r)=i\sigma_2^{ij}\ , \tag{3.11}$$

where σ_2 is the usual Pauli matrix.

Note that we are using for the massive case (3.8) the same scalar field wave function as in the conformal case (3.5). Since in the semiclassical limit of quantum cosmology we obtain quantum field theory in curved spacetime in the Schrödinger picture [15,30], this wave function is the Heisenberg state corresponding to an n-particle state of the conformal particle model, in the usual formulation of quantum field theory in curved spacetime [34]. Therefore, particle creation arises because we are using approximate (zero-mass) modes to expand the scalar field, and that leads to creation and annihilation operators which depend on x. In fact, the analogous situation in quantum field theory in curved spacetime leads to the conclusion that creation and annihilation operators at two times are related via a Bogoliubov transformation [16].

Since we have one differential equation (2.4) for two unknown functions α_i, we may add the condition

$$F^i(x,r)\partial_x\alpha_i(x,r)=0\ . \tag{3.12}$$

Taking this into account, and substituting (3.8) into the Wheeler-DeWitt equation (2.4), we get

$$i\partial_x\alpha_i(x,p)=\sum_r\mathcal{H}_i^k(x,p,r)\alpha_k(x,r)\ , \tag{3.13}$$

with

$$\mathcal{H}_i^k(x,p,r)\equiv\left[\frac{m}{m_{\rm P}}\right]^2 x^2\omega_i^k(x,p,r)\sum_n A_n(p,r)\ , \tag{3.14}$$

and

$$\omega_i^k(x,p,r)\equiv(\sigma_2)_{ji}F^j(x,p)F^k(x,r)\ . \tag{3.15}$$

Equation (3.13) represents the evolution in the interaction picture of the wave-function "components" (in the uncoupled basis of solutions F^i). As stated before, this equation becomes trivial when the interaction is suppressed ($m=0$), since $\mathcal{H}_i^k(x,p,r)$ vanishes. Therefore, particle creation appears when the components α_i depend on x. To study the dynamics of these components, we shall define a density matrix. This provides a natural way to follow the evolution and also allows the implementation of coarse-graining techniques.

IV. THE DENSITY MATRIX: EVOLUTION IN THE INTERACTION PICTURE

The Wheeler-DeWitt equation (2.4) corresponds to a Klein-Gordon equation in a Minkowski spacetime; therefore it preserves the inner product

$$(\Theta,\Psi)=i\int\prod_n d\phi_n(\Theta^*\partial_x\Psi-\Psi\partial_x\Theta^*)\ . \tag{4.1}$$

Recalling (3.8), we obtain

$$(\Psi,\Psi)=\sum_p\sigma_2^{ij}\alpha_i(x,p)\alpha_j^*(x,p)\ . \tag{4.2}$$

From (4.2) we define the diagonal elements of the density matrix as [6]

$$\rho(x,p,p)\equiv\sigma_2^{ij}\alpha_i(x,p)\alpha_j^*(x,p)\ . \tag{4.3}$$

This definition has the advantage of constant total "weight"; i.e., the sum of diagonal elements remains constant as the scale factor a varies. However, we must notice that the definition (4.3) has a serious drawback, namely, that the diagonal elements are not positive definite. Therefore, we shall not attempt to give them a probabilistic interpretation [35]; it will be enough to consider them as giving a characterization of the quantum field state at "time" x.

More generally, we shall define the density matrix as

$$\rho(x,p,q)\equiv\sigma_2^{ij}\alpha_i(x,p)\alpha_j^*(x,q)\ . \tag{4.4}$$

Although this definition is somewhat arbitrary, it will suffice to study the dynamics of the diagonal elements. From Eq. (3.13) it is straightforward to find an equation for the matrix,

$$\rho_{ij}(x,p,q)\equiv\alpha_i(x,p)\alpha_j^*(x,q)\ , \tag{4.5}$$

and, introducing the vector

$$\rho_\mu\equiv\sigma_\mu^{ji}\rho_{ij} \tag{4.6}$$

($\mu=0,1,2,3;\sigma_0$ is the identity matrix and the others are the Pauli matrices), we get

$$i\partial_x\rho_\nu(x,p,q)=\sum_s\sigma_\nu^{ji}[\mathcal{H}_i^l(x,p,s)\rho_\mu(x,s,q)\sigma_{lj}^\mu+\mathcal{H}_j^l(x,q,s)\rho_\mu(x,p,s)\sigma_{il}^\mu]\ . \tag{4.7}$$

We are only interested in the evolution equation for ρ_2. Unfortunately, (4.7) indicates that each component ρ_μ is coupled to the others. To find a closed equation for ρ_2, we would have to apply reduction techniques to the system of coupled equations (4.7). Nevertheless, we shall consider in a first approximation that we can neglect the irrelevant components (ρ_0,ρ_1,ρ_3), and keep the equation $(\rho\equiv\rho_2)$

$$i\partial_x\rho(x,p,q)=\sum_s[\mathcal{H}(x,p,s)\rho(x,s,q)-\rho(x,p,s)\mathcal{H}(x,s,q)]\ , \tag{4.8}$$

with

$$\mathcal{H}(x,p,s)=\left[\frac{mx}{m_{\rm P}}\right]^2\omega(x,p,s)\sum_n A_n(s,p)\ , \tag{4.9}$$

and

$$\omega(x,p,s)=\omega^*(x,s,p)=-\omega(x,s,p)\equiv\tfrac{1}{2}\omega_l^l(p,s)=\frac{i}{2}[F^2(x,p)F^1(x,s)-F^1(x,p)F^2(x,s)]\ . \tag{4.10}$$

Owing to the antisymmetry property, the first term in (3.7) does not contribute to $\mathcal{H}$, and therefore $\mathcal{H}$ has only extradiagonal elements. Observe that total "weight" is still conserved, i.e., from (4.8) we get $\partial_x \sum_p \rho(x,p,p)=0$. On the other hand, the condition (3.12) leads (in the decoupling approximation) to

$$\mathcal{H}(x,p,q)\partial_x\rho(x,p,q)=0 \ , \tag{4.11}$$

which, due to the antisymmetry of $\mathcal{H}$, means that the nondiagonal elements of ρ remain constant during the evolution. Therefore, the neglect of (ρ_0,ρ_1,ρ_3) will be acceptable if the extradiagonal elements of ρ are "slowly varying." This can be justified from the relevance concept we shall use and by the approximation that the bath is "sluggish" [6]. Under these hypotheses, Eq. (4.8) represents the evolution of the density matrix in the interaction picture.

V. THE RELEVANT DENSITY MATRIX: EVOLUTION IN THE INTERACTION PICTURE

Now we shall specify our concept of relevance and find the dynamics of the relevant density matrix in the interaction picture. To reach this end, it is convenient to start defining the tetradic operator

$$\hat{L}(x,p,q,r,s)\equiv\mathcal{H}(x,p,r)\delta(s,q)-\delta(p,r)\mathcal{H}(x,s,q) \ ; \tag{5.1}$$

thus, Eq. (4.8) resembles a Liouville–Von Neumann equation:

$$i\partial_x\rho(x,p,q)=\sum_{r,s}\hat{L}(x,p,q,r,s)\rho(x,r,s) = [\hat{L}(x)\rho(x)](p,q) \ . \tag{5.2}$$

As discussed in Sec. II, we shall define our irrelevant variables from the scalar field modes. First, we have to choose the basis in which the division between relevant and irrelevant portions of the density matrix is going to be made. We adopt for this purpose (as we have been using so far) the "particle number representation," since in the limit of weak particle creation (to which it will suffice to restrict ourselves to demonstrate the existence of dissipation) the number of particles is an adiabatic invariant. On the other hand, one could work in a complementary basis, such as that associated with the phase of each mode [36] or the coherent-state basis [17]. However, we shall deal with particle creation in the first stages of the cosmic evolution, when occupation numbers are small and spontaneous particle creation dominates over stimulated creation. In this case, the uncertainty in the particle number is much less than that in the phase [17].

Concerning the specification of the relevant density matrix, recall that the information about particle number sequences is much more accessible from the "observational" point of view than that related with the interference among distinct quantum states, since these relative phases could be lost as a consequence of interactions, decays, and annihilations that would destroy the coherence of the state, but presumably not the probability distribution of the occupation numbers [18,26,37]. A good example is the spectrum of the cosmic background radiation, which is characterized by a thermal spectrum (i.e., a state represented by a diagonal density matrix in the number representation).

Therefore, we shall consider as a relevant density matrix the diagonal part of the density matrix defined in (4.4), since these elements give the "weight" of a given state specified by its sequence of particle numbers. Note that the specification of this concept of relevance does not imply neglecting the extradiagonal elements of the density matrix; in fact, it is the back reaction of these elements into the relevant ones that cause dissipation, as we will see below.

Observe that, in contrast with other work [5], we are not considering irrelevant the whole scalar field, but only the extradiagonal elements of the density matrix. On the other hand, this concept of relevance is the most important within quantum mechanics [10], since it leads to Pauli's master equation and its generalizations [10,12].

In this connection, it is interesting to observe that, in the usual derivation of Pauli's equation, decoherence is invoked to justify discarding nondiagonal terms in the density matrix [10]. In the approach we shall follow, leading to a generalized master equation, those terms are not neglected, although eventually we shall assume that the density matrix is diagonal at the initial "time." This choice of initial data, and the reasons behind it, will be discussed below [cf. Eq. (5.10)].

To obtain the dynamics of the relevant density matrix, we begin defining the projection operator $\hat{P}$ that corresponds to our concept of relevance:

$$\hat{P}(p,q,r,s)\equiv\delta(p,r)\delta(q,s)\delta(p,q) \ , \tag{5.3}$$

and the complementary operator

$$(1-\hat{P})(p,q,r,s)\equiv\delta(p,r)\delta(q,s)[1-\delta(p,q)] \ . \tag{5.4}$$

The single "Liouville–Von Neumann" equation (5.2) is equivalent to the coupled system:

$$i\partial_x\rho_R(x)=\hat{P}\hat{L}(x)\rho_R(x)+\hat{P}\hat{L}(x)\rho_I(x) \ , \tag{5.5}$$

$$i\partial_x\rho_I(x)=(1-\hat{P})\hat{L}(x)\rho_R(x)+(1-\hat{P})\hat{L}(x)\rho_I(x) \ , \tag{5.6}$$

where $\rho_R(x,p,q)\equiv\rho(x,p,p)\delta(p,q)$ is the relevant density matrix, and $\rho_I(x,p,q)\equiv\rho(x,p,q)[1-\delta(p,q)]$ is the irrelevant density matrix ($\rho_R+\rho_I=\rho$). In terms of an initial condition at "time" x_0, Eq. (5.6) can be formally solved to yield

$$\rho_I(x)=\hat{G}(x,x_0)\rho_I(x_0)-i\int_{x_0}^{x}dy\ \hat{G}(x,y)(1-\hat{P})\hat{L}(y)\rho_R(y) \ , \tag{5.7}$$

where

$$\hat{G}(x,x_0)\equiv T\exp\left[-i\int_{x_0}^{x}dy(1-\hat{P})\hat{L}(y)(1-\hat{P})\right] \ , \tag{5.8}$$

and T denotes a time-ordering operator. By inserting this formal solution back into Eq. (5.5), we get an exact closed equation for ρ_R:

$$i\partial_x\rho_R(x)=\hat{P}\hat{\mathcal{L}}(x)\rho_R(x)+\hat{P}\hat{\mathcal{L}}(x)\hat{G}(x,x_0)\rho_I(x_0)-i\int_{x_0}^{x}dy\,\hat{P}\hat{\mathcal{L}}(x)\hat{G}(x,y)(1-\hat{P})\hat{\mathcal{L}}(y)\rho_R(y)\ . \tag{5.9}$$

Let us look into the meaning of each term in the right-hand side of (5.9). The first term is the trivial part of the relevant dynamics and takes the form of an instantaneous "self-interaction." This term does not contribute to our concept of relevance, i.e., from (5.1) and (5.3) we obtain $\hat{P}\hat{\mathcal{L}}\hat{P}=0$.

The second term of (5.9) arises from the irrelevant density matrix at "initial time" x_0. To evaluate this contribution, we must specify the initial conditions. Within the framework of quantum cosmology, one would not be free to choose the initial conditions arbitrarily, but in agreement with a fundamental principle that defines the quantum state of the Universe [38]. No such principle has been definitely established yet. For simplicity, we shall assume that the quantum state of the Universe is consistent with the hypothesis that our system can be described initially only in terms of relevant variables, and impose the initial condition:

$$\rho_I(x_0)\equiv 0\ . \tag{5.10}$$

Although this "generalized molecular chaos hypothesis" is stronger than the molecular chaos assumption, it is assumed to hold only at the initial "time". Using this method we can be sure that the evolution is consistent with Eq. (5.2). Moreover, (5.10) corresponds (in those cases where a probabilistic interpretation exists) to the usual initial condition of equal fine-grained and coarse-grained probabilities [39].

The last and essential term in (5.9) takes the form of a (non-Markovian) "memory term," since it describes the dependence of the "time" derivative on the previous history of ρ_R throughout the interval $x_0<y<x$. Finally, introducing the kernel

$$\hat{K}(x,y)\equiv\hat{P}\hat{\mathcal{L}}(x)\hat{G}(x,y)(1-\hat{P})\hat{\mathcal{L}}(y)\ , \tag{5.11}$$

[which, in view of (5.1) satisfies $\sum_r\hat{K}(x,y,p,p,r,r)=0$] we may rewrite the evolution equation for the relevant density matrix in interaction representation in the final form:

$$\partial_x\rho_R(x,p,p)=-\int_{x_0}^{x}dy\sum_r\hat{K}(x,y,p,p,r,r)\times[\rho_R(y,r,r)-\rho_R(y,p,p)]\ . \tag{5.12}$$

VI. EFFECTIVE EVOLUTION FOR "SMALL UNIVERSES"

Now we shall attempt to derive a simpler effective evolution equation from the approximation of "small universes" to Eq. (5.12). To reach this end, we must analyze the structure of the kernel $\hat{K}$ in (5.12). We begin writing

$$\hat{G}(x,y,s,t,u,v)=\delta(s,u)\delta(t,v)+\hat{g}(x,y,s,t,u,v)[1-\delta(s,u)][1-\delta(t,v)]\ , \tag{6.1}$$

since in the expansion of (5.8) the only diagonal term is the unit tetradic operator. In terms of this characterization of $\hat{G}$, we may rewrite $\hat{K}$ as

$$\hat{K}(x,y,p,p,r,r)=\sum_{s\neq t}\hat{\mathcal{L}}(x,p,p,s,t)\hat{\mathcal{L}}(y,s,t,r,r)+\sum_{s\neq t,u;u\neq v,t}\hat{\mathcal{L}}(x,p,p,s,t)\hat{g}(x,y,s,t,u,v)\hat{\mathcal{L}}(y,u,v,r,r)\ . \tag{6.2}$$

Recalling (3.7), (4.9), and (5.1), we may interpret the first term in (6.2) as giving the "transition rate" between "states" of ρ_R that differ in the creation of a particle pair, and the second term as coming from the contribution of states that differ in the creation of more than one pair. Let us see that for "small universes," the first term in (6.1) and (6.2) is dominant.

Taking into account that $\hat{G}$ is the propagator for Eq. (5.6) when ρ_R is zero, we can see that $\hat{g}\approx x|\mathcal{H}(x)|$ or, in the limit of small x, $\hat{g}\approx(m^2\omega A/m_P^2)x^3$, where $\omega\equiv|\omega(x\to 0)|$ and $A\equiv\sum_n A_n$. Using the expressions of F^1 and F^2 for small x [33] (e.g., for x smaller than the classical turning point $x_{tp}\approx 2\rho_D m_P^2$), and assuming the creation of only one pair from vacuum in the homogeneous mode, we may estimate

$$\hat{g}\approx m^2\omega A x_{tp}^3/m_P^2\approx m^2/m_P^2<<1\ , \tag{6.3}$$

for $m_P^2\rho_D\approx 0.5-1$, and reasonable values of the mass of the field's quanta. Within this approximation, we may assume that ρ_R and $\hat{\mathcal{L}}$ change slowly and put $y\approx x$ [18] in (5.12) to obtain

$$\partial_x\rho_R(x,p,p)=-2(x-x_0)\sum_r\mathcal{H}^2(x,p,r)[\rho_R(x,r,r)-\rho_R(x,p,p)]\ . \tag{6.4}$$

This is the evolution equation for the relevant density matrix in the "small universes" approximation. Since $\mathcal{H}$ is imaginary, this is a "Pauli-type" equation and an H theorem could be proved for $H\equiv\mathrm{Tr}(\rho_R\ln\rho_R)$ if one assumes the positiveness of the diagonal elements of ρ. To avoid this hypothesis, one may verify instead the dissipative behavior from (6.4) through the definition of a functional Ω according to

$$\Omega(x) \equiv \mathrm{Tr}[\rho_R(x)^\dagger \rho_R(x)] \ . \quad (6.5)$$

From (6.4) we confirm that $\Omega(x)$ is a Lyapunov functional, since

$$\partial_x \Omega(x) = 2(x - x_0) \sum_{p,r} \mathcal{H}^2(x,p,r) \times [\rho_R(x,r,r) - \rho_R(x,p,p)]^2 \leq 0 \ , \quad (6.6)$$

which indicates that the relevant density matrix obeys, for "small universes," a dissipative evolution equation.

VII. CONCLUSIONS

We implemented the "system-bath" splitting in the context of quantum cosmology, for a Friedmann-Robertson-Walker model with both classical radiation and a massive inhomogeneous (conformally coupled) quantum scalar field. Despite its simplicity, the model we have presented has the basic ingredients that allow the specification of a physically meaningful concept of relevance.

In this model, particle creation appears when conformal invariance is broken by the scalar field's mass. This feature allowed us to work in the "interaction picture" (using the mass as a coupling constant), in which particle creation appears as a dependance of the wave-function components (with respect to the zero-mass solutions of the Wheeler-DeWitt equation) on x.

To follow the evolution of these components, we defined a density matrix. This provides a context suitable for the application of coarse-graining techniques. The effective dynamics of the relevant subsystem is described in this case by a generalized master equation for the relevant density matrix.

The specification of a concept of relevance, from which we constructed the projection operator, was based on our interest in following the evolution of a certain combination of the wave-function components, i.e., that associated with the "weight" of a given configuration of the wave function (characterized by a sequence of particle numbers). Thus, working in the "particle number" basis, we defined the diagonal part of the density matrix in this representation as the relevant density matrix. This election is justified because the relative phases are not "accessible" in the physical situations relevant to cosmology (for example, the observation of thermal spectra).

This concept of relevance is more "fine-grained" than the usual one when dealing with decoherence [5]. Here the "environment" is constituted by the nondiagonal elements of the density matrix in the number representation; in this way we retain part of the scalar field modes as relevant information.

Once we have obtained the evolution equation for the relevant density matrix in the interaction representation (using the condition that only "relevant information" is present initially), the "small universes" approximation led to the evolution equation (6.4), which is manifestly dissipative. To confirm the "dissipative" evolution of the relevant subsystem, we have constructed a Lyapunov functional Ω from the relevant density matrix.

In this model, "dissipation" results into the building of a correlation between the size of the Universe and the distribution of occupation numbers of the scalar field. In effect, as we consider universes larger than the "initial size" x_0, the distribution of occupation numbers "spreads out" with increasing Universe size.

The use of coarse-graining techniques makes it possible to focus on relevant physical phenomena (in this case, the correlation between the size of the Universe and the physically accessible occupation numbers of the matter field), as described by effective evolution equations [e.g., Eq. (6.4)] much simpler than the original Wheeler-DeWitt equation (2.4). In this sense, coarse-graining techniques are a valuable tool for concrete model building in quantum cosmology. We are continuing our research into their manifold applications.

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