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Nonequilibrium Field Theory Description of the Bose-Einstein Condensate

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We study the detailed out-of-equilibrium time evolution of a homogeneous Bose-Einstein condensate (BEC). We consider a nonrelativistic quantum theory for a self-interacting complex scalar field, immersed in a thermal bath, as an effective microscopic model for the description of the BEC. The interaction between fluctuations proves to be crucial in the mechanism of instability generation. We show the existence of two regimes in k space, with a crossover for $k^2/2m \sim 2\lambda|\varphi_0|^2$, where λ is the coupling constant and $|\varphi_0|^2$ is the condensate density. We deduce and solve a set of coupled equations that completely determines the nonequilibrium dynamics of the condensate density.

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The experimental verification of the phenomenon of Bose-Einstein condensation in weakly interacting gases has boosted a large number of theoretical investigations on the dynamics of weakly interacting dilute gas systems [for a recent review, see, e.g., Ref. [1], and references therein]. Current experiments and planned ones make it possible to probe different aspects of the Bose-Einstein condensate formation, with great control over interactions, trapping potentials, etc. Nevertheless, a basic problem not yet fully understood is the following: given an initial state, how will the condensate evolve with time? Of special note, the time scales for the condensate formation and its final size are important quantities involved in recent experiments with dilute atomic gases [2].

On the theoretical side, however, only restricted progress has been achieved concerning the problems above. Previous studies by Stoof [3] were able to give a qualitative idea of the various time scales involved during the condensate formation. In fact, they were the first attempts to analyze the problem from a microscopic point of view, by using the Schwinger-Keldysh closed time-path formalism (for reviews, see, for instance, Refs. [4,5]) in the quantum field theory description of Bose-Einstein condensation. Regarding the condensate growth problem, Gardiner *et al.* [6] have used a quantum kinetic theory to construct a master

equation for a density operator describing the state of the condensate, which is equivalent to a Boltzmann equation describing a quasiequilibrium growth of the condensate.

In this work we will study the quantum field time evolution of an interacting homogeneous condensate. Although nonhomogeneity is inherent to current experiments on Bose-Einstein condensation of atomic gases in trapping potentials, we believe that a full understanding of the time evolution of even the simpler case of a homogeneous gas is still lacking. Besides, as pointed out by Stoof in [3], the simplest formulations based on kinetic theory do not allow for the observation of a macroscopic occupation of the one-particle ground state, and the question of the instability of the Bose gas system in the homogeneous case is a nontrivial one. This makes its study an interesting problem, which may shed some light on the analysis of the systems under experimental investigation.

We consider the simplest model for a nonrelativistic complex Bose field, with a hard-core interaction potential, whose Lagrangian density is given by (throughout this work we use units such that $\hbar = 1$)

$$\mathcal{L} = \phi^* \left(i \frac{d}{dt} + \frac{1}{2m} \nabla^2 \right) \phi + \mu \phi^* \phi - \lambda (\phi^* \phi)^2, \quad (1)$$

where the complex scalar field $\phi(\mathbf{x}, t)$ represents complex spinless bosons of mass m , and λ is the coupling constant, related to the s -wave scattering length a by $\lambda = 4\pi a/m$. In (1) we have also explicitly introduced a chemical potential μ that produces a constant total density of particles $\langle \phi^* \phi \rangle = n$. We also assume that the system is coupled to a heat bath environment with inverse temperature $\beta = 1/k_B T$.

We may now perform the standard decomposition [7] of the fields (ϕ, ϕ^*) into a condensate (uniform) part (φ_0, φ_0^*) and a fluctuation (nonuniform) part (φ, φ^*) that describes the atoms outside the condensate, as $\phi(\mathbf{x}, t) = \varphi_0(t) + \varphi(\mathbf{x}, t)$ and $\phi^*(\mathbf{x}, t) = \varphi_0^*(t) + \varphi^*(\mathbf{x}, t)$, where we have assumed a homogeneous condensate. Note that we take at first $\varphi_0(t)$ as an arbitrary function of time that will be determined by the dynamics of the system.

Substituting the fields above in (1), we can readily obtain the Bogoliubov spectrum for quasiparticles [8]. In particular, the quadratic part of the Lagrangian for the fluctuation fields is the Bogoliubov approximation for quasiparticles. However, this approximation has a flaw: there is no interaction between the fluctuations, which is only reasonable at temperatures well below the critical temperature for the condensate formation. Our aim in this work is the study of the condensate evolution and, therefore, we must go beyond the Bogoliubov approximation. The simplest extension is to implement a mean-field approximation in the interactions between the fluctuation field. In this way, as we show below, one can make clear the appearance of instability modes towards the condensation formation once the interactions between fluctuations are taken into account. With the decomposition above, the interaction term for fluctuations in the Lagrangian becomes $\lambda(\varphi^* \varphi)^2$. The mean-field approximation amounts to the following:

$$\lambda(\varphi^* \varphi)^2 = 4\lambda \langle \varphi^* \varphi \rangle \varphi^* \varphi + [\lambda(\varphi^* \varphi)^2 - 4\lambda \langle \varphi^* \varphi \rangle \varphi^* \varphi], \quad (2)$$

where the first term in the right-hand side is taken as part of the quadratic Lagrangian for fluctuations, and the term inside the square brackets is taken as part of the interaction Lagrangian.

From the decomposition of the fields and (2), the quadratic part of the Lagrangian density for the fluctuations, $\mathcal{L}_0(\varphi, \varphi^*)$, may be written as

$$\begin{aligned} \mathcal{L}_0(\varphi, \varphi^*) = & \varphi^* \left[i \frac{d}{dt} + \frac{1}{2m} \nabla^2 \right] \varphi + \varphi^* (-\lambda \varphi_0^2) \varphi^* \\ & + \varphi (-\lambda \varphi_0^{*2}) \varphi. \end{aligned} \quad (3)$$

Here, we have used the fact that, under the field decomposition in the condensate and out of the condensate modes, the density constraint then becomes $\langle \phi^* \phi \rangle = |\varphi_0|^2 + \langle \varphi^* \varphi \rangle = n$. Additionally, assuming that at the initial time the system is mostly composed of particles outside the condensate, $\langle \phi^* \phi \rangle \simeq \langle \varphi^* \varphi \rangle$ (at $t = 0$), simple relations involving the generating functional for the correlation functions (see, for instance, the last section of

Chap. 2 in [9]) allow us to write the total number density n of particles in terms of the chemical potential μ , valid in the mean-field approximation for the potential, as $\mu = 4\lambda n$. Note that this is just the expression obtained also in the Hartree-Popov approximation [10], which turns out to satisfy the Hugenholtz-Pines relation [11] that would be obtained in the equilibrium problem. These considerations lead to the quadratic Lagrangian for the fluctuations shown above.

The scenario we have in mind is that for time $t < 0$ the initial state is in *equilibrium* at a temperature $T_i \gg T_c$. At $t = 0$ the system is then abruptly quenched to a much lower temperature $T_f \ll T_c$. T_f is the temperature of the thermal bath in which the system is immersed and, of course, it will be the equilibrium temperature which the system will reach asymptotically. This kind of quench is easily attained in the experiments of Bose-Einstein condensation of atomic gases, where the typical relaxation time scales are long enough (around ~ 0.1 s, depending on the temperature [12]) to allow for a fast drop in the temperature of the system that evolves afterwards out of equilibrium. With this choice of initial state, it is reasonable to approximate the dynamics of the buildup of the condensate state, which at the initial time is $n_{\text{cond}}(t = 0) = |\varphi_0(t = 0)|^2 \approx 0$, and the depletion of the excited states [which at $t = 0$ it is given by $n \approx n_{\text{exc}}(t = 0) = \langle \varphi^* \varphi \rangle$] as essentially a two-level problem. It is clear that this approximation breaks down for temperatures close to the critical temperature, where the detailed treatment would require a thorough study of the dynamics among the many levels of excited states. In the above approximation, the condensate builds up subject to the density constraint relation, which may be expressed in terms of the averages of the real and the imaginary parts of φ and φ^* ($\varphi = \varphi_1 + i\varphi_2$ and $\varphi^* = \varphi_1 - i\varphi_2$, respectively). Spatial translational invariance yields

$$\begin{aligned} |\varphi_0(t)|^2 + n_{\text{exc}}(t) &= n, \\ n_{\text{exc}}(t) &= \langle \varphi_1(t) \varphi_1(t) \rangle + \langle \varphi_2(t) \varphi_2(t) \rangle. \end{aligned} \quad (4)$$

The field averages above can be expressed in terms of the Green's functions for φ_1 and φ_2 as ($j = 1, 2$)

$$\langle \varphi_j(t) \varphi_j(t) \rangle = \int \frac{d^3 k}{(2\pi)^3} \left[-i G_{jj}^>(\mathbf{k}, t, t) \right], \quad (5)$$

where $G_{jj}^>(\mathbf{k}, t, t)$ is defined from the Green's functions for the fields in the closed-time path [3,5] (in momentum space)

$$\begin{aligned} G_{jj}^{++}(\mathbf{k}, t, t') &= G_{jj}^>(\mathbf{k}, t, t') \theta(t - t') \\ &\quad + G_{jj}^<(\mathbf{k}, t, t') \theta(t' - t), \\ G_{jj}^{--}(\mathbf{k}, t, t') &= G_{jj}^>(\mathbf{k}, t, t') \theta(t' - t) \\ &\quad + G_{jj}^<(\mathbf{k}, t, t') \theta(t - t'), \\ G_{jj}^{+-}(\mathbf{k}, t, t') &= -G_{jj}^<(\mathbf{k}, t, t'), \\ G_{jj}^{-+}(\mathbf{k}, t, t') &= -G_{jj}^>(\mathbf{k}, t, t'). \end{aligned} \quad (6)$$

The functions $G^>$ and $G^<$ satisfy the property $G_{jj}^<(\mathbf{k}, t, t') = G_{jj}^>(\mathbf{k}, t - i\beta, t')$, which is recognized as the periodicity condition in imaginary time [Kubo-Martin-Schwinger (KMS) condition]. β here is the inverse of the temperature of the thermal bath and appears here as a consequence of the boundary conditions arising from the construction of the complex time path. $G^>$ and $G^<$ are constructed from the homogeneous solutions to the operator of quadratic fluctuation modes, which, using Eq. (3) expressed in terms of φ_1 and φ_2 , are given by (in momentum space)

$$\begin{aligned} \frac{d\chi_2(\mathbf{k}, t)}{dt} + \left(\frac{\mathbf{k}^2}{2m} + 2\lambda|\varphi_0|^2 \right) \chi_1(\mathbf{k}, t) &= 0, \\ \frac{d\chi_1(\mathbf{k}, t)}{dt} - \left(\frac{\mathbf{k}^2}{2m} - 2\lambda|\varphi_0|^2 \right) \chi_2(\mathbf{k}, t) &= 0. \end{aligned} \quad (7)$$

The boundary conditions for the solutions of the equations above are such that, for $t < 0$, $|\varphi_0(t)|^2 = 0$, $\chi_1(\mathbf{k}, t) = \cos(\varepsilon_{\mathbf{k}} t)$, and $\chi_2(\mathbf{k}, t) = -\sin(\varepsilon_{\mathbf{k}} t)$, where $\varepsilon_{\mathbf{k}} = \mathbf{k}^2/(2m)$. In terms of these fluctuations modes, the Green's functions are expressed as

$$\begin{aligned} G_{jj}^>(\mathbf{k}, t, t') &= \frac{i}{2(1 - e^{-\beta\varepsilon_{\mathbf{k}}})} \\ &\times [\chi_j(\mathbf{k}, t)\chi_j^*(\mathbf{k}, t') \\ &+ e^{-\beta\varepsilon_{\mathbf{k}}}\chi_j^*(\mathbf{k}, t)\chi_j(\mathbf{k}, t')] \end{aligned} \quad (8)$$

and $G_{jj}^<(\mathbf{k}, t, t') = G_{jj}^>(\mathbf{k}, t', t)$.

By decoupling the set of equations in (7), we can readily identify that those modes with $(\mathbf{k}^2/2m) < 2\lambda|\varphi_0|^2$ are unstable and drive the excited particles towards condensation. Note also that not all the excited particles condense, since there will always be a fraction (which depends on various parameters for a particular system and on the temperature of the thermal bath) of excited modes, with high enough frequency, that remains stable. This will be clear from our numerical results shown later.

Using Eqs. (7) and (8) and the boundary conditions on the Green's functions, Eq. (6), together with the initial condition on the density (at $t = 0$, as defined before), one can then show that $n_{\text{exc}}(t)$ can be expressed as (by subtracting the zero point divergent contribution)

$$\begin{aligned} n_{\text{exc}}(t) &= \left(\frac{\beta}{\beta_c} \right)^{3/2} \int \frac{d^3k}{(2\pi)^3} \\ &\times [|\chi_1(\mathbf{k}, t)|^2 + |\chi_2(\mathbf{k}, t)|^2] n_{\mathbf{k}}(\beta), \end{aligned} \quad (9)$$

where $n_{\mathbf{k}}(\beta) = (e^{\beta\varepsilon_{\mathbf{k}}} - 1)^{-1}$, and β_c is the inverse of the equilibrium critical temperature, defined in terms of the total gas density n [13]. It should also be noted that in our out of equilibrium approach there are no infrared divergences since the finite time is a natural regulator. However, for the equilibrium $t \rightarrow \infty$, the critical temperature will be modified by the interactions as pointed out in Ref. [14].

The expression above can also be obtained directly in terms of the Green's functions for the complex fields φ, φ^* :

$$\langle \varphi(t)\varphi^*(t) \rangle = \int \frac{d^3k}{(2\pi)^3} [-iG_{\varphi\varphi^*}^>(\mathbf{k}, t, t)], \quad (10)$$

$$\langle \varphi^*(t)\varphi(t) \rangle = \int \frac{d^3k}{(2\pi)^3} [-iG_{\varphi^*\varphi}^>(\mathbf{k}, t, t)]. \quad (11)$$

In terms of (10) and (11), we have $\langle \varphi_1(t)\varphi_1(t) \rangle + \langle \varphi_2(t)\varphi_2(t) \rangle = (\langle \varphi(t)\varphi^*(t) \rangle + \langle \varphi^*(t)\varphi(t) \rangle)/2$, and the KMS condition can be expressed, in this case, as $G_{\varphi\varphi^*}^>(\mathbf{k}, t - i\beta, t') = [G_{\varphi^*\varphi}^>(\mathbf{k}, t, t')]^*$, or $G_{\varphi^*\varphi}^>(\mathbf{k}, t - i\beta, t') = [G_{\varphi\varphi^*}^>(\mathbf{k}, t, t')]^*$.

Equation (9) is the first order term in the finite temperature quantum many-body perturbation expansion for $\langle \varphi_j^2 \rangle$. Higher-order corrections for the equal-time two-point field averages can be expressed in terms of the coincidence limit of the (causal) two-point Green's functions $G_{\varphi\varphi^*}$ and $G_{\varphi^*\varphi}$, which satisfy the Dyson equations (the indices stand for φ and φ^*):

$$G_{ij} = G_{ij}^0 + G_{ik}^0 \Sigma_{kl} G_{lj}, \quad (12)$$

where Σ_{ij} is the (matrix) self-energy, and G_{ij}^0 is the zeroth-order noninteracting Green's function, satisfying the equation (in momentum space)

$$\left[\pm i \frac{d}{dt} - \varepsilon_{\mathbf{k}} \right] G_{\varphi\varphi^*}^0(\mathbf{k}, t, t') = \delta(t - t'). \quad (13)$$

One of the advantages of expressing the Green's functions in terms of the solutions of (7) is the possibility of obtaining, in an unambiguous way, all higher-order corrections to the two-point and many-point functions [15].

By using Eq. (9), we can rewrite the constraint on the density as

$$\begin{aligned} |\varphi_0(t)|^2 &= \frac{(\beta/\beta_c)^{3/2}}{2\pi^2} \int_0^{\sqrt{16\pi a|\varphi_0(t)|^2}} dk k^2 \\ &\times \{1 - [|\chi_1(\mathbf{k}, t)|^2 + |\chi_2(\mathbf{k}, t)|^2] n_{\mathbf{k}}(\beta)\}, \end{aligned} \quad (14)$$

that reproduces the result obtained by Stoof [3] for the limit $t \rightarrow \infty$. Equations (7) and (14) form an integrodifferential system that may be solved for $\varphi_0(t)$ numerically, given the initial conditions for $\varphi_0(t)$, $\chi_1(k, t)$, and $\chi_2(k, t)$ mentioned before. Indeed, this system of equations determines completely the time evolution of the condensate density as a function of the temperature and of the total density of the gas. Explicit results for different temperatures are shown in Fig. 1. It is important to point out at this stage that the evolution of the condensate is completely driven by the interactions between the microscopic fluctuations of the field around the condensate.

Throughout this Letter, we have developed an out-of-equilibrium nonperturbative quantum field theory description of the condensation process of an interacting

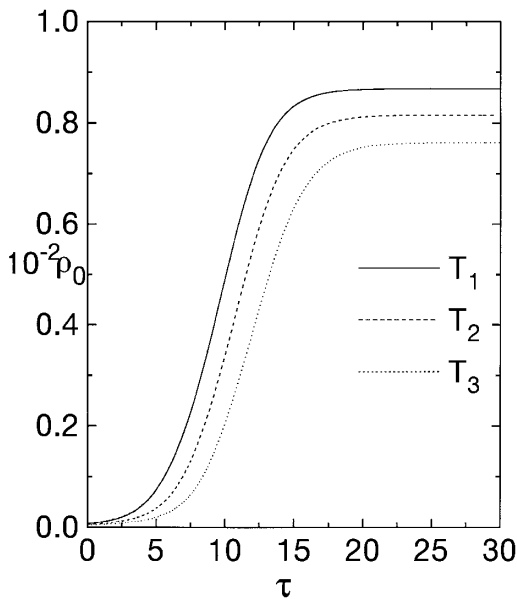


FIG. 1. Condensate density as a function of time for $na^3 = 0.01$ and $T_1/T_c = 0.06$, $T_2/T_c = 0.08$, and $T_3/T_c = 0.1$. Here, $\tau \equiv (\hbar/ma^2)t$ is a dimensionless time and $\rho_0 \equiv a^3|\varphi_0|^2$ is a dimensionless density.

homogeneous Bose-Einstein gas quenched below the critical temperature. In summary, this approach yielded the following main results: (i) The interaction between fluctuations proved to be crucial in the mechanism of instability generation; without it, there is simply no macroscopic condensate at all. (ii) There are essentially two regimes in the k space: for $(k^2/2m) \ll 2\lambda|\varphi_0^2|$ we have unstable modes that decay exponentially, while for $(k^2/2m) \gg 2\lambda|\varphi_0^2|$ we have stable modes that oscillate, with a crossover for $(k^2/2m) \sim 2\lambda|\varphi_0^2|$. (iii) Equations (7) and (14) come from a microscopic model for the weak-interaction gas, and determine completely the dynamics of the condensate. In fact, they are nonperturbative and certainly implement a resummation of the ladder Feynman diagrams mentioned by Stoof in [3]. Indeed, the highly nonequilibrium character of this description should complement the usual approach via Boltzmann equation.

Although we focused this Letter on the instability process that generates the condensate (i.e., the short time behavior), for $t \rightarrow \infty$ our results confirm the behavior predicted in Ref. [3] for this limit. However, the equilibrium ($t \rightarrow \infty$) values of the condensate fraction are lower than the experimental results [12] and the calculations of Dalfovo *et al.* [1]. This may be due to our approximation of neglecting incoherent collisional processes, which is a valid approximation in an infinite homogeneous gas at very low temperatures and densities, but otherwise may give an important contribution. We expect that the self-consistent inclusion of pair terms should account for most of these contributions. We will report on these improve-

ments of our mean-field approximation in a future publication [15].

In spite of the absence of nonhomogeneity effects, we hope that the approach developed here may be useful in the analysis of transients in realistic Bose-Einstein condensation experiments with atomic gases. Moreover, with a suitable generalization of the formalism presented above, we could be able to develop a theoretical description of the dynamical aspects of a recently proposed experiment [16] (currently in progress), regarding the Bose-Einstein condensation in a weakly interacting photon gas in a nonlinear Fabry-Perot cavity [17].

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