# Nonequilibrium evolution of scalar fields in FRW cosmologies

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We derive the effective equations for the out of equilibrium time evolution of the order parameter and the fluctuations of a scalar field theory in spatially flat FRW cosmologies. The calculation is performed both to one loop and in a nonperturbative, self-consistent Hartree approximation. The method consists of evolving an initial functional thermal density matrix in time and is suitable for studying phase transitions out of equilibrium. The renormalization aspects are studied in detail and we find that the counterterms depend on the initial state. We investigate the high temperature expansion and show that it breaks down at long times. We also obtain the time evolution of the initial Boltzmann distribution functions, and argue that to one-loop order or in the Hartree approximation the time evolved state is a "squeezed" state. We illustrate the departure from thermal equilibrium by numerically studying the case of a free massive scalar field in de Sitter and radiation-dominated cosmologies. It is found that a suitably defined nonequilibrium entropy per mode increases linearly with comoving time in a de Sitter cosmology, whereas it is *not* a monotonically increasing function in the radiation-dominated case.

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## I. INTRODUCTION AND MOTIVATION

Since its creation more than a decade ago, the inflationary Universe scenario [1-3] has become an integral part of the standard model of cosmology. However, to a great extent, this scenario is incomplete. One of the problems is the lack of a model of inflation that is adequate both from the inflationary and the particle physics viewpoints. While many models [4] exist that do all the things an inflationary model needs to do, such as inflating, ending inflation gracefully, reheating the Universe, and generating safe density fluctuations, none of these models really is part of any reasonable extension of the standard model of particle physics.

What we address in this work, however, is a more serious problem. This has to do with the dynamics of inflation, and more generally, the dynamics of scalar fields in an expanding Universe. By and large, the various models of inflation make the assumption that the dynamics of the spatial zero mode of the (so-called) inflaton field is governed by some approximation to the effective potential which incorporates the effects of quantum fluctuations of the field. Thus the equation of motion is usually of the form

$$\ddot{\phi} + 3\frac{\dot{a}}{a}\dot{\phi} + V'_{\text{eff}}(\phi) = 0.$$
(1.1)

The problem here is that the effective potential is really only suited for analyzing *static* situations; it is the effective action evaluated for a field configuration that is constant in time [5]. Thus, it is inconsistent to use the effective potential in a *dynamical* situation. Notice that such inconsistency appears for *any* inflationary scenario (old, new, chaotic, ...).

More generally, the standard methods of high temperature field theory are based on an equilibrium formalism [6,7]; there is no time evolution in such a situation. Such techniques preclude us from treating nonequilibrium situations such as surely exist for very weakly coupled theories in the early Universe.

In this work we try to rectify this situation by addressing three issues: (a) obtaining the evolution equations for the order parameter including the *quantum fluctuations*; (b) studying departures from thermal equilibrium if the initial state is specified as a thermal ensemble; (c) understanding the renormalization aspects and the validity of the high temperature expansion.

Our ultimate goal is to study the dynamics of phase transitions in the early Universe, in particular, the formation and evolution of correlated domains and symmetry breaking in an expanding Universe. From some of our previous studies on the dynamics of phase transitions [8,9] in Minkowski space, we have learned that the familiar picture of "rolling" is drastically modified when the fluctuations are taken into account. As the phase transition proceeds fluctuations become large and correlated regions (domains) begin to grow. This enhancement of the fluctuations modifies substantially the evolution equation of the order parameter. Thus the time dependence of the order parameter is not enough to understand the dynamical aspects of the phase transition; it must be studied in conjunction with that of the fluctuations. Vilenkin and Ford [15] and Linde [16] studied the fluctuations in a free scalar field theory in de Sitter space and Guth and Pi [17] studied the growth of fluctuations by approximating a broken symmetry situation with an inverted parabolic potential in de Sitter space. However, we are not aware of any previous attempt to incorporate the growth of fluctuations (arising from the nonlinearities) in the dynamics of the order parameter during cosmological phase transitions.

Our approach is to use the functional Schrödinger formulation, wherein we specify the initial wave functional  $\Psi[\Phi(\cdot);t]$  (or more generally a density matrix  $\rho[\Phi(\cdot), \tilde{\Phi}(\cdot);t]$ ), and then use the Schrödinger equation to evolve this state in time. We can then use this state to compute all of the expectation values required in the construction of the effective equations of motion for the order parameter of the theory, as well as that for the fluctuations. The Schrödinger approach has already been used in the literature at zero temperature [10] and to study nonequilibrium aspects of field theories [11].

One advantage of this approach is that it is truly a dynamical one; we set up initial conditions at some time  $t_0$ by specifying the initial state and then we follow the evolution of the order parameter  $\phi(t) \equiv \langle \Phi(\mathbf{x}) \rangle$  and of the fluctuations as this state evolves in time. Another advantage is that it allows for departures from equilibrium. Thus, issues concerning the restoration of symmetries in the early Universe can be addressed in a much more general setting.

There have been several attempts [12–14] to obtain the evolution equations in expanding cosmologies. Our motivations, goals, and many technical aspects differ substantially from those of previous treatments. In particular, we not only obtain the evolution equations for the order parameter to one-loop approximation, but we also find them in a nonperturbative self-consistent Hartree approximation. Within these approximation schemes, we obtain the evolution of the fluctuations (quantum and thermal), departures from equilibrium, study in detail the subtle aspects of renormalization and the validity of a high-temperature expansion. Our analysis applies quite generally to any arbitrary spatially flat FRW cosmology. We also determine the time evolution of the initial (Boltzmann) distribution functions, relate the time evolution to "squeezed states," and perform a numerical integration in the case of free fields for de Sitter and radiation-dominated cosmologies. We expect to provide a numerical analysis of the evolution of the order parameter and the dynamics of phase transitions for interacting fields in a forthcoming article.

In the next section, we set up the formalism for determining the dynamics of the order parameter  $\phi(t)$ . This involves constructing the order  $\hbar$  equations of motion for  $\phi(t)$  incorporating quantum fluctuations, and then constructing an ansatz for the time evolved density matrix we need to use to evaluate the various expectation values in the problem. We then consider a self-consistent (Hartree) approximation to the equations of motion (Sec. III) and deal with the issue of renormalization of these equations (Sec. IV).

The initial state we pick for the field  $\Phi(\mathbf{x},t)$  is that corresponding to a thermal density matrix centered at  $\phi(t)$ . It is then useful to try to understand the high temperature limit of our calculations. We are able to compute both the leading and subleading terms in the high T expansion of  $\langle \Phi^2(\mathbf{x},t) \rangle$ . From this we show that the high T expansion cannot be valid for all time, but breaks down in the large time limit (Sec. V).

In Sec. VI we compute the time evolution of the Boltzmann distribution function (initially specified as thermal) as a function of time, and find that to one-loop order and in the Hartree approximation, the density matrix describes a "squeezed" state. Section VII provides a numerical analysis of the departure from equilibrium in the simpler case of a free massive scalar field in de Sitter and radiation dominated cosmologies. We point out that a coarse-grained entropy used in the literature is not a monotonically increasing function of time in the radiation-dominated case. Section VIII contains our conclusions. There are two appendixes; the first contains some technical results that are necessary in order to compute the time evolved density matrix. The second appendix treats some of the results of the paper in conformal instead of comoving time.

### **II. EVOLUTION EQUATIONS**

We start by setting up the Schrödinger formalism for spatially flat FRW cosmologies. Consider a scalar field in such a cosmology where the metric is

$$ds^{2} = dt^{2} - a^{2}(t)d\mathbf{x}^{2}.$$
 (2.1)

The action and Lagrangian density are given by

$$S = \int d^4x \mathcal{L}.$$
 (2.2)

$$\mathcal{L} = a^{3}(t) \left[ \frac{1}{2} \dot{\Phi}^{2}(\mathbf{x}, t) - \frac{1}{2} \frac{[\boldsymbol{\nabla} \Phi(\mathbf{x}, t)]^{2}}{a(t)^{2}} - V[\Phi(\mathbf{x}, t)] \right],$$

$$V(\Phi) = \frac{1}{2} [m^2 + \xi \mathcal{R}] \Phi^2(\mathbf{x}, t) + \frac{\lambda}{4!} \Phi^4(\mathbf{x}, t), \qquad (2.4)$$

$$\mathcal{R} = 6\left(\frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right),\tag{2.5}$$

with  $\mathcal{R}$  the Ricci scalar. The canonical momentum conjugate to  $\Phi$  is

$$\Pi(\mathbf{x},t) = a^3(t)\dot{\Phi}(\mathbf{x},t) \tag{2.6}$$

and the Hamiltonian becomes

$$H(t) = \int d^3x \left\{ \frac{\Pi^2}{2a^3(t)} + \frac{a(t)}{2} (\nabla \Phi)^2 + a^3(t) V(\Phi) \right\}.$$
(2.7)

In the Schrödinger representation (at an arbitrary fixed

time  $t_0$ ), the canonical momentum is represented as

$$\Pi(\mathbf{x}) = -i\hbarrac{\delta}{\delta\Phi(\mathbf{x})}.$$

Wave functionals obey the time-dependent functional Schrödinger equation

$$i\hbar \frac{\partial \Psi[\Phi, t]}{\partial t} = H\Psi[\Phi, t].$$
 (2.8)

Since we shall eventually consider a "thermal ensemble" it is convenient to work with a functional density matrix  $\hat{\rho}$  with matrix elements in the Schrödinger representation  $\rho[\Phi(\cdot), \tilde{\Phi}(\cdot); t]$ . We will assume that the density matrix obeys the functional Liouville equation

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$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [H(t), \hat{\rho}]$$
 (2.9)

whose formal solution is

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$$\hat{\rho}(t) = U(t, t_0)\hat{\rho}(t_0)U^{-1}(t, t_0),$$

where  $U(t, t_0)$  is the time evolution operator, and  $\hat{\rho}(t_0)$  the density matrix at the arbitrary initial time  $t_0$ .

The diagonal density matrix elements  $\rho[\Phi, \Phi; t]$  are interpreted as a probability density in functional space. Since we are considering a homogeneous and isotropic background, the functional density matrix may be assumed to be translationally invariant. Normalizing the density matrix such that  $\text{Tr}\hat{\rho} = 1$ , the "order parameter" is defined as

$$\begin{split} \phi(t) &= \frac{1}{\Omega} \int d^3x \langle \Phi(\mathbf{x}, t) \rangle \\ &= \frac{1}{\Omega} \int d^3x \operatorname{Tr} \hat{\rho}(t) \Phi(\mathbf{x}) \\ &= \frac{1}{\Omega} \int d^3x \operatorname{Tr} \hat{\rho}(t_0) U^{-1}(t, t_0) \Phi(\mathbf{x}, t_0) U(t, t_0), \end{split}$$
(2.10)

where  $\Omega$  is the comoving volume, and the scale factors cancel between the numerator (in the integral) and the denominator. Note that we have used the fact that the field operator does not evolve in time in this picture. The evolution equations for the order parameter are

$$\begin{aligned} \frac{d\phi(t)}{dt} &= \frac{1}{a^3(t)\Omega} \int d^3x \langle \Pi(\mathbf{x},t) \rangle \\ &= \frac{1}{a^3(t)\Omega} \int d^3x \operatorname{Tr} \hat{\rho}(t) \Pi(\mathbf{x}) \\ &= \frac{\pi(t)}{a^3(t)}, \end{aligned}$$
(2.11)

$$\frac{d\pi(t)}{dt} = -\frac{1}{\Omega} \int d^3x a^3(t) \left\langle \frac{\delta V(\Phi)}{\delta \Phi(\mathbf{x})} \right\rangle.$$
(2.12)

It is now convenient to write the field in the Schrödinger picture as

$$\Phi(\mathbf{x}) = \phi(t) + \eta(\mathbf{x}, t), \qquad (2.13)$$

$$\langle \eta(\mathbf{x},t) \rangle = 0. \tag{2.14}$$

Expanding the right-hand side of (2.12) we find the effective equation of motion for the order parameter:

$$\frac{d^2\phi(t)}{dt^2} + 3\frac{\dot{a}(t)}{a(t)}\frac{d\phi(t)}{dt} + V'[\phi(t)]$$
$$+ \frac{V'''(\phi(t))}{2\Omega}\int d^3x \langle \eta^2(\mathbf{x},t)\rangle + \dots = 0, \quad (2.15)$$

where primes stand for derivatives with respect to  $\phi$ . To leading order in the loop expansion we need that  $\langle \eta^2(\mathbf{x},t) \rangle = O(\hbar)$ . This will be guaranteed to this order if the density matrix is assumed to be Gaussian with a covariance (width)  $O(1/\hbar)$ . If (2.13) is introduced in the Hamiltonian, we arrive at

$$H(t) = \int d^3x \left\{ -\frac{\hbar^2}{2a^3(t)} \frac{\delta^2}{\delta\eta^2} + \frac{a(t)}{2} \left( \nabla \eta \right)^2 + a^3(t) \left[ V(\phi) + V'(\phi)\eta + \frac{1}{2}V''(\phi)\eta^2 + \cdots \right] \right\}.$$
 (2.16)

Keeping only the terms quadratic in  $\eta$  in (2.16) gives the first-order term in the loop expansion. It is convenient to introduce the discrete Fourier transform of the fields in the comoving frame as

$$\eta(\mathbf{x},t) = \frac{1}{\sqrt{\Omega}} \sum_{\mathbf{k}} \eta_{\mathbf{k}}(t) e^{-i\mathbf{k}\cdot\mathbf{x}}.$$
(2.17)

In this representation, the quadratic approximation to the Hamiltonian (2.16) becomes the Hamiltonian of a collection of independent harmonic oscillators for each mode **k**:

$$H_{q} = \Omega a^{3}(t) V[\phi(t)] + \frac{1}{2} \sum_{\mathbf{k}} \left\{ -\frac{\hbar^{2}}{a^{3}(t)} \frac{\delta^{2}}{\delta \eta_{\mathbf{k}} \delta \eta_{-\mathbf{k}}} + 2a^{3}(t) V_{\mathbf{k}}'[\phi(t)] \eta_{-\mathbf{k}} + \omega_{k}^{2}(t) \eta_{\mathbf{k}} \eta_{-\mathbf{k}} \right\},$$
(2.18)

$$V'_{\mathbf{k}}[\phi(t)] = V'[\phi(t)]\sqrt{\Omega}\delta_{\mathbf{k},0}, \quad \omega_{\mathbf{k}}^{2}(t) = a(t)\mathbf{k}^{2} + a^{3}(t)V''[\phi(t)].$$
(2.19)

We propose the following Gaussian ansatz for the functional density matrix elements in the Schrödinger representation:

(2.21)(2.22)

$$\rho[\Phi, \tilde{\Phi}, t] = \prod_{\mathbf{k}} \mathcal{N}_{\mathbf{k}}(t) \exp\left\{-\left[\frac{A_{\mathbf{k}}(t)}{2\hbar}\eta_{\mathbf{k}}(t)\eta_{-\mathbf{k}}(t) + \frac{A_{\mathbf{k}}^{*}(t)}{2\hbar}\tilde{\eta}_{\mathbf{k}}(t)\tilde{\eta}_{-\mathbf{k}}(t) + \frac{B_{\mathbf{k}}(t)}{\hbar}\eta_{\mathbf{k}}(t)\tilde{\eta}_{-\mathbf{k}}(t)\right] + \frac{i}{\hbar}\pi_{\mathbf{k}}(t)\left[\eta_{-\mathbf{k}}(t) - \tilde{\eta}_{-\mathbf{k}}(t)\right]\right\},$$

$$(2.20)$$

$$\eta_{k}(t) = \Phi_{k} - \phi(t) \sqrt{\Omega} \delta_{k,0},$$
$$\tilde{\eta}_{k}(t) = \tilde{\Phi}_{k} - \phi(t) \sqrt{\Omega} \delta_{k,0},$$

where  $\phi(t) = \langle \Phi(\mathbf{x}) \rangle$  and  $\pi_k(t)$  is the Fourier transform of  $\langle \Pi(\mathbf{x}) \rangle$ . This form of the density matrix is dictated by the Hermiticity condition  $\rho^{\dagger}[\Phi, \tilde{\Phi}, t] = \rho^*[\tilde{\Phi}, \Phi, t]$ ; as a result of this,  $B_k(t)$  is real. The kernel  $B_k(t)$  determines the amount of "mixing" in the density matrix, since if  $B_k = 0$ , the density matrix corresponds to a pure state because it is a wave functional times its complex conjugate.

In order to solve for the time evolution of the density matrix (2.9) we need to specify the density matrix at some initial time  $t_0$ . It is at this point that we have to assume some physically motivated initial condition. We believe that this is a subtle point that has not received proper consideration in the literature. A system in thermal equilibrium has time-independent ensemble averages (as the evolution Hamiltonian commutes with the density matrix) and there is no memory of any initial state. However, in a time dependent background, the density matrix will evolve in time, departing from the equilibrium state and correlation functions or expectation values may depend on details of the initial state.

We will assume that at early times the initial density matrix is thermal for the modes that diagonalize the Hamiltonian at  $t_0$  (we call these the adiabatic modes). The effective temperature for these modes is  $k_B T_0 = 1/\beta_0$ . It is only in this initial state that the notion of "temperature" is meaningful. As the system departs from equilibrium one cannot define a thermodynamic temperature. Thus in this case the "temperature" refers to the temperature defined in the initial state.

The initial values of the order parameter and average canonical momentum are  $\phi(t_0) = \phi_0$  and  $\pi(t_0) = \pi_0$ , respectively. Defining the adiabatic frequencies as

$$W_k^2(t_0) = \frac{\omega_k^2(t_0)}{a^3(t_0)} = \frac{\mathbf{k}^2}{a^2(t_0)} + V''[\phi_{\rm cl}(t_0)]$$
(2.23)

we find that the initial values of the time dependent pa-

rameters in the density matrix (2.20) are

$$A_{k}(t_{0}) = A_{k}^{*}(t_{0}) = W_{k}(t_{0})a^{3}(t_{0}) \coth\left[\beta_{0}\hbar W_{k}(t_{0})\right],$$
(2.24)

$$B_{k}(t_{0}) = -\frac{W_{k}(t_{0})a^{3}(t_{0})}{\sinh\left[\beta_{0}\hbar W_{k}(t_{0})\right]},$$
(2.25)

$$\mathcal{N}_{\boldsymbol{k}}(t_0) = \left[\frac{W_{\boldsymbol{k}}(t_0)a^3(t_0)}{\pi\hbar} \tanh\left(\frac{\beta_0\hbar W_{\boldsymbol{k}}(t_0)}{2}\right)\right]^{\frac{1}{2}}, \quad (2.26)$$

$$\phi(t_0) = \phi_0 \ , \ \pi(t_0) = \pi_0.$$
 (2.27)

The initial density matrix is normalized such that  $\text{Tr}\rho(t_0) = 1$ . Since time evolution is unitary such a normalization will be constant in time. For  $T_0 = 0$  the density matrix describes a pure state since  $B_k = 0$ .

As an example, consider the case of de Sitter space. The scale factor is given by  $a(t) = a_0 e^{Ht}$  and for  $T_0 \rightarrow 0$ ,  $t_0 \rightarrow -\infty$  we recognize the ground-state wave functional for the Bunch-Davies vacuum [10,18]. For  $T_0 \neq 0$  this initial density matrix corresponds to a thermal ensemble of Bunch-Davies modes. Certainly this choice is somewhat arbitrary but it physically describes the situation in which at very early times the adiabatic modes are in *local thermodynamic equilibrium*. Whether or not this situation actually obtains for a given system has to be checked explicitly. In the cosmological setting, the nature of the initial condition will necessarily have to result from a deeper understanding of the relationship between particle physics, gravitation, and statistical mechanics at very large energy scales.

Although we will continue henceforth to use this thermal initial state, it should be emphasized that our formalism is quite general and can be applied to *any initial* state.

In the Schrödinger picture, the Liouville equation (2.9) becomes

$$i\hbar\frac{\partial\rho[\Phi,\tilde{\Phi},t]}{\partial t} = \sum_{k} \left\{ -\frac{\hbar^2}{2a^3(t)} \left( \frac{\delta^2}{\delta\eta_k \delta\eta_{-k}} - \frac{\delta^2}{\delta\tilde{\eta}_k \delta\tilde{\eta}_{-k}} \right) + a^3(t)V'_{-k}[\phi(t)](\eta_k - \tilde{\eta}_k) + \frac{1}{2}\omega_k^2(t)(\eta_k \eta_{-k} - \tilde{\eta}_k \tilde{\eta}_{-k}) \right\} \rho[\Phi,\tilde{\Phi},t].$$

$$(2.28)$$

Since the modes do not mix in this approximation to the Hamiltonian, the equations for the kernels in the density matrix are obtained by comparing the powers of  $\eta$  on both sides of the above equation. We obtain the following equations for the coefficients:

$$i\frac{\dot{\mathcal{N}}_{k}}{\mathcal{N}_{k}} = \frac{1}{2a^{3}(t)}(A_{k} - A_{k}^{*}), \qquad (2.29)$$

$$i\dot{A}_{k} = \left[\frac{A_{k}^{2} - B_{k}^{2}}{a(t)^{3}} - \omega_{k}^{2}(t)\right], \qquad (2.30)$$

$$i\dot{B}_{k} = \frac{B_{k}}{a^{3}(t)}(A_{k} - A_{k}^{*}),$$
 (2.31)

$$-\dot{\pi}_{\mathbf{k}} = V'[\phi(t)]a^3(t)\sqrt{\Omega}\delta_{\mathbf{k},0}, \qquad (2.32)$$

$$\dot{\phi} = \frac{\pi}{a^3(t)}.\tag{2.33}$$

The last two equations are identified with the *classical* equations of motion for the order parameter (2.15). The equation for  $B_k(t)$  reflects the fact that a pure state  $B_k = 0$  remains pure under time evolution.

Writing  $A_k$  in terms of its real and imaginary components  $A_k(t) = A_{Rk}(t) + iA_{Ik}(t)$  (and because  $B_k$  is real) we find that

$$\frac{B_k(t)}{A_{Rk}(t)} = \frac{B_k(t_0)}{A_{Rk}(t_0)}$$
(2.34)

and that the time evolution is unitary (as it should be), that is

$$\frac{\mathcal{N}_k(t)}{\sqrt{[A_{Rk}(t) + B_k(t)]}} = \text{const.}$$
(2.35)

The initial conditions (2.24) and (2.25) and the invariance of the ratio (2.34) suggest that the solution for the real part of A and for B may be obtained by introducing a complex function  $\mathcal{A}_k(t) = \mathcal{A}_{Rk}(t) + i\mathcal{A}_{Ik}(t)$ 

$$\mathcal{A}_{Rk}(t) = A_{Rk}(t) \tanh \left[\beta_0 \hbar W_k(t_0)\right]$$
  
=  $-B_k(t) \sinh \left[\beta_0 \hbar W_k(t_0)\right],$  (2.36)

$$\mathcal{A}_{Rk}(t_0) = W_k(t_0) \ a^3(t_0), \tag{2.37}$$

$$\mathcal{A}_{Ik}(t) = A_{Ik}(t). \tag{2.38}$$

In this form, the real and imaginary parts of  $\mathcal{A}$  satisfy the equations

$$\dot{\mathcal{A}}_{Rk}(t) = \frac{2}{a^3(t)} \mathcal{A}_{Rk}(t) \mathcal{A}_{Ik}(t), \qquad (2.39)$$

$$-\dot{\mathcal{A}}_{Ik}(t) = \frac{1}{a^3(t)} \left[ \mathcal{A}_{Rk}^2(t) - \mathcal{A}_{Ik}^2(t) - \omega_k^2(t) a^3(t) \right].$$
(2.40)

These two equations may be combined in one complex equation for the combination  $\mathcal{A}_{k}(t) = \mathcal{A}_{Rk}(t) + i\mathcal{A}_{Ik}(t)$  that obeys the Riccati-type equation

$$i\dot{\mathcal{A}}_{k}(t) = \frac{1}{a^{3}(t)} \left[ \mathcal{A}_{k}^{2}(t) - \omega_{k}^{2}(t)a^{3}(t) \right]$$
(2.41)

with the initial conditions

$$\mathcal{A}_{Rk}(t_0) = W_k(t_0)a^3(t_0), \qquad (2.42)$$

$$\mathcal{A}_{Ik}(t_0) = 0. \tag{2.43}$$

The Riccati equation (2.41) becomes a more amenable differential equation by the change of variables

$$\mathcal{A}_{k}(t) = -ia^{3}(t)\frac{\dot{\varphi}_{k}(t)}{\varphi_{k}(t)}.$$
(2.44)

The solution to the Ricatti equation with the above initial conditions is detailed in Appendix A. We find that it is convenient to introduce two real mode functions (for each wave vector k) and write

$$\varphi_{k}(t) = \frac{\mathcal{U}_{k1}(t) + i\mathcal{U}_{k2}(t)}{\sqrt{a^{3}(t)W_{k}(t_{0})}}.$$
(2.45)

These mode functions obey a Schrödinger-like equation. The initial conditions on  $\varphi_k(t_0)$  are (see Appendix A)

$$egin{aligned} arphi_{m{k}}(t_0) &= rac{1}{\sqrt{a^3(t_0)W_{m{k}}(t_0)}}, \ \dot{arphi}_{m{k}}(t) \mid_{t_0} &= i\sqrt{rac{W_{m{k}}(t_0)}{a^3(t_0)}}, \end{aligned}$$

 $\mathcal{A}_{Rk}(t)$  is given by Eq. (A14) in Appendix A, so that

$$A_{Rk}(t) = \frac{1}{\mid \varphi_k(t) \mid^2} \coth\left[\beta_0 \hbar W_k(t_0)\right], \qquad (2.46)$$

$$B_{k}(t) = -\frac{1}{|\varphi_{k}(t)|^{2}} \left[ \frac{1}{\sinh \left[\beta_{0} \hbar W_{k}(t_{0})\right]} \right].$$
(2.47)

The equal time two-point function for the fluctuation becomes

$$\langle \eta_{k}(t)\eta_{-k}(t) \rangle = \frac{\hbar}{2 \left[ A_{Rk}(t) + B_{k}(t) \right]}$$
  
=  $\frac{\hbar}{2} |\varphi_{k}(t)|^{2} \coth \left[ \beta_{0} \hbar W_{k}(t_{0}) / 2 \right].$  (2.48)

The one-loop equation of motion for the order parameter thus becomes

$$\ddot{\phi} + 3\frac{\dot{a}}{a}\dot{\phi} + V'(\phi) + V'''(\phi)\frac{\hbar}{2} \\ \times \int \frac{d^3k}{(2\pi)^3} \frac{|\varphi_k(t)|^2}{2} \coth\left[\beta_0 \hbar W_k(t_0)/2\right] = 0 \quad (2.49)$$

with the function  $\varphi_k(t)$  defined in Appendix A by (A7) and (A8) in which, to this order in  $\hbar$ , only the *classical solution*  $\phi_{cl}(t)$  enters. A consistent numerical solution of these equations to  $O(\hbar)$  would involve splitting  $\phi(t) = \phi_{cl}(t) + \hbar \phi_{(1)}(t)$  and keeping only the  $O(\hbar)$  terms in the evolution equation. This will result in two simultaneous equations, one for the classical evolution of the order parameter and another for  $\phi_{(1)}(t)$ .

This equation of motion is clearly *very* different from the one obtained by using the effective potential. It may be easily seen (by writing the effective action as the classical action plus the logarithm of the determinant of the quadratic fluctuation operator) that this is the equation of motion obtained by the variation of the one-loop effective action.

The *static* effective potential is clearly not the appropriate quantity to use to describe scalar field dynamics in an expanding Universe. Although there may be some time regime in which the time evolution is slow and fluctuations rather small, this will certainly *not* be the case at the onset of a phase transition. As the phase transition takes place, fluctuations become dominant and grow in time signaling the onset of long-range correlations [8,9].

#### **III. HARTREE EQUATIONS**

Motivated by our previous studies in Minkowski space [8,9] which showed that the growth of correlation and enhancement of fluctuations during a phase transition may not be described perturbatively, we now proceed to obtaining the equations of motion in a Hartree approximation. This approximation is nonperturbative in the sense that it sums up infinitely many diagrams of the cactustype [6]. The Hartree approximation becomes exact in the  $N \to \infty$  limit of an O(N) vector theory. Although its validity is not warranted in the present case, it at least provides a consistent nonperturbative framework in which correlations and fluctuations can be studied. It is conceivable that this approximation could be implemented beyond the lowest (cactus) order in a consistent fashion.

Vilenkin [19] has previously studied an approximate version of the Hartree equations.

The Hartree self-consistent approximation is implemented as follows. We decompose the field as in (2.13), using a potential as in (2.4). We find that the Hamiltonian becomes

$$H = \int d^3x \left\{ -\frac{\hbar^2}{2a^3(t)} \frac{\delta^2}{\delta\eta^2} + \frac{a(t)}{2} \left( \nabla \eta \right)^2 + a^3(t) \left( V(\phi) + V'(\phi)\eta + \frac{1}{2!} V''(\phi)\eta^2 + \frac{1}{3!} \lambda \phi \eta^3 + \frac{1}{4!} \lambda \eta^4 \right) \right\}.$$
 (3.1)

The Hartree approximation is obtained by assuming the factorization

$$\eta^{3}(\mathbf{x},t) \to 3\langle \eta^{2}(\mathbf{x},t) \rangle \eta(\mathbf{x},t),$$
 (3.2)

$$\eta^4(\mathbf{x},t) \to 6\langle \eta^2(\mathbf{x},t) \rangle \eta^2(\mathbf{x},t) - 3\langle \eta^2(\mathbf{x},t) \rangle^2,$$
 (3.3)

where angular brackets denote the average using the time evolved density matrix. This average will be determined self-consistently (see below). Translational invariance shows that  $\langle \eta^2(\mathbf{x}, t) \rangle$  can only be a function of time. This approximation makes the Hamiltonian quadratic at the expense of a self-consistent condition. In the timeindependent (Minkowski) case this approximation sums up all the "daisy" (or "cactus") diagrams and leads to the self-consistent gap equation [6]. In this approximation the Hamiltonian becomes

$$H = \Omega a^{3}(t) \mathcal{V}(\phi) + \int d^{3}x \Biggl\{ -\frac{\hbar^{2}}{2a^{3}(t)} \frac{\delta^{2}}{\delta\eta^{2}} + \frac{a(t)}{2} \left( \nabla \eta \right)^{2} + a^{3}(t) \left[ \mathcal{V}^{(1)}(\phi)\eta + \frac{1}{2} \mathcal{V}^{(2)}(\phi)\eta^{2} \right] \Biggr\}, \quad (3.4)$$

$$\mathcal{V}(\phi) = V(\phi) - \frac{1}{8}\lambda\langle\eta^2\rangle^2, \qquad (3.5)$$

$$\mathcal{V}^{(1)}(\phi) = V'(\phi) + \frac{1}{2}\lambda\phi\langle\eta^2\rangle, \qquad (3.6)$$

$$\mathcal{V}^{(2)}(\phi) = V''(\phi) + \frac{1}{2}\lambda\langle\eta^2\rangle. \tag{3.7}$$

We can now introduce the Fourier transform of the field as in (2.17). The Hamiltonian will have the same form as (2.18) but the time dependent frequencies (2.19) and linear term in  $\eta$  become

$$\omega_k^2(t) = a(t)\mathbf{k}^2 + a^3(t)\mathcal{V}^{(2)}[\phi(t)], \qquad (3.8)$$

$$\mathcal{V}_{\mathbf{k}}^{(1)}[\phi(t)] = \mathcal{V}^{(1)}[\phi(t)]\sqrt{\Omega}\delta_{\mathbf{k},0}.$$
(3.9)

The ansatz for the Gaussian density matrix is the same as before (2.20), as are the evolution equations for the coefficients  $A_k(t)$ ,  $B_k(t)$ ,  $\mathcal{N}_k(t)$ . However, the frequencies are now given by (3.8). The *classical* equations of motion (2.32) and (2.33) now become

$$-\dot{\pi} = \mathcal{V}^{(1)}[\phi(t)]a^3(t), \qquad (3.10)$$

$$\dot{\phi} = \frac{\pi}{a^3(t)}.\tag{3.11}$$

The equations for the coefficients  $A_k(t)$ ,  $B_k(t)$ ,  $\mathcal{N}_k(t)$  are again solved in terms of the mode functions given in Appendix A but with  $V''[\phi_{\rm cl}(t)]$  now replaced by  $\mathcal{V}^{(2)}[\phi(t)]$ and the following replacement of the adiabatic frequencies:

$$W_k(t_0) \to \mathcal{W}_k(t_0) = \frac{\left[\mathbf{k}^2 + m^2(T_0)\right]^{\frac{1}{2}}}{a(t_0)},$$
 (3.12)

$$\frac{m^2(T_0)}{a^2(t_0)} = \mathcal{V}^{(2)}[\phi(t_0)]. \tag{3.13}$$

The mode functions of Appendix A obey the differential equations and initial conditions with this replacement and

$$\mid arphi_{m{k}}(t)\mid^{2} 
ightarrow \mid arphi_{m{k}}^{H}(t)\mid^{2}$$
 .

The initial conditions at  $t_0$  are now given in terms of these new adiabatic frequencies (see Appendix A). The equal time two-point function thus becomes

$$\langle \eta^2(\mathbf{x},t) \rangle = \frac{\hbar}{2} \int \frac{d^3k}{(2\pi)^3} \mid \varphi_k^H(t) \mid^2 \coth\left[\beta_0 \hbar \mathcal{W}_k(t_0)/2\right],$$
(3.14)

which leads to the following set of self-consistent time dependent Hartree equations:

$$\ddot{\phi} + 3\frac{a}{a}\dot{\phi} + V'(\phi)$$

$$+\lambda\phi\frac{\hbar}{2}\int\frac{d^3k}{(2\pi)^3}\frac{|\varphi_k^H(t)|^2}{2}\coth\left[\beta_0\hbar\mathcal{W}_k(t_0)/2\right] = 0,$$
(3.15)

$$\varphi_{k}^{H}(t_{0}) = \frac{1}{\sqrt{a^{3}(t_{0})\mathcal{W}_{k}(t_{0})}},$$
(3.17)

$$\dot{\varphi}_{k}^{H}(t) \mid_{t_{0}} = i \sqrt{\frac{\mathcal{W}_{k}(t_{0})}{a^{3}(t_{0})}}.$$
 (3.18)

#### **IV. RENORMALIZATION**

In either the one-loop approximation or the Hartree self-consistent approximation, the renormalization aspects are contained in the momentum integrals of the mode functions. Because the Bose-Einstein distribution functions are exponentially suppressed at large momenta, the finite temperature contribution will be convergent and we need only address the zero temperature contribution. The study of renormalization is more conveniently performed in terms of the following mode function satisfying a Schrödinger-like equation (see Appendix A):

$$\mathcal{U}_{k}^{H}(t) = a^{\frac{3}{2}}(t)\varphi_{k}^{H}(t)\sqrt{\mathcal{W}_{k}(t_{0})}, \qquad (4.1)$$

$$\mathcal{U}_k^H(t_0) = 1, \tag{4.2}$$

$$\dot{\mathcal{U}}_{k}^{H}(t) = \frac{3\dot{a}(t_{0})}{2a(t_{0})} + i\mathcal{W}_{k}(t_{0}).$$
(4.3)

The one-loop case may be obtained by making the replacement  $\mathcal{W}_k(\phi) \to W_k(\phi)$ .

We will now analyze the renormalization aspects for the Hartree approximation; the one-loop case may be obtained easily from this more general case. We need to understand the divergences in the integral

$$I = \int \frac{d^3k}{(2\pi)^3} \frac{|\mathcal{U}_k^H(t)|^2}{2a^3(t)\mathcal{W}_k(t_0)}.$$
(4.4)

The divergences in this integral will be determined from the large-k behavior of the mode function that is a solution to the differential equation obtained from (3.16) with the initial conditions (4.2) and (4.3). The largek behavior of this function may be obtained in a WKB approximation by introducing the function  $\mathcal{D}_k(t)$ ;

$$\mathcal{D}_{k}(t) = \exp\left[\int_{t_{0}}^{t} R(t')dt'\right], \qquad (4.5)$$

$$\mathcal{D}_{\boldsymbol{k}}(t_0) = 1, \tag{4.6}$$

satisfying the differential equation

$$\left[\frac{d^2}{dt^2} - \frac{3}{2}\left(\frac{\ddot{a}}{a} + \frac{1}{2}\frac{\dot{a}^2}{a^2}\right) + \frac{\mathbf{k}^2}{a^2(t)} + V''[\phi(t)] + \frac{\lambda}{2}\langle\eta^2(\mathbf{x},t)\rangle\right]\mathcal{D}_k(t) = 0 \quad (4.7)$$

with  $\langle \eta^2(\mathbf{x}, t) \rangle$  being the self-consistent integral in the Hartree equation (3.16). The one-loop approximation is obtained by setting  $\langle \eta^2(\mathbf{x}, t) \rangle = 0$  in the above equation. The mode function  $\mathcal{U}^H$  is obtained as a linear combination of the function  $\mathcal{D}_k(t)$  and its complex conjugate; the coefficients are to be determined from the initial conditions (see below). The function R(t) obeys a Riccati equation

$$\begin{split} \dot{R} + R^2 - \frac{3}{2} \left( \frac{\ddot{a}}{a} + \frac{1}{2} \frac{\dot{a}^2}{a^2} \right) + \frac{\mathbf{k}^2}{a^2(t)} + V''[\phi(t)] \\ + \frac{\lambda}{2} \langle \eta^2(\mathbf{x}, t) \rangle = 0. \end{split}$$
(4.8)

We propose a WKB solution to this equation of the form

$$R = \frac{-ik}{a(t)} + R_0(t) - \frac{iR_1(t)}{k} + \frac{R_2(t)}{k^2} + \cdots$$
(4.9)

and find the time dependent coefficients by comparing powers of k. This yields

$$R_0(t) = \frac{\dot{a}(t)}{2a(t)},$$
(4.10)

$$R_1(t) = \frac{a(t)}{2} \left[ -\frac{\mathcal{R}}{6} + V''[\phi(t)] + \frac{\lambda}{2} \langle \eta^2(\mathbf{x}, t) \rangle \right], \quad (4.11)$$

$$R_2(t) = -\frac{1}{2} \frac{d}{dt} \left[ a(t) R_1(t) \right].$$
(4.12)

Finally, we write

$$\mathcal{U}_{k}^{H}(t) = \frac{1}{2}[1+\gamma]\mathcal{D}_{k}^{*}(t) + \frac{1}{2}[1-\gamma]\mathcal{D}_{k}(t), \qquad (4.13)$$

where  $\gamma$  is determined from the initial condition (4.3):

$$\gamma = 1 - i \frac{\dot{a}(t_0)}{k} + \frac{m(T_0)^2}{2k^2} - \frac{a(t_0)R_1(t_0)}{k^2} + O(1/k^3) + \cdots$$
(4.14)

Thus in the  $k \to \infty$  limit we find

$$\frac{|\varphi_k^H(t)|^2}{2} \to \left\{ \frac{1}{2a^2(t)k} + \frac{1}{4k^3} \left[ \frac{\dot{a}^2(t_0)}{a^2(t)} - \left( -\frac{\mathcal{R}}{6} + V''(\phi) + \frac{\lambda}{2} \langle \eta^2(\mathbf{x}, t) \rangle \right) \right] + O(1/k^4) + \cdots \right\}.$$
(4.15)

Introducing an upper momentum cutoff  $\Lambda$  we obtain

$$\langle \eta^{2}(\mathbf{x},t) \rangle = \hbar \int \frac{d^{3}k}{(2\pi)^{3}} \frac{|\varphi_{k}^{H}(t)|^{2}}{2} \coth\left[\beta_{0}\hbar \mathcal{W}_{k}(t_{0})/2\right]$$

$$= \frac{\hbar}{8\pi^{2}} \frac{\Lambda^{2}}{a^{2}(t)} + \frac{\hbar}{8\pi^{2}} \ln\left(\frac{\Lambda}{K}\right) \left[\frac{\dot{a}^{2}(t_{0})}{a^{2}(t)} - \left(-\frac{\mathcal{R}}{6} + V''[\phi(t)] + \frac{\lambda}{2} \langle \eta^{2}(\mathbf{x},t) \rangle\right)\right] + \text{ finite },$$

$$(4.16)$$

where we have introduced a renormalization point K, and the finite part depends on time, temperature, and K. In the one-loop approximation,  $\langle \eta^2(\mathbf{x},t) \rangle$  does not appear in the logarithmic divergent term in (4.16) (as it does not appear in the differential equation for the mode functions up to one loop).

There are several physically important features of the divergent structure obtained above. First, the quadratically divergent term reflects the fact that the physical momentum cutoff is being redshifted by the expansion. This term will not appear in dimensional regularization.

Second, the logarithmic divergence contains a term that reflects the initial condition (the derivative of the expansion factor at the initial time  $t_0$ ). The initial condition breaks any remnant symmetry. For example, in de Sitter space there is still invariance under the de Sitter group, but this is also broken by the initial condition at an arbitrary time  $t_0$ . Thus this term is not forbidden, and its appearance does not come as a surprise. As a consequence of this term, we need a time dependent term in the bare mass proportional to  $1/a^2(t)$ .

We are now in a position to present the renormalization prescription within the Hartree approximation. In this approximation there are no interactions, since the Hamiltonian is quadratic. The nonlinearities are encoded in the self-consistency condition. Because of this, there are no counterterms with which to cancel the divergences and the differential equation for the mode functions (3.16)*must be finite.* Thus the renormalization conditions are obtained from

$$m_B^2(t) + \frac{\lambda_B}{2}\phi^2(t) + \xi_B \mathcal{R} + \frac{\lambda_B}{2}\langle \eta^2 \rangle_B$$
$$= m_R^2 + \frac{\lambda_R}{2}\phi^2(t) + \xi_R \mathcal{R} + \frac{\lambda_R}{2}\langle \eta^2 \rangle_R, \quad (4.17)$$

where the subscripts B, R refer to bare and renormalized quantities, respectively, and  $\langle \eta^2 \rangle_B$  is read from (4.16):

$$\langle \eta^2 \rangle_B = \frac{\hbar}{8\pi^2} \frac{\Lambda^2}{a^2(t)} + \frac{\hbar}{8\pi^2} \ln\left(\frac{\Lambda}{K}\right) \left[\frac{\dot{a}^2(t_0)}{a^2(t)} - \left(-\frac{\mathcal{R}}{6} + m_R^2 + \frac{\lambda_R}{2}\phi^2(t) + \xi_R \mathcal{R} + \frac{\lambda_R}{2}\langle \eta^2 \rangle_R\right)\right] + \text{ finite} .$$
(4.18)

Using the renormalization conditions (4.17) we obtain

γ

$$n_B^2(t) + \frac{\lambda_B \hbar}{16\pi^2} \frac{\Lambda^2}{a^2(t)} + \frac{\lambda_B \hbar}{16\pi^2} \ln\left(\frac{\Lambda}{K}\right) \frac{\dot{a}^2(t_0)}{a^2(t)} = m_R^2 \left[1 + \frac{\lambda_B \hbar}{16\pi^2} \ln\left(\frac{\Lambda}{K}\right)\right],\tag{4.19}$$

$$\lambda_B = \frac{\lambda_R}{1 - \frac{\lambda_R \hbar}{16\pi^2} \ln\left(\frac{\Lambda}{K}\right)},\tag{4.20}$$

$$\xi_B = \xi_R + \frac{\lambda_B \hbar}{16\pi^2} \ln\left(\frac{\Lambda}{K}\right) \left(\xi_R - \frac{1}{6}\right),\tag{4.21}$$

$$\langle \eta^2 \rangle_R = I_R + J, \tag{4.22}$$

where

$$I_{R} = \hbar \int \frac{d^{3}k}{(2\pi)^{3}} \left\{ \frac{|\varphi_{k}^{H}(t)|^{2}}{2} - \frac{1}{2ka^{2}(t)} + \frac{\theta(k-K)}{4k^{3}} \left[ -\frac{\mathcal{R}}{6} - \frac{\dot{a}^{2}(t_{0})}{a^{2}(t)} + m_{R}^{2} + \frac{\lambda_{R}}{2}\phi^{2}(t) + \xi_{R}\mathcal{R} + \frac{\lambda_{R}}{2}\langle\eta^{2}\rangle_{R} \right] \right\}, \quad (4.23)$$

$$J = \hbar \int \frac{d^3k}{(2\pi)^3} \frac{|\varphi_k^H(t)|^2}{\exp\beta_0 \hbar \mathcal{W}_k(t_0) - 1}.$$
(4.24)

The conformal coupling  $\xi = 1/6$  is a fixed point under renormalization [18]. In dimensional regularization the terms involving  $\Lambda^2$  are absent and  $\ln \Lambda$  is replaced by a simple pole at the physical dimension. Even in such a regularization scheme, however, a time dependent bare mass is needed. The presence of this new renormalization allows us to introduce a new renormalized mass term of the form

$$\frac{\Sigma}{a^2(t)}$$

This counterterm may be interpreted as a squared mass redshifted by the expansion of the Universe. However, we shall set  $\Sigma = 0$  for simplicity.

It is clear that there is no wave function renormaliza-

tion. This is a consequence of the approximations invoked. There is, in fact, no wave function renormalization in either the one-loop or the Hartree approximation for a scalar field theory in three spatial dimensions.

Notice that there is a weak cutoff dependence on the effective equation of motion for the order parameter.

For fixed  $\lambda_R$ , as the cutoff  $\Lambda \to \infty$ ,

$$\lambda_B \approx -\frac{(4\pi)^2}{\ln\left(\frac{\Lambda}{K}\right)}.$$
 (4.25)

In addition,

$$\xi_B = \frac{1}{6} + O\left(\frac{1}{\ln\Lambda}\right) \tag{4.26}$$

$$m_B^2(t) = \frac{1}{a^2(t)} \left[ \frac{\Lambda^2}{\ln\left(\frac{\Lambda}{K}\right)} + \dot{a}^2(t_0) \right] + O\left(\frac{1}{\ln\Lambda}\right). \quad (4.27)$$

This approach to  $0^-$  of the bare coupling as the cutoff is removed translates into an instability in the bare theory. This is a consequence of the fact that the *N*component  $\Phi^4$  theory for  $N \to \infty$  is asymptotically free (see Ref. [20]), which is not relieved in curved space-time. Clearly this theory is sensible only as a low-energy cutoff effective theory, and it is in this restricted sense that we will ignore the weak cutoff dependence and neglect the term proportional to the bare coupling in (4.28).

The renormalized self-consistent Hartree equations thus become after letting  $\Lambda = \infty$ :

$$\begin{split} \ddot{\phi} + 3\frac{\dot{a}}{a}\dot{\phi} + m_R^2\phi + \xi_R\mathcal{R}\phi + \frac{\lambda_R}{2}\phi^3 + \frac{\lambda_R\phi}{2}\langle\eta^2\rangle_R &= 0, \\ (4.28) \\ \left[\frac{d^2}{dt^2} + 3\frac{\dot{a}(t)}{a(t)}\frac{d}{dt} + \frac{\mathbf{k}^2}{a^2(t)} + m_R^2 + \xi_R\mathcal{R} \\ + \frac{\lambda_R}{2}\phi^2 + \frac{\lambda_R}{2}\langle\eta^2\rangle_R\right]\varphi_k^H(t) &= 0, \quad (4.29) \end{split}$$

where  $\langle \eta^2 \rangle_R$  is given by Eqs. (4.23) and (4.24).

For completeness we quote the renormalized equation of motion for the order parameter to one loop:

$$\ddot{\phi} + 3\frac{\dot{a}}{a}\dot{\phi} + m_R^2\phi + \xi_R\mathcal{R}\phi + \frac{\lambda_R}{2}\phi^3 + \frac{\lambda_R\phi}{2}\langle\eta^2\rangle_R = 0,$$
(4.30)
$$\left[\frac{d^2}{dt^2} + 3\frac{\dot{a}(t)}{a(t)}\frac{d}{dt} + \frac{\mathbf{k}^2}{a^2(t)} + m_R^2 + \xi_R\mathcal{R} + \frac{\lambda_R}{2}\phi^2(t)\right]\varphi_k(t) = 0. \quad (4.31)$$

The one-loop coupling constant renormalization differs from that in the Hartree approximation by a factor of 3. This is a consequence of the fact that the Hartree approximation is equivalent to a large-N approximation and only sums up the *s*-channel bubbles.

#### V. HIGH TEMPERATURE LIMIT

One of the payoffs of understanding the large-k behavior of the mode functions (as obtained in the previous section via the WKB method) is that it permits the evaluation of the high temperature limit. We shall perform our analysis of the high temperature expansion for the Hartree approximation. The one-loop case may be read off from these results.

The finite temperature contribution is determined by the integral

$$J = \hbar \int \frac{d^3k}{(2\pi)^3} \frac{|\varphi_k^H(t)|^2}{e^{\beta_0 \hbar W_k(t_0)} - 1}.$$
 (5.1)

For large temperature, only momenta  $k \ge T_0$  contribute. Thus the leading contribution is determined by the first term of the function R(t) [eq.(4.9)] of the previous section. We find

$$J = \frac{1}{12\hbar} \left[ \frac{k_B T_0 a(t_0)}{a(t)} \right]^2 \left[ 1 + O(1/T_0) + \cdots \right].$$
 (5.2)

Thus we see that the leading high temperature behavior reflects the physical redshift in the cosmological background and it results in an effective time dependent temperature

$$T_{ ext{eff}}(t) = T_0 \left[ rac{a(t_0)}{a(t)} 
ight].$$

To leading order, the expression obtained for the time dependent effective temperature corresponds to what would be obtained for an *adiabatic* (isentropic) expansion for blackbody-type radiation consisting of massless relativistic particles evolving in the cosmological background.

This behavior only appears at *leading* order in the high temperature expansion. There are subleading terms that must be taken into account. These can be calculated within the high temperature expansion and we do this below. To avoid cluttering of notation, we will set  $k_B = \hbar = 1$  in what follows.

We define

$$m^{2}(T_{0}) \equiv m_{R}^{2} + \xi_{R}\mathcal{R}(t_{0}) + \frac{\lambda_{R}}{2}\phi^{2}(t_{0}) + \frac{\lambda_{R}}{2}\langle\eta^{2}(t_{0})\rangle_{R}$$
(5.3)

and we will assume that  $m^2(T_0) \ll T_0^2$ . Since we are interested in the description of a phase transition, we will write

$$m_R^2 + \xi_R \mathcal{R}(t_0) + \frac{\lambda_R}{2} \phi^2(t_0) = -\frac{\lambda_R T_c^2}{24}, \quad T_c^2 > 0.$$
 (5.4)

Thus, to leading order in  $T_0$ ,

$$m^{2}(T_{0}) = \frac{\lambda_{R}}{24} (T_{0}^{2} - T_{c}^{2}).$$
 (5.5)

Our high temperature expansion will assume fixed  $m(T_0)$ and  $m(T_0)/T_0 \ll 1$ .

It becomes convenient to define the variable

$$\begin{aligned} x^2 &= \frac{k^2}{T_0^2 a^2(t_0)} + \frac{m^2(T_0)}{T_0^2}, \\ &|\varphi_k^H(t)|^2 = \left|\varphi^H\left(a(t_0)\sqrt{x^2T_0^2 - m^2(T_0)}; t\right)\right|^2. \end{aligned}$$

Recall from our WKB analysis that the leading behavior for  $k \to \infty$  is [see Eq. (4.15)]

$$\frac{\mid \varphi^H_k(t)\mid^2}{2} \rightarrow \frac{1}{2a^2(t)k}$$

adding and subtracting this leading term in the integral J and performing the above change of variables, we have

$$J = J_1 + J_2,$$

$$J_1 = \left[\frac{a(t_0)}{a(t)}\right]^3 \left(\frac{T_0}{\pi}\right)^2 \int_{\frac{m(T_0)}{T_0}}^{\infty} \frac{xdx}{e^x - 1} \left[a^3(t)\sqrt{x^2T_0^2 - m^2(T_0)} \frac{|\varphi_k^H(t)|^2}{2} - \frac{a(t)}{2a(t_0)}\right],$$
(5.6)

We now must study the high temperature expansion of  $J_1$ . We will restrict ourselves to the determination of the linear and logarithmic dependence on  $T_0$ . For this purpose, it becomes convenient to introduce yet another change of variables

$$x = \frac{m(T_0)}{T_0} z$$

and use the fact that, in the limit  $T_0 \gg m(T_0)$ ,

$$\frac{z}{e^{\frac{m(T_0)}{T_0}z}-1}\approx \frac{T_0}{m(T_0)}\left(1-\frac{m(T_0)}{2T_0}z+\cdots\right).$$

This yields the following linear and logarithmic terms in  $T_0$ :

$$J_{1 \text{ lin}} = \left[\frac{a(t_0)}{a(t)}\right]^3 \frac{T_0 m(T_0)}{\pi^2} \int_1^\infty dz \left\{ a^3(t) m(T_0) \sqrt{z^2 - 1} \frac{|\varphi_k^H(t)|^2}{2} - \frac{a(t)}{2a(t_0)} \right\}.$$
(5.8)

Note that the above integral is finite.

The logarithmic contribution is obtained by keeping the  $O(1/k^3)$  in the large momentum expansion of  $|\varphi_k^H(t)|^2$  given by Eq. (4.15) (in terms of the new variable z). We obtain, after some straightforward algebra,

$$J_{1 \log} = -\frac{\ln\left[\frac{m(T_0)}{T_0}\right]}{8\pi^2} \left\{ -\frac{\mathcal{R}}{6} - \frac{\dot{a}^2(t_0)}{a^2(t)} + \left[\frac{a(t_0)}{a(t)}\right]^2 \left[m^2(T_0) + \frac{\lambda_R T_c^2}{24}\right] - \frac{\lambda_R T_c^2}{24} \right\}.$$
(5.9)

That is, in the limit  $T_0 \gg m(T_0)$ ,  $J_1 = J_1 \lim_{l \to 0} + J_1 \log + O((T_0)^0)$ .

Comparing the  $O(T_0^2, T_0, \ln T_0)$  contributions it becomes clear that they have very different time dependences through the scale factor a(t). Thus the high temperature expansion as presented will not remain accurate at large times since the term quadratic in  $T_0$  may become of the same order or smaller than the linear or logarithmic terms. The high temperature expansion and the long time limit are thus not interchangeable, and any high temperature expansion is thus bound to be valid only within some time regime that depends on the initial value of the temperature and the initial conditions.

As an illustration of this observation, we calculate  $J_{1 \text{ lin}}$  explicitly in the case of de Sitter space. We need to obtain  $|\varphi_k^H(t)|^2$  in order to evaluate the integral in (5.8). Inserting the term proportional to  $T_0^2$  in the Hartree equations, we find that  $|\varphi_k^H(t)|^2$  obeys the differential equation

$$\left[\frac{d^2}{dt^2} + 3H\frac{d}{dt} + \left(\frac{k^2}{a_0^2} + m^2(T_0) + \frac{\lambda_R T_c^2}{24}\right)e^{-2Ht} - \frac{\lambda_R T_c^2}{24}\right]\varphi_k^H(t) = 0.$$
(5.10)

The solution of this equation is given by

$$\varphi_{k}^{H}(t) = \left[ C_{1}H_{3/2}^{(1)}(B_{k}e^{-Ht}) + C_{2}H_{3/2}^{(2)}(B_{k}e^{-Ht}) \right] e^{-\frac{3}{2}Ht},$$
(5.11)

$$B_{k} = \frac{1}{H} \left[ \frac{k^{2}}{a_{0}^{2}} + m^{2}(T_{0}) + \frac{\lambda_{R}T_{c}^{2}}{24} \right]^{\frac{1}{2}},$$

where  $H_{3/2}^{(1,2)}$  are the Hankel functions and we have assumed

$$m^2(T_0)$$
,  $\frac{\lambda_R T_c^2}{24} \ll H.$ 

The coefficients  $C_1, C_2$  are determined by the initial conditions on  $\varphi_k^H(t)$  described above. We finally obtain

$$J_{1 \text{ lin}} = \frac{m(T_0)T_0}{8\pi^2} \left(He^{Ht_0}\right)^4 \int_1^\infty \frac{dz}{z} \frac{\sqrt{z^2 - 1}}{\left[\frac{\lambda_R T_c^2}{24} + m^2(T)z\right]^2}.$$
(5.12)

This term is time independent, finite, and positive. This example clearly illustrates the fact that different powers of  $T_0$  enter in the expansion with different functions of time and that the high temperature expansion is nonuniform as a function of time.

## VI. EVOLUTION OF THE INITIAL DISTRIBUTION

The initial density matrix at  $t = t_0$  was assumed to be thermal for the adiabatic modes. This corresponds to a Boltzmann distribution for the uncoupled harmonic oscillators for the adiabatic modes of momentum **k**, and frequencies  $\mathcal{W}_k(t_0)$  [in the Hartree approximation; as usual, the one-loop result can be found by replacing this with  $W_k(t_0)$ ]. That is

$$\rho(t_0) = \frac{e^{-\beta_0 H_0}}{\text{Tr}e^{-\beta_0 H_0}},$$
(6.1)

$$H_0 = \sum_{\mathbf{k}} \hbar \mathcal{W}_{\mathbf{k}}(t_0) \left[ \alpha_{\mathbf{k}}^{\dagger}(t_0) \alpha_{\mathbf{k}}(t_0) + \frac{1}{2} \right].$$
(6.2)

The creation and annihilation operators define the initial occupation number of the adiabatic modes:

$$\hat{N}_{\boldsymbol{k}}(t_0) = \alpha_{\boldsymbol{k}}^{\dagger}(t_0)\alpha_{\boldsymbol{k}}(t_0), \qquad (6.3)$$

$$\langle \hat{N}_k(t_0) \rangle = \frac{1}{e^{\beta_0 \hbar \mathcal{W}_k(t_0)} - 1},\tag{6.4}$$

where the expectation value in (6.4) is in the initial density matrix at time  $t_0$ .

In a time dependent gravitational background the concept of particle is ill-defined. However, by postulating an equilibrium initial density matrix of the above form, a preferred "pointer" basis is singled out at the initial time. It is this basis that provides a natural definition of particles at the initial time and we can use it to ask: how does the expectation value of *this* number operator evolve in time?

At any time t, this expectation value is given by

$$\langle \hat{N}_{k} \rangle(t) = \frac{\mathrm{Tr}\alpha_{k}^{\dagger}(t_{0})\alpha_{k}(t_{0})\rho(t)}{\mathrm{Tr}\rho(t_{0})}.$$
(6.5)

This quantity gives information on how the original Boltzmann distribution function for the adiabatic modes evolves with time. The  $\mathbf{k} = 0$  mode will receive a contribution from the order parameter, but since the number of particles is not conserved (no charge) there is no Bose condensation and the  $\mathbf{k} = 0$  mode will give a negligible contribution to the total number of particles. Thus we only concentrate on the  $\mathbf{k} \neq 0$  modes.

The expectation value (6.5) may be easily computed by writing the creation and annihilation operators in terms of  $\eta_k$ ,  $\Pi_k = \delta/\delta\eta_{-k}$  in the Schrödinger picture at  $t_0$ . The result of doing this is

$$\alpha_{k}^{\dagger}(t_{0}) = \frac{1}{\sqrt{2\hbar}} \left[ -\frac{1}{\sqrt{a^{3}(t_{0})}\mathcal{W}_{k}(t_{0})}} \frac{\delta}{\delta\eta_{k}} + \sqrt{a^{3}(t_{0})}\mathcal{W}_{k}(t_{0})}\eta_{-k} \right], \tag{6.6}$$

$$\alpha_k(t_0) = \frac{1}{\sqrt{2\hbar}} \left[ \frac{1}{\sqrt{a^3(t_0)\mathcal{W}_k(t_0)}} \frac{\delta}{\delta\eta_{-k}} + \sqrt{a^3(t_0)\mathcal{W}_k(t_0)}\eta_k \right].$$
(6.7)

After some straightforward algebra we find

$$\langle \hat{N}_{k} \rangle(t) + \frac{1}{2} = \left[ 2 \mid \mathcal{F}_{k}(t, t_{0}) \mid^{2} - 1 \right] \left[ \langle \hat{N}_{k} \rangle(t_{0}) + \frac{1}{2} \right],$$
(6.8)

$$\mathcal{F}_{k}(t,t_{0})|^{2} = \frac{1}{4} \frac{|\varphi_{k}^{H}(t)|^{2}}{|\varphi_{k}^{H}(t_{0})|^{2}} \left[ 1 + \frac{a^{6}(t)}{a^{6}(t_{0})\mathcal{W}_{k}^{2}(t_{0})} \frac{|\dot{\varphi}_{k}^{H}(t)|^{2}}{|\varphi_{k}^{H}(t)|^{2}} \right] + \frac{1}{2},$$
(6.9)

where we have made use of (A14) and (A15). This result exhibits the two contributions from "spontaneous" (proportional to the initial thermal occupation) and "induced" (independent of it).

We now show that this result may be understood as a Bogoliubov transformation. To do this, consider the expansion of the field in the *Heisenberg* picture:

$$\eta_{k}(t) = \frac{1}{\sqrt{2}} \left( \tilde{\alpha}_{k} \varphi_{k}^{H\dagger}(t) + \tilde{\alpha}_{k}^{\dagger} \varphi_{k}^{H}(t) \right), \qquad (6.10)$$

where the mode functions satisfy

$$\frac{d^2\varphi_k^H}{dt^2} + 3\frac{\dot{a}}{a}\frac{d\varphi_k^H}{dt} + \left[\frac{\mathbf{k}^2}{a^2} + \mathcal{V}^{(2)}[\phi(t)]\right]\varphi_k^H = 0 \quad (6.11)$$

together with the self-consistency relation. Then the Heisenberg field  $\eta_k(t)$  is a solution of the Hartree Heisenberg equations of motion and the  $\tilde{\alpha}_k^{\dagger}$ ,  $\tilde{\alpha}_k$  create and destroy the Hartree-Fock states. Notice that in the Heisenberg picture, these creation and annihilation operators

do not depend on time. Using the Wronskian properties of the functions  $\varphi_k^H(t)$  (see Appendix A) we can invert and find the creation and annihilation operators in terms of  $\eta_k(t)$  and its canonically conjugate momentum  $\Pi_{-k}(t)$ . Once we have expressed these operators in the Heisenberg picture in terms of the field and its canonically conjugate momentum, we can go to the Schrödinger picture at time  $t_0$ . In this picture the creation and annihilation operators depend on time and are given by

$$\tilde{\alpha}_{k}(t) = \frac{i}{\sqrt{2}} \left[ \Pi_{k}(t_{0})\varphi_{k}^{H}(t) - a^{3}(t)\eta_{k}(t_{0})\dot{\varphi}_{k}^{H}(t) \right],$$
(6.12)
$$\tilde{\alpha}_{-k}^{\dagger}(t) = \frac{-i}{\sqrt{2}} \left[ \Pi_{k}(t_{0})\varphi_{k}^{H\dagger}(t) - a^{3}(t)\eta_{k}(t_{0})\dot{\varphi}_{k}^{H\dagger}(t) \right].$$
(6.13)

The Schrödinger picture fields at  $t_0$  can be written in terms of the operators (6.6) and (6.7) and we finally find

the creation and destruction operators at time t to be related to those at time  $t_0$  by a Bogoliubov transformation:

$$\tilde{\alpha}_{k}(t) = \mathcal{F}_{+,k}(t,t_{0})\alpha_{k}(t_{0}) + \mathcal{F}_{-,k}(t,t_{0})\alpha_{-k}^{\dagger}(t_{0}). \quad (6.14)$$

If we now compute the average of the new creation and annihilation operators in the initial density matrix and write the mode functions  $\varphi_k(t)$  in terms of the real functions  $\mathcal{U}_{1,2}$  as defined in Appendix A, we recognize  $|\mathcal{F}_{+,k}(t,t_0)|^2$  to be the same as  $|\mathcal{F}_k(t,t_0)|^2$  given by (6.9).

We also find that

$$| | \mathcal{F}_{+, \boldsymbol{k}}(t, t_0) |^2 - | \mathcal{F}_{-, \boldsymbol{k}}(t, t_0) |^2 = 1$$

as is required for a Bogoliubov transformation.

One way to interpret this result is that, at least within the one-loop or Hartree approximations, time evolution corresponds to a Bogoliubov transformation. This interpretation is, in fact, consistent with the result that in these approximation schemes, the density matrix remains Gaussian with the only change being that the covariance and mixing terms change with time.

Thus within the one-loop or Hartree approximation, time evolution corresponds to a "squeezing" of the initial state. The covariance changes with time and this corresponds to a Bogoliubov transformation. As argued by Grishchuk and Sidorov [21] the amplification of quantum fluctuations during inflation is a process of quantum squeezing and it corresponds to a Bogoliubov transformation. The properties of these "squeezed" quantum states have been investigated in Refs. [22–24].

Hu and Pavon [25], Hu and Kandrup [26], and Kandrup [27] have introduced a nonequilibrium, coarsegrained entropy that grows in time as a consequence of particle production and "parametric amplification." This definition was generalized by Brandenberger *et al.* [22], and Gasperini and collaborators [23] to give a measure of the entropy of the gravitational field. The growth of this entropy is again a consequence of the parametric amplification of fluctuations and the "squeezing" of the quantum state under time evolution.

These authors argue that the nonequilibrium coarsegrained entropy in the mode of (comoving) wave vector  $\mathbf{k}$  is

$$s_k \approx \ln\left(\langle N_k \rangle(t)\right)$$
 (6.15)

in the case when  $\langle N_k \rangle(t) \gg 1$ . Thus the growth of entropy is directly associated with "particle production" or in our case to the evolution of the initial Boltzmann distribution function.

The coefficient of parametric amplification is related to the Bogoliubov coefficient given by Eq. (6.9). Thus this coefficient directly determines the time dependence of the nonequilibrium coarse-grained entropy.

#### VII. TWO SIMPLE EXAMPLES

As an example of the method that allows the out-of equilibrium time evolution, we solve numerically the simple cases of a free massive scalar field in two relevant cosmologies.

## A. de Sitter cosmology

In this case the scale factor is  $a(t) = a_0 e^{Ht}$  with H being Hubble's constant. The important quantities that encode the out-of-equilibrium evolution are the mode functions  $\varphi_k(t)$  that obey Eq. (A2) with  $V''(\phi) = m^2$ . With these mode functions we construct the real and imaginary parts of  $A_k(t)$  and the kernels of the density matrix [see Eq. 2.36] and the parametric amplification factor (6.9). It is convenient to rescale the differential equation and functions and define

$$z = H(t - t_0), \ q = \frac{ke^{-Ht_0}}{a_0H}, \ \epsilon = \frac{m}{H},$$
 (7.1)

the variable q is recognized as the physical wave vector at the initial time  $t_0$  multiplied by the horizon size (or equivalently, horizon size divided by physical wavelength). At the same time it is convenient to rescale the mode functions (in terms of their real and imaginary parts)

$$\Psi_q^{R,I}(z) = (a_0^3 H)^{\frac{1}{2}} \varphi_k^{R,I}(t), \qquad (7.2)$$

$$\Psi_q^R(0) = \left[q^2 + \epsilon^2\right]^{-\frac{1}{4}}, \ \Psi_q^I(0) = 0, \tag{7.3}$$

$$\frac{d\Psi_{q}^{R}(z)}{dz}\bigg|_{z=0} = 0 \ , \ \frac{d\Psi_{q}^{I}(z)}{dz}\bigg|_{z=0} = \left[q^{2} + \epsilon^{2}\right]^{\frac{1}{4}}.$$
 (7.4)

The differential equation becomes

$$\left[\frac{d^2}{dz^2} + 3\frac{d}{dz} + q^2 e^{-2z} + \epsilon^2\right] \Psi_q^{R,I}(z) = 0.$$
(7.5)

We have numerically integrated these equations with the above boundary conditions choosing as representative parameters m = 1 GeV;  $H = 10^{10}$  GeV, q =0.01, 0.1, 1, 10, 100. In Fig. 1 we show  $\mathcal{A}_{Rk}/(a_0^3 H)$  for q = 0.1, 1.0, 10 as function of z for  $\epsilon = 10^{-10}$ . Figure 2 shows the logarithm of  $\mathcal{A}_{Ik}e^{-3Ht_0}/(a_0^3H)$  for q =0.01, 0.1, 1.0, 10, 100 as a function of z. Whereas the real part tends to (a q-dependent) constant at large times, the imaginary part grows at long times as  $\approx e^{H(t-t_0)}$ (the slope on the graph is 1). Figure 3 shows the logarithm of the parametric amplification factor (6.9) for the above values of q as a function of z. The slope of the lines at long times is 2, thus the parametric amplification factor grows as  $\approx e^{2H(t-t_0)}$  at large times. Thus we clearly see that if the distribution function at some initial time  $t_0$  was determined by an equilibrium Boltzmann factor (in terms of the comoving wavelengths), this distribution function evolves in time out of equilibrium and grows with time approximately as  $\approx e^{2\hat{H}(t-t_0)}$  at long times but with different rates for different wave vectors.

From the numerical integration we see that in the case of de Sitter expansion, at late times [when the number of "particles produced" is large and the expression for the entropy (6.15) is valid] the entropy per mode grows *linearly* with comoving time.



FIG. 1. (a)  $A_R/a_0^3 H$  vs z for q = 0.1,  $m/H = 10^{-10}$ . (b)  $A_R/a_0^3 H$  vs z for de Sitter for q = 1.0,  $m/H = 10^{-10}$ . (c)  $A_R/a_0^3 H$  vs z for de Sitter for q = 10,  $m/H = 10^{-10}$ .



FIG. 2.  $\ln \left( \mathcal{A}_I e^{-3Ht_0}/a_0^3 H \right)$  vs z for de Sitter for q = 0.01; 0.1; 1; 10; 100,  $m/H = 10^{-10}$ . The slopes of the lines at long times is 1.

### B. Radiation-dominated cosmology

For a radiation-dominated cosmology the scale factor is given by

$$a(t)=a_0\left(rac{t}{t_0}
ight)^{rac{1}{2}}.$$

For this case, a convenient rescaling is in terms of the variables

$$s = mt \;\;,\;\; q = rac{k}{ma_0} \;\;,\;\; \Psi_q(s) = \left(a_0^3 m
ight)^{rac{1}{2}} arphi_k(t).$$

The differential equation for the mode functions, and



FIG. 3.  $\ln | \mathcal{F} |$  vs z for de Sitter for  $q = 0.01; 0.1; 10; 100, m/H = 10^{-10}$ . The slope of the lines at long times is 2.

boundary conditions thus become

$$\left[\frac{d^2}{ds^2} + \frac{3}{2s}\frac{d}{ds} + \frac{q^2}{s} + 1\right]\Psi_q^{R,I}(s) = 0,$$
(7.6)

$$\Psi_q^R(s_0) = \left[q^2 + 1\right]^{-\frac{1}{4}} , \ \Psi_q^I(s_0) = 0, \tag{7.7}$$

$$\frac{d\Psi_q^R(s)}{ds}\bigg|_{s=s_0} = 0 \ , \ \frac{d\Psi_q^I(s)}{ds}\bigg|_{s=s_0} = \left[q^2 + 1\right]^{\frac{1}{4}}.$$
 (7.8)

There are several noteworthy features in the radiationdominated case as exhibited by Figs. 4 and 5. There is a strong dependence on the initial condition as parametrized by  $t_0$  ( $s_0 = mt_0$ ) and also a strong dependence on the initial physical wave number q. Perhaps the most notable features are the oscillations in both the real and imaginary parts of the covariance  $\mathcal{A}$  that translate into an oscillatory behavior in the parametric amplification factor. As result, at long times the entropy per mode (6.15) is not a monotonically increasing function of comoving time.

### VIII. CONCLUSIONS

Nonequilibrium aspects of the dynamics of scalar fields in spatially flat FRW cosmologies were studied by means of a functional Schrödinger approach. The initial state was specified as a thermal density matrix at some early initial time assuming local thermodynamic equilibrium for the adiabatic modes at that particular time. This density matrix was evolved in time and the evolution equations for the order parameter (ensemble average of the scalar field) and the fluctuations were obtained both to one-loop and in a nonperturbative self-consistent Hartree approximation. The renormalization aspects were studied in detail and it was pointed out that the renormal-



FIG. 4. (a)  $\mathcal{A}_R/a_0^3 m$  vs s for radiation dominated for q = 1 (solid line) and q = 10 (dashed line);  $s_0 = 1.0$ . (b)  $\mathcal{A}_I/a_0^3 m$  vs s for radiation dominated for q = 1 (solid line) and q = 10 (dashed line);  $s_0 = 1$ . (c)  $\mathcal{A}_R/a_0^3 m$  vs s for radiation dominated for q = 1 (solid line);  $s_0 = 10$ . (d)  $\mathcal{A}_I/a_0^3 m$  vs s for radiation dominated for q = 1 (solid line);  $s_0 = 10$ . (d)  $\mathcal{A}_I/a_0^3 m$  vs s for radiation dominated for q = 1 (solid line);  $s_0 = 10$ .

ization counterterms contain a dependence on the initial conditions through the scale factor and its derivatives at the initial time.

The high temperature expansion was investigated and it was found that the limit of high temperatures and long times are not interchangeable. As a consequence of the redshift of the initial temperature the coefficients of the different powers of temperature are different timedependent functions. The high temperature expansion is only valid within a short time interval after the initial time and certainly breaks down at long times.

The time evolution of the Boltzmann distribution functions (initially the thermal equilibrium distribution functions) is obtained. It is pointed out that to one-loop order and also in the Hartree approximation, the time evolved density matrix describes quantum "squeezed" states and time evolution corresponds to a Bogoliubov transformation.

To illustrate the departure of equilibrium, we have



FIG. 5. (a)  $|\mathcal{F}|^2$  vs s for radiation dominated for q = 1 (solid line) and q = 10 (dashed line);  $s_0 = 1$ . (b)  $|\mathcal{F}|^2$  vs s for radiation dominated for q = 1 (solid line) and q = 10 (dashed line);  $s_0 = 10$ .

studied numerically the case of a free massive scalar field in de Sitter and radiation-dominated cosmologies. It was found that a suitably defined coarse-grained nonequilibrium entropy (per  $\mathbf{k}$  mode) grows linearly with time in the de Sitter case but it is not a monotonically increasing function of time in the radiation-dominated case. This result may cast some doubt on the applicability of this definition of the nonequilibrium entropy. There still remain some (open) fundamental questions regarding the connection of this entropy and the thermodynamic entropy of the Universe, in particular whether the amount of entropy produced is consistent with the current bounds.

This work sets the stage for a numerical study of the dynamics of phase transitions in cosmology fully incorporating the nonequilibrium aspects in the evolution of the order parameter and which at the same time can account for the dynamics of the fluctuations which will necessarily become very important during the phase transition.

We expect to report on the numerical study of the phase transition in a forthcoming paper [28].

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## APPENDIX A

The Riccati equation (2.41) can be transformed into a linear differential equation by the change of variables

$$\mathcal{A}_{k}(t) = -ia^{3}(t)\frac{\dot{\varphi}_{k}(t)}{\varphi_{k}(t)}.$$
(A1)

We find that  $\varphi_k(t)$  obeys a simple evolution equation

$$\frac{d^2\varphi_k}{dt^2} + 3\frac{\dot{a}}{a}\frac{d\varphi_k}{dt} + \left[\frac{\mathbf{k}^2}{a^2} + V''[\phi_{\rm cl}(t)]\right]\varphi_k = 0 \qquad (A2)$$

with  $\phi_{\rm cl}(t)$  the solution to the *classical* equation of motion (2.32) and (2.33). In the Hartree approximation  $V''[\phi_{\rm cl}(t)]$  should be replaced by  $\mathcal{V}^{(2)}[\phi(t)]$  with  $\phi(t)$  the full solution of the self-consistent equations:  $\frac{d^2\varphi_k^H}{dt^2} + 3\frac{\dot{a}}{a}\frac{d\varphi_k^H}{dt} + \left[\frac{\mathbf{k}^2}{a^2} + \mathcal{V}^{(2)}[\phi(t)]\right]\varphi_k^H = 0.$ (A3)

The Wronskian for two arbitrary solutions to the above differential equation is

$$\mathbf{W}[\varphi_1,\varphi_2] = \dot{\varphi_2}(t)\varphi_1(t) - \dot{\varphi_1}(t)\varphi_2(t) = \frac{C}{a^3(t)} \qquad (A4)$$

with C a constant. Then writing  $\varphi_k(t) = \varphi_{1k}(t) + i\varphi_{2k}(t)$ with  $\varphi_{1,2}$  real solutions we find

$$\mathcal{A}_{Rk}(t) = \frac{C}{[\varphi_{1k}^2 + \varphi_{2k}^2]},\tag{A5}$$

$$\mathcal{A}_{Ik}(t) = -a^3(t) \left[ \frac{\dot{\varphi_{1k}} \varphi_{1k} + \dot{\varphi_{2k}} \varphi_{2k}}{\varphi_{1k}^2 + \varphi_{2k}^2} \right].$$
(A6)

It proves convenient to introduce (for all **k**) the real functions  $\mathcal{U}_{1,2}(t)$  as

$$\varphi_{1,2}(t) = [a(t)]^{-\frac{3}{2}} \frac{\mathcal{U}_{1,2}(t)}{\sqrt{W_k(t_0)}}.$$
 (A7)

The  $\mathcal{U}_{\alpha k}$  for  $\alpha = 1, 2$  are real and satisfy the Schrödingerlike differential equation

$$\left[rac{d^2}{dt^2}-rac{3}{2}\left(rac{\ddot{a}}{a}+rac{1}{2}rac{\dot{a}^2}{a^2}
ight)+rac{\mathbf{k}^2}{a^2(t)}+V^{\prime\prime}(\phi_{ ext{cl}})(t)
ight]\mathcal{U}_{mlpham k}(t)=0,$$

(A8)

$$W[\mathcal{U}_{1,k},\mathcal{U}_{2,k}] = CW_k(t_0), \tag{A9}$$

with  $W[\cdots]$  the Wronskian, and C is the same constant as above. Since the choice of C corresponds to a choice of normalization of these functions, we choose C = 1. The initial conditions (2.42) and (2.43) still leave one free condition on these functions, we choose

$$\mathcal{U}_{1k}(t_0) \neq 0, \tag{A10}$$

$$\mathcal{U}_{2k}(t_0) = 0. \tag{A11}$$

The boundary conditions on the mode functions  $\mathcal{U}_{\alpha,k}$  are

$$\mathcal{U}_{1k}(t_0) = 1 \quad , \quad \mathcal{U}_{2k}(t_0) = 0, \tag{A12}$$

$$\dot{\mathcal{U}}_{1k}(t_0) = \frac{3}{2} \frac{a(t_0)}{a(t_0)},$$
(A13)

$$\dot{\mathcal{U}}_{2m{k}}(t_0) = W_{m{k}}(t_0) = \left[rac{m{k}^2}{a^2(t_0)} + V''[\phi_{
m cl}(t_0)]
ight]^{rac{1}{2}},$$

and the corresponding replacement for the Hartree case. Thus the final solution to the Riccati equation (2.41) with the given initial conditions is

$$\mathcal{A}_{Rk}(t) = \frac{a^{3}(t)W_{k}(t_{0})}{[\mathcal{U}_{1k}^{2}(t) + \mathcal{U}_{2k}^{2}(t)]},$$
(A14)

$$\mathcal{A}_{Ik}(t) = -a^{3}(t) \left[ \frac{\mathcal{U}_{1k} \left( \dot{\mathcal{U}}_{1k} - \frac{3\dot{a}}{2a} \mathcal{U}_{1k} \right) + \mathcal{U}_{2k} \left( \dot{\mathcal{U}}_{2k} - \frac{3\dot{a}}{2a} \mathcal{U}_{2k} \right)}{\mathcal{U}_{1k}^{2}(t) + \mathcal{U}_{2k}^{2}(t)} \right].$$
(A15)

In terms of the original functions  $\varphi_k(t)$  (A1) the initial conditions are simply

$$\varphi_{k}(t_{0}) = \frac{1}{\sqrt{a^{3}(t_{0})W_{k}(t_{0})}},$$
 (A16)

$$\dot{\varphi}_{k}(t) \mid_{t_{0}} = i \sqrt{\frac{W_{k}(t_{0})}{a^{3}(t_{0})}}.$$
 (A17)

Then the initial conditions for  $\varphi_k(t)$ ;  $\varphi_k^*(t)$  are naturally interpreted as those for negative and positive (adiabatic) frequency modes at the initial time  $t_0$ .

The reason for introducing the functions  $\mathcal{U}_{\alpha,k}(t)$  is because these obey a simpler second-order Schrödinger-like equation which is amenable to be studied in the asymptotic regime via WKB approximations (see the section on renormalization).

## **APPENDIX B: CONFORMAL TIME ANALYSIS**

It is interesting to see how some of our results can be obtained by rewriting the metric in terms of the conformal time defined by

$$\eta = \int^t \frac{dt'}{a(t')}.$$
 (B1)

The first thing we should note is that the physics should not depend on what time coordinate is used, since the theory should be generally coordinate invariant (there are no gravitational anomalies in four dimensions [29]). Thus, the field amplitude and the canonical momentum in conformal time should be related to those in comoving time via a canonical transformation. We now show that this is indeed the case.

Using the conformal time version of the line element  $ds^2 = a^2(\eta)(d\eta^2 - d\mathbf{x}^2)$ , the scalar field action can be written as

$$S[\Phi] = \int d\eta d^3x a^4(\eta) \Biggl[ rac{1}{2a^2(\eta)} [(\partial_\eta \Phi)^2 - (
abla \Phi)^2] - V[\Phi(\eta, \mathbf{x})] \Biggr],$$
 (B2)

where the potential term is as in the text (i.e., it could include a coupling to the curvature scalar). Following the standard procedure for obtaining the canonical momentum  $\Pi(\eta, \mathbf{x})$  to  $\Phi(\eta, \mathbf{x})$ , and to get at the Hamiltonian density yields

$$\Pi(\eta, \mathbf{x}) = a^2(\eta)\Phi'(\eta, \mathbf{x}),$$
  
$$\mathcal{H} = \frac{\Pi^2}{2a^2(\eta)} + \frac{a^2(\eta)}{2}(\nabla\Phi) + a^4(\eta)V(\Phi).$$
(B3)

Here conformal time derivatives are denoted by a prime. The generator H of displacements in conformal time is the spatial integral of  $\mathcal{H}$  above. Thus the conformal time Liouville equation reads

$$i\frac{\partial\rho}{\partial\eta} = [H,\rho].$$
 (B4)

If we label the field and its conjugate momentum in the comoving time frame (i.e., that of the text) as  $\hat{\Phi}$ ,  $\hat{\Pi}$ , respectively, the results of Sec. II are

$$\hat{\Pi}(\mathbf{x},t) = a^{3}(t)\hat{\Phi}(\mathbf{x},t),$$
$$\hat{H} = \int d^{3}x \left\{ \frac{\hat{\Pi}^{2}}{2a^{3}} + \frac{a}{2} (\boldsymbol{\nabla}\hat{\Phi})^{2} + a^{3}V(\hat{\Phi}) \right\}.$$
(B5)

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The Liouville equation in comoving time can be rewritten in conformal time using the relation  $\partial/\partial t = a(\eta)^{-1}\partial/\partial \eta$ . After doing this we find that Eq. (2.9) becomes

$$i\frac{\partial\hat{\rho}(\hat{\Pi},\hat{\Phi})}{\partial\eta} = \left[a(\eta)\hat{H},\hat{\rho}(\hat{\Pi},\hat{\Phi})\right].$$
 (B6)

But

$$a(\eta)\hat{H} = \int d^3x \left[ \frac{\hat{\Pi}}{2a^2(\eta)} + \frac{1}{2}a^2(\eta)(\nabla\hat{\Phi})^2 + a^4(\eta)V(\hat{\Phi}) \right].$$
(B7)

Comparing this with Eq. (B3), we see that we can make the identifications  $\Pi = \hat{\Pi}$ ,  $\Psi = \hat{\Psi}$ . Thus not only is the physics equivalent in both coordinate systems (as must have been the case), but the physics in the two coordinate systems related by a trivial canonical transformation.

We can rewrite all of the comoving time results in terms of conformal time. Some of the equations take on a much simpler form in conformal time than in comoving time. This will be important when numerical issues are tackled, such as an analysis of the back-reaction problem. This work is in progress [28].

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