Nucleation of Bose-Einstein condensation

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Using a functional formulation of the Keldysh theory we investigate the time evolution of a dilute Bose gas through the critical point. We determine the critical region of the gas and show that if the system is quenched inside this region, Bose-Einstein condensation is nucleated on a time scale of $O(\hbar/k_BT_c)$ by means of a coherent population of the one-particle ground state. We also examine the subsequent buildup of the condensate density, taking place on a much longer time scale. However, in the experimentally interesting case of spin-polarized atomic hydrogen or cesium it is still short compared to the lifetime of the gas.

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I. INTRODUCTION

Perhaps the most important issue in connection with experiments aiming at the achievement of Bose-Einstein condensation in a gas of weakly interacting atoms is the time scale for the appearance of the condensate. The solution of this problem is particularly pressing since in the most promising experiments, using magnetically trapped atomic hydrogen [1,2] or cesium [3], the gas is essentially isolated from its surroundings and the only way to populate the ground state is by means of interatomic collisions, which (if an electron or nuclear spin is flipped in the process [4]) also lead to decay of the sample. Hence, it is not immediately evident that the condensation takes place within the lifetime of the system.

However, in a recent publication [5] we showed that the time scale for the onset of the phase transition, after the system is quenched into the critical region, is short and of $O(\hbar/k_B T_c)$. Therefore, the time evolution of the system through the critical point can be divided into three stages. In the first stage the gas evolves from a highly nonequilibrium situation, that depends on the precise way in which the system is cooled experimentally, to an equilibrium inside the critical region. This kinetic stage of the evolution can be described by a Boltzmann equation and has been studied analytically by Levich and Yakhot [6] and numerically by Snoke and Wolfe [7]. As expected they find that equilibrium is reached on a scale of $O(1/n \langle v\sigma \rangle)$, which in the region of interest is of $O((\Lambda_c/a)^2\hbar/k_BT_c)$. Here n is the density of the gas, $\langle v\sigma \rangle$ the thermal average of the relative velocity v of two colliding atoms times their elastic cross section σ, a the corresponding scattering length, and Λ_c the thermal deBroglie wavelength $(2\pi\hbar^2/mk_BT)^{1/2}$ at the critical temperature T_c . In the following coherent stage the system needs only a short time of $O(\hbar/k_B T_c)$ to develop the instability associated with the phase transition, although the actual buildup of the condensate density is governed by a time scale of $O((\Lambda_c/a)^2\hbar/k_BT_c)$ as will be shown below. In the final stage the thermalization between condensate and quasiparticles takes place. This part of the problem was analyzed by Eckern [8], who found a relaxation time of $O((\Lambda_c/a)^3\hbar/k_BT_c)$, which in the case of atomic hydrogen or cesium is comparable to the lifetime of the system.

In this paper we are mainly concerned with the coherent stage, which for the issue at hand is the most important one since here the actual phase transition occurs. In Sec. II we present a functional formulation of the nonequilibrium theory that is needed in Sec. III to derive a time-dependent Landau-Ginzburg theory for the order parameter of the phase transition. In this manner we are not only able to study the condensation time, which we focused our attention on in Ref. 5, but also the time evolution of the condensate density and the final distribution of (quasi)particles. We will, in particular, show how the constraint of particle-number conservation is enforced on the system even though the symmetry that gives rise to this conservation law is broken spontaneously. Finally, Sec. IV summarizes the conclusions of this work.

II. NONEQUILIBRIUM THEORY

The time evolution of a Bose gas that initially is described by the density matrix $\rho(t_0)$, can be studied very elegantly in the framework of the Keldysh formalism [9], which has been reviewed by Danielewics [10] using canonical operator methods. However, for our purposes it is convenient to formulate this nonequilibrium theory in a functional form, because the time-dependent Landau-Ginzburg equation for the order parameter $\langle \psi_H(\mathbf{x},t) \rangle$ of the phase transition can then be derived in a physically more transparent way. Moreover, it naturally leads to a (long-wavelength) effective action for the gas, which will enable us in Sec. III to study also the influence of the condensation on the particles with a nonzero momentum.

Our derivation of the functional form of the theory starts with the observation that the generating functional of all Green's functions can be written as a functional integral

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$$Z[J,J^*] = \int d[\psi^*]d[\psi] \exp\left\{\frac{i}{\hbar}S[\psi^*,\psi]\right\} + \left\{i\int_c dt\int d\mathbf{x}[\psi^*(\mathbf{x},t)J(\mathbf{x},t) + J^*(\mathbf{x},t)\psi(\mathbf{x},t)]\right\},\tag{1}$$

where $J(\mathbf{x},t)$ and $J^*(\mathbf{x},t)$ are c-number sources and the time integration over the Keldysh contour C runs along the chronological branch from t_0 to infinity and subsequently along the antichronological branch from infinity to t_0 [10]. In addition, it should be noted that we have implicitly assumed the fields $\psi(\mathbf{x},t)$ and $\psi(\mathbf{x},t')$ to be independent if the times t and t' are located on different branches.

The action $S[\psi^*, \psi]$ consists of a part

$$S_0[\psi^*,\psi] = \int_C dt \int d\mathbf{x} \,\psi^*(\mathbf{x},t) \left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2 \nabla^2}{2m} \right] \psi(\mathbf{x},t) , \qquad (2)$$

describing an ideal gas of spinless bosons with mass m, and a part due to the repulsive interaction $V(\mathbf{x} - \mathbf{x}')$ between the particles

$$S_{I}[\psi^{*},\psi] = -\frac{1}{2} \int_{C} dt \int d\mathbf{x} \int d\mathbf{x}' \psi^{*}(\mathbf{x},t) \psi^{*}(\mathbf{x}',t) V(\mathbf{x}-\mathbf{x}') \psi(\mathbf{x}',t) \psi(\mathbf{x},t) .$$
(3)

Because of this separation the generating functional $Z[J,J^*]$ can formally be written as

$$Z[J,J^*] = \exp\left\{\frac{1}{\hbar}S_I\left[\frac{\delta}{i\delta J}, \frac{\delta}{i\delta J^*}\right]\right\} Z_0[J,J^*], \qquad (4)$$

with $Z_0[J,J^*]$ the generating functional of the noninteracting theory, using the action $S_0[\psi^*,\psi]$. It is given by

$$Z_0[J,J^*] = \exp\left\{-i\int_C dt\int d\mathbf{x}\int_C dt'\int d\mathbf{x}' J^*(\mathbf{x},t)G_0(\mathbf{x},t;\mathbf{x}',t')J(\mathbf{x}',t')\right\},$$
(5)

and the noninteracting Green's function

$$iG_{0}(\mathbf{x},t;\mathbf{x}',t') = \left\langle T\left[\psi_{I}(\mathbf{x},t)\psi_{I}^{\dagger}(\mathbf{x}',t')\right] \right\rangle$$
$$\equiv \operatorname{Tr}\left[\rho(t_{0})T\left[\psi_{I}(\mathbf{x},t)\psi_{I}^{\dagger}(\mathbf{x}',t')\right]\right], \qquad (6)$$

that explicitly depends on the initial state $\rho(t_0)$ of the system. In the last equation we denote the time-ordering operator along the Keldysh contour by T, and the creation and annihilation operators in the interaction picture by $\psi_I^{\dagger}(\mathbf{x},t)$ and $\psi_I(\mathbf{x},t)$, respectively. In contrast, the field operators in the Heisenberg picture have the subscript H.

Expanding the exponential in Eq. (4) we can derive the Feynman rules of the theory simply by differentiating. In particular for the one-particle connected Green's function in momentum space, which plays an important role in Sec. III, they are schematically

$$iG_{c}^{(2)} = \sum_{D} \int_{C} \prod_{v=1}^{V} dt_{v} \int \prod_{i=1}^{V} \frac{d\mathbf{k}_{i}}{(2\pi)^{3}} \left\{ \prod_{v'=1}^{V} \left[-\frac{i}{\hbar} V(t_{v'}) \right] \prod_{l=1}^{L} iG_{0} \right\},$$

where the sum is over all connected and topologically distinct Feynman diagrams with V vertices and L=2V+1 lines. Notice that we have not performed a Fourier expansion on the time dependence, since in a nonequilibrium formalism the *n*-particle Green's functions $G_c^{(2n)}$ are only defined on the Keldysh contour, which consists of two half-infinite time intervals. However, it is convenient to perform a transformation from coordinate space to momentum space, because we are dealing with a homogeneous system.

To discuss Bose-Einstein condensation we need the generating functional of all connected Green's functions $W[J,J^*] \equiv -i \ln\{Z[J,J^*]\}$ and, in particular, its Legendre transform $\Gamma[\phi^*,\phi]$ obtained from

$$\Gamma[\phi^*,\phi] = \int_C dt \int d\mathbf{x} \left[\phi^*(\mathbf{x},t) J(\mathbf{x},t) + J^*(\mathbf{x},t) \phi(\mathbf{x},t) \right] - W[J,J^*] , \qquad (7)$$

with $\phi(\mathbf{x},t) \equiv \delta W[J,J^*]/\delta J^*(\mathbf{x},t) = \langle \psi_H(\mathbf{x},t) \rangle$ and the complex-conjugate expression for $\phi^*(\mathbf{x},t)$. The functional $\Gamma[\phi^*,\phi]$, which generates all one-particle irreducible diagrams, has two possible interpretations. First, we see from Eq. (7) that $-\pi\Gamma[\phi^*,\phi]$ is the effective action $S[\phi^*,\phi]$ of the gas, where we should keep in mind that any quantity obtained from this action in perturbation theory must be evaluated by using only one-particle reducible diagrams to avoid including the same graph twice. Secondly, the time evolution of both the magnitude and the phase of the order parameter is specified by the coupled equations

$$\frac{\delta\Gamma[\phi^*,\phi]}{\delta\phi^*(\mathbf{x},t)} = J(\mathbf{x},t), \quad \frac{\delta\Gamma[\phi^*,\phi]}{\delta\phi(\mathbf{x},t)} = J^*(\mathbf{x},t)$$
(8)

in the limit $J, J^* \rightarrow 0$. This clearly shows the importance of $\Gamma[\phi^*, \phi]$ for the topic of this paper.

We are left with the actual calculation of $\Gamma[\phi^*, \phi]$ in perturbation theory, which requires the relation between the 2*n*-point vertex function $\Gamma^{(2n)}$ and the connected Green's functions $G_c^{(2n)}$. This can most easily be derived by functional differentiation [11]. Remembering that $\phi(\mathbf{x},t) = \delta W[J,J^*]/\delta J^*(\mathbf{x},t)$, taking the derivative of this equation with respect to $\phi(\mathbf{x}',t')$, and using Eq. (8), we have in the limit of vanishing sources

$$\delta(\mathbf{x} - \mathbf{x}')\delta(t, t') = \int_{C} dt'' \int d\mathbf{x}'' \frac{\delta^{2} W[J, J^{*}]}{\delta J(\mathbf{x}, t) \delta J^{*}(\mathbf{x}'', t'')} \frac{\delta^{2} \Gamma[\phi^{*}, \phi]}{\delta \phi(\mathbf{x}'', t'') \delta \phi^{*}(\mathbf{x}', t')}$$
$$= -\int_{C} dt'' \int d\mathbf{x}'' \Gamma^{(2)}(\mathbf{x}', t'; \mathbf{x}'', t'') G_{c}^{(2)}(\mathbf{x}'', t''; \mathbf{x}, t) , \qquad (9)$$

where the δ function on the Keldysh contour is defined by $\int_C dt' \delta(t,t') = 1$. Using a representation independent notation we thus find $\Gamma^{(2)} = -(G_c^{(2)})^{-1}$ or equivalently $iG_c^{(2)} = (iG_c^{(2)})i\Gamma^{(2)}(iG_c^{(2)})$. In a similar way we can show that the four-point vertex function obeys $i^2G_c^{(4)} = -(iG_c^{(2)})^2i\Gamma^{(4)}(iG_c^{(2)})^2$. This proves the one-particle irreducible nature of $\Gamma^{(2)}$ and $\Gamma^{(4)}$, which is a property of all vertex functions $\Gamma^{(2n)}$ as mentioned previously. Although the general proof is not difficult, we will not present it here, since only $\Gamma^{(2)}$ and $\Gamma^{(4)}$ are needed for an accurate discussion of a dilute gas.

III. NUCLEATION

A weakly interacting Bose gas is characterized by $na^3 \ll 1$. Physically this means that it is very unlikely for three (or more) particles to interact with each other simultaneously. Hence, only two-body processes are of importance and it suffices to evaluate the effective action within the *T*-matrix (or ladder) approximation, which is summarized diagrammatically in Fig. 1. Introducing the self-energy Σ by the Dyson equation $G_c^{(2)} = G_0 + G_0 \Sigma G_c^{(2)}$ this corresponds in momentum space to

$$\Gamma^{(2)}(\mathbf{k};t,t') = -\frac{1}{\hbar} \left\{ \left[i\hbar \frac{\partial}{\partial t} - \frac{\hbar^2 \mathbf{k}^2}{2m} \right] \delta(t,t') - \hbar \Sigma(\mathbf{k};t,t') \right\},$$
(10a)

$$\Gamma^{(4)}(\mathbf{k},\mathbf{k}',\mathbf{K};t,t') = \frac{1}{\hbar} \left\{ T(\mathbf{k},\mathbf{k}',\mathbf{K};t,t') + T(-\mathbf{k},\mathbf{k}',\mathbf{K};t,t') \right\},$$
(10b)

$$\Gamma^{(2n)} = 0 \quad \text{for } n \ge 3 , \tag{10c}$$

where the self-energy is given by

$$\Sigma(\mathbf{k};t,t') = \frac{i}{\hbar} \int \frac{d\mathbf{k}'}{(2\pi)^3} \left[T\left[\frac{\mathbf{k} - \mathbf{k}'}{2}, \frac{\mathbf{k} - \mathbf{k}'}{2}, \mathbf{k} + \mathbf{k}'; t, t' \right] + T\left[-\frac{\mathbf{k} - \mathbf{k}'}{2}, \frac{\mathbf{k} - \mathbf{k}'}{2}, \mathbf{k} + \mathbf{k}'; t, t' \right] \right] G_0(\mathbf{k}'; t', t) , \qquad (11)$$

and the T matrix, which describes the scattering of two particles with momenta $\hbar(\frac{1}{2}\mathbf{K}+\mathbf{k}')$ and $\hbar(\frac{1}{2}\mathbf{K}-\mathbf{k}')$ to the momenta $\hbar(\frac{1}{2}\mathbf{K}+\mathbf{k})$ and $\hbar(\frac{1}{2}\mathbf{K}-\mathbf{k})$, obeys

$$T(\mathbf{k},\mathbf{k}',\mathbf{K};t,t') = V(\mathbf{k}-\mathbf{k}')\delta(t,t') + \frac{i}{\hbar} \int_{C} dt'' \int \frac{d\mathbf{k}''}{(2\pi)^{3}} V(\mathbf{k}-\mathbf{k}'')G_{0} \left[\frac{\mathbf{K}}{2} + \mathbf{k}'';t,t'' \right] \times G_{0} \left[\frac{\mathbf{K}}{2} - \mathbf{k}'';t,t'' \right] T(\mathbf{k}'',\mathbf{k}',\mathbf{K};t'',t') .$$
(12)

Equations (10)-(12) summarize the procedure for the evaluation of the effective action in lowest order of the gas parameter na^3 . However, before following this procedure, we notice that Eq. (12) is actually a complicated set of coupled equations since a function F(t,t') on the Keldysh contour can be decomposed into its analytic pieces by means of

$$F(t,t') \equiv F^{\delta}(t)\delta(t,t') + F^{>}(t,t')\Theta(t,t') + F^{<}(t,t')\Theta(t',t) , \qquad (13)$$

and the Heaviside function on the contour $\Theta(t, t')$ [10,12]. Introducing the retarded and advanced quantities

$$F^{(\pm)}(t,t') = F^{\delta}(t)\delta(t-t')\pm\Theta(\pm(t-t'))(F^{>}(t,t')-F^{<}(t,t')), \qquad (14)$$

defined on the real axis, we find from Eq. (12) that $T^{(\pm)}(\mathbf{k},\mathbf{k}',\mathbf{K};t,t')$ depends only on the time difference t-t' and that the Fourier-transformed function $T^{(\pm)}(\mathbf{k},\mathbf{k}',\mathbf{K};E)$ obeys the (bosonic) Bethe-Salpeter equation

$$T^{(\pm)}(\mathbf{k},\mathbf{k}',\mathbf{K};E) = V(\mathbf{k}-\mathbf{k}') + \int \frac{d\mathbf{k}''}{(2\pi)^3} V(\mathbf{k}-\mathbf{k}'') \frac{\left[1+N\left[\frac{\mathbf{K}}{2}+\mathbf{k}''\right]+N\left[\frac{\mathbf{K}}{2}-\mathbf{k}''\right]\right]}{E\pm i0-\epsilon(\mathbf{k}'',\mathbf{K})} T^{(\pm)}(\mathbf{k}'',\mathbf{k}',\mathbf{K};E) , \qquad (15)$$

using $\epsilon(\mathbf{k}'',\mathbf{K}) = (\hbar^2/m)(\mathbf{k}''^2 + \frac{1}{4}\mathbf{K}^2)$ for the total kinetic energy of the relative and center-of-mass motion and $N(\mathbf{k}) \equiv iG_0^{<}(\mathbf{k};t,t)$ for the average number of particles with momentum $\hbar \mathbf{k}$ at $t = t_0$. In addition, we find that

$$T^{\leq}(\mathbf{k},\mathbf{k}',\mathbf{K};t,t') = \frac{i}{\hbar} \int_{t_0}^{\infty} d\tau' \int_{t_0}^{\infty} d\tau'' \int \frac{d\mathbf{k}''}{(2\pi)^3} T^{(+)}(\mathbf{k},\mathbf{k}'',\mathbf{K};t,\tau') \times G_0^{\leq} \left[\frac{\mathbf{K}}{2} + \mathbf{k}'';\tau',\tau''\right] G_0^{\leq} \left[\frac{\mathbf{K}}{2} - \mathbf{k}'';\tau',\tau''\right] T^{(-)}(\mathbf{k}'',\mathbf{k}',\mathbf{K};\tau'',t') , \qquad (16)$$

which completes the discussion of Eq. (12) and explicitly shows that in contrast with $T^{(\pm)}$, $T^{<}$ and $T^{>}$ depend on t and t' separately and not only on their difference. This will be of some importance in the following sections.

A. Effective action

According to the principle of causality we expect the effective action of the gas to depend only on the retarded part of $\Gamma^{(2n)}$, which we denote by $\Gamma^{(+)}_{2n}$. Formally, this comes about because $\langle \psi_H(\mathbf{x},t) \rangle$ is independent of the branch on which the time t is located. The action $S[\phi^*, \phi]$ then acquires the explicitly causal form

$$S[\phi^{*},\phi] = \int_{t_{0}}^{\infty} dt \int_{t_{0}}^{\infty} dt' \left\{ \int \frac{d\mathbf{k}}{(2\pi)^{3}} \phi^{*}(\mathbf{k},t) \Gamma_{2}^{(+)}(\mathbf{k};t,t') \phi(\mathbf{k},t') + \frac{1}{(2!)^{2}} \int \frac{d\mathbf{K}}{(2\pi)^{3}} \int \frac{d\mathbf{k}}{(2\pi)^{3}} \int \frac{d\mathbf{k}'}{(2\pi)^{3}} \phi^{*}\left[\frac{\mathbf{K}}{2} + \mathbf{k},t\right] \phi^{*}\left[\frac{\mathbf{K}}{2} - \mathbf{k},t\right] \times \Gamma_{4}^{(+)}(\mathbf{k},\mathbf{k}',\mathbf{K};t,t') \phi\left[\frac{\mathbf{K}}{2} + \mathbf{k}',t'\right] \phi\left[\frac{\mathbf{K}}{2} + \mathbf{k}',t'\right] \right\}.$$
 (17)

A further simplification is possible because for a Bose gas we are especially interested in momenta $\hbar k < \hbar \sqrt{na}$, which are much smaller than the thermal momenta of $O(\hbar/\Lambda)$ due to the smallness of the parameter a/Λ at the low temperatures envisaged in magnetic trap experiments. [In the critical region we have $n\Lambda^3 = O(1)$ and thus $na\Lambda^2 \ll 1$.] We are therefore justified in neglecting the momentum dependence of $\Gamma_2^{(+)}$ and $\Gamma_4^{(+)}$, leading to

$$\Gamma_{2}^{(+)}(\mathbf{k};t,t') \simeq -\frac{1}{\hbar} \left\{ \left[i\hbar \frac{\partial}{\partial t} - \frac{\hbar^{2}\mathbf{k}^{2}}{2m} \right] \delta(t-t') - \hbar \Sigma^{(+)}(\mathbf{0};t,t') \right\},$$
(18a)

$$\Gamma_4^{(+)}(\mathbf{k},\mathbf{k}',\mathbf{K};t,t') \simeq \frac{2}{\hbar} T^{(+)}(\mathbf{0},\mathbf{0},\mathbf{0};0)\delta(t-t') , \qquad (18b)$$

where the retarded part of the self-energy is found from Eq. (11) and equals

$$\Sigma^{(+)}(\mathbf{0};t,t') = \frac{i}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} \left\{ \left[T^{(+)} \left[\frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2}, \mathbf{k}; t, t' \right] + T^{(+)} \left[-\frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2}, \mathbf{k}; t, t' \right] \right] G_0^<(\mathbf{k};t',t) + \left[T^< \left[\frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2}, \mathbf{k}; t, t' \right] + T^< \left[-\frac{\mathbf{k}}{2}, \frac{\mathbf{k}}{2}, \mathbf{k}; t, t' \right] \right] G_0^{(-)}(\mathbf{k};t',t) \right\}.$$
(19)

Physically, the first term is due to the possibility of decay of a zero-momentum particle into two particles and one hole whereas the second term corresponds to the production of zero-momentum particles by means of the time-reversed process. This interpretation shows that the imaginary part of $\Sigma^{(+)}$ describes the rate of change of the condensate density caused by incoherent scattering processes, which cannot nucleate the condensation [5]. These processes are only of importance on a time scale that is much longer than the one we are interested in and will thus be neglected in the following. Furthermore, Eq. (19) shows that the non-Markovian character of the self-energy leads only to a very small, and typically of $O(na\Lambda^2)$, renormalization of the time-derivative term in the effective action. Hence, memory effects can also be neglected and we only have to deal with the quantity

$$S^{(+)}(\mathbf{0};t) \equiv \hbar \int_{t_0}^t dt' \operatorname{Re} \left[\Sigma^{(+)}(\mathbf{0};t,t') \right] .$$
⁽²⁰⁾

Combining Eqs. (17), (18), and (20) we see that the long-wavelength action for a dilute Bose gas corresponds to a timedependent Landau-Ginzburg theory for a second-order phase transition [13]

$$S[\phi^*,\phi] = \int_{t_0}^{\infty} dt \int d\mathbf{x} \,\phi^*(\mathbf{x},t) \left\{ i \hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 - S^{(+)}(\mathbf{0};t) - \frac{T^{(+)}(\mathbf{0},\mathbf{0},\mathbf{0};0)}{2} |\phi(\mathbf{x},t)|^2 \right\} \phi(\mathbf{x},t) \,, \tag{21}$$

with complex order parameter. Clearly, when $S^{(+)}(0;t)$ becomes negative, the global U(1) gauge symmetry is broken

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spontaneously and the system develops an instability, which will be removed by the formation of a condensate.

To evaluate $S^{(+)}(\mathbf{0};t)$ we note that in the momentum integral of Eq. (19) the main contribution comes from thermal momenta. Therefore, we can neglect the dependence of $T^{(\pm)}(\mathbf{k},\mathbf{k}',\mathbf{K};E)$ on the relative momenta $\hbar\mathbf{k}$ and $\hbar\mathbf{k}'$, but not its dependence on the center of mass momentum $\hbar\mathbf{K}$, which is a consequence of the fact that the particles scatter inside a medium and not in a vacuum. The T matrix is thus well approximated by the on-shell quantity $T^{(\pm)}(\mathbf{0},\mathbf{0},\mathbf{K};\hbar^2\mathbf{K}^2/4m)$. Using the Bethe-Salpeter equation it can easily be shown that in terms of the genuine two-body T-matrix $T^{(\pm)}(\mathbf{k},\mathbf{k}';E)$ we have

$$T^{(\pm)}(\mathbf{0},\mathbf{0},\mathbf{K};\hbar^{2}\mathbf{K}^{2}/4m) = T^{(\pm)}(\mathbf{0},\mathbf{0};0) - \int \frac{d\mathbf{k}''}{(2\pi)^{3}} T^{(\pm)}(\mathbf{0},\mathbf{k}'';0) - \frac{N\left[\frac{\mathbf{K}}{2} + \mathbf{k}''\right] + N\left[\frac{\mathbf{K}}{2} - \mathbf{k}''\right]}{\hbar^{2}\mathbf{k}''^{2}/m} \times T^{(\pm)}(\mathbf{k}'',\mathbf{0},\mathbf{K};\hbar^{2}\mathbf{K}^{2}/4m) .$$
(22)

In the latter integral the relative momentum dependence can again be neglected and we obtain the convenient formula

$$T^{(\pm)}(\mathbf{0},\mathbf{0},\mathbf{K};\hbar^{2}\mathbf{K}^{2}/4m) = \frac{T^{(\pm)}(\mathbf{0},\mathbf{0};0)}{1+T^{(\pm)}(\mathbf{0},\mathbf{0};0)\mathbf{\Xi}(\mathbf{K})} , \qquad (23)$$

with $T^{(\pm)}(0,0;0) = 4\pi\hbar^2 a / m$ and

$$\Xi(\mathbf{K}) = \int \frac{d\mathbf{k}''}{(2\pi)^3} \frac{m}{\hbar^2 k''^2} \left\{ N \left[\frac{\mathbf{K}}{2} + \mathbf{k}'' \right] + N \left[\frac{\mathbf{K}}{2} - \mathbf{k}'' \right] \right\}.$$
(24)

An important first conclusion that can immediately be drawn from this result is that the scattering length a should be positive for the Landau-Ginzburg theory derived above to be stable and thus useful. In the opposite case a < 0, we expect instead of a Bose-Einstein condensation a phase transition of the BCS type and the pair wave function $\langle \psi_H(\mathbf{x},t)\psi_H(\mathbf{x}',t)\rangle$ as the order parameter [14]. A more detailed discussion of this interesting case, for which there is strong evidence that it is relevant to the experiments with atomic.cesium [15], is deferred to a following paper. Here we will consider only the (repulsive) case with a > 0.

Secondly, Eq. (24) shows that for thermal momenta $T^{(+)}(\mathbf{0},\mathbf{0};\mathbf{0})\Xi(\mathbf{K})$ is of $O(na\Lambda^2)$ and negligible. Therefore, the contribution of the $T^{(+)}G^{<}$ term to $S^{(+)}(\mathbf{0};t)$ is well approximated by the time-independent (Hartree-Fock) result $2nT^{(+)}(\mathbf{0},\mathbf{0};0)$. The contribution of the $T^{<}G^{(-)}$ term is, however, more difficult. Introducing the integration variables $\mathbf{p} = \frac{1}{2}\mathbf{k} + \mathbf{k}''$ and $\mathbf{p}' = \frac{1}{2}\mathbf{k} - \mathbf{k}''$, and neglecting the dependence of the many-body T matrix on the relative momenta as explained above we find first of all the result

$$-2\int \frac{d\mathbf{p}}{(2\pi)^3} \int \frac{d\mathbf{p}'}{(2\pi)^3} |T^{(+)}(\mathbf{0},\mathbf{0},\mathbf{p}+\mathbf{p}';\hbar^2(\mathbf{p}+\mathbf{p}')^2/4m)|^2 N(\mathbf{p}) N(\mathbf{p}') \frac{1-\cos(\hbar\mathbf{p}\cdot\mathbf{p}'(t-t_0)/m)}{\hbar^2\mathbf{p}\cdot\mathbf{p}'/m}$$

Note that if we neglect also the center of mass dependence of $T^{(\pm)}$ this contribution vanishes and a phase transition cannot occur. Therefore, we consider $T^{(\pm)}(\mathbf{0},\mathbf{0};\mathbf{0})\Xi(\mathbf{p}+\mathbf{p}')$ as a small quantity and expand the above expression up to first nonvanishing order. In this manner we obtain finally

$$S^{(+)}(\mathbf{0};t) = 2nT^{(+)}(\mathbf{0},\mathbf{0};0) - 4[T^{(+)}(\mathbf{0},\mathbf{0};0)]^{3} \\ \times \int \frac{d\mathbf{p}}{(2\pi)^{3}} \int \frac{d\mathbf{p}'}{(2\pi)^{3}} N(\mathbf{p}) N(\mathbf{p}') \frac{1 - \cos(\hbar\mathbf{p} \cdot \mathbf{p}'(t-t_{0})/m)}{\hbar^{2}\mathbf{p} \cdot \mathbf{p}'/m} [\Xi(\mathbf{0}) - \Xi(\mathbf{p}+\mathbf{p}')] , \qquad (25)$$

in agreement with Ref. 5 if we take $t_0 = 0$.

B. Critical region

Before we discuss the dynamics of the phase transition it is useful to consider first the equilibrium situation and calculate the critical temperature T_c of the gas. In our real-time formalism this can be accomplished by taking the limit $t \to \infty$ and using the Bose distribution $N(\mathbf{k}) = \{\xi^{-1} \exp[\beta \epsilon(\mathbf{k})] - 1\}^{-1}$, with chemical potential μ , $\epsilon(\mathbf{k}) = \hbar^2 \mathbf{k}^2 / 2m$ and the fugacity ξ defined by $\xi \equiv \exp(\beta \mu)$. The critical temperature is then determined by $S^{(+)}(\mathbf{0}; \infty) = 0$, since in that case the correlation length $\xi = \hbar [2mS^{(+)}(\mathbf{0}; \infty)]^{-1/2}$ diverges.

For temperatures large compared to the critical temperature T_0 of the ideal (noninteracting) Bose gas the second term in the right-hand side of Eq. (25) is a factor of $O((a/\Lambda)^2)$ smaller than the first term and cannot lead to a zero result for $S^{(+)}(\mathbf{0}; \infty)$. However, for temperatures very close to T_0 this argument does not hold any longer because the various momentum integrations diverge if $T \searrow T_0$ or similarly $\zeta \nearrow 1$. Therefore, we are especially interested in the asymptotic behavior of the function

$$I(\zeta) \equiv \int \frac{d\mathbf{p}}{(2\pi)^3} \int \frac{d\mathbf{p}'}{(2\pi)^3} N(\mathbf{p}) N(\mathbf{p}') \frac{m}{\hbar^2 \mathbf{p} \cdot \mathbf{p}'} [\Xi(\mathbf{0}) - \Xi(\mathbf{p} + \mathbf{p}')]$$

in this limit. Considering $\Xi(\mathbf{K})$ first we find, due to the properties of the Bose functions $g_n(z)$ [16], that

$$T^{(+)}(\mathbf{0},\mathbf{0};0) \Xi(\mathbf{K}) \sim_{\zeta \neq 1} \begin{cases} 4 \frac{a}{\Lambda} \frac{\pi^{1/2}}{(1-\zeta)^{1/2}} - \frac{1}{4\pi^{1/2}} \frac{a}{\Lambda} \frac{(K\Lambda)^2}{(1-\zeta)^{3/2}} & \text{for } K\Lambda \ll \sqrt{1-\zeta} \\ 8\pi^2 \frac{a}{\Lambda} \frac{1}{K\Lambda} & \text{for } \sqrt{1-\zeta} \ll K\Lambda \ll 1 \\ 32\pi g_{3/2}(\zeta) \frac{a}{\Lambda} \frac{1}{(K\Lambda)^2} & \text{for } 1 \ll K\Lambda \end{cases}$$

which leads to the conclusion that the main contribution to $I(\zeta)$ comes from the region where $\sqrt{1-\zeta}/\Lambda \ll |\mathbf{p}+\mathbf{p}'| < O(1/\Lambda)$ and we can use the approximation

$$T^{(+)}(\mathbf{0},\mathbf{0};\mathbf{0})\Xi(\mathbf{p}+\mathbf{p}') \simeq 8\pi^2 \frac{a}{\Lambda} \frac{1}{\eta(1-\zeta)^{1/2}+|\mathbf{p}+\mathbf{p}'|\Lambda}$$

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The term $\eta\sqrt{1-\zeta}$ in the denominator provides the correct low-momentum cutoff, which is required to regulate the resulting expression. Ultimately, we take the limit $\eta \rightarrow 0$. In this manner the asymptotic behavior of $I(\zeta)$ can be extracted and results in

$$I(\zeta) \underset{\zeta \nearrow 1}{\sim} \frac{n}{2\pi} \left[\frac{m}{\Lambda \hbar^2} \right]^2 \frac{1}{1 - \zeta} , \qquad (27)$$

the density being equal to $g_{3/2}(\zeta)/\Lambda^3$. The condition $S^{(+)}(\mathbf{0}; \infty) = 0$ is thus equivalent to $\sqrt{1-\zeta} = 4\sqrt{\pi}(a/\Lambda)$ and gives a critical temperature that is slightly higher than the value for the ideal Bose gas, i.e.,

$$T_{c} = T_{0} \left\{ 1 + \frac{16\pi}{3g_{3/2}(1)} \frac{a}{\Lambda_{0}} \right\}, \qquad (28)$$

with $g_{3/2}(1) = \zeta(3/2) \simeq 2.612$.

It is of interest to point out that this result implies that at the critical temperature $|T^{(+)}(0,0;0)| \equiv (0) = 4(a/\Lambda)g_{1/2}(\zeta) = 1$, which is identical to the Thouless criterion [17] for the onset of superconductivity if a < 0 [cf. Eq. (23)] and, more importantly, shows that indeed $T^{(\pm)}(0,0;0) \equiv (\underline{p+p'}) \ll 1$ for the relevant momenta $\hbar |\mathbf{p+p'}| \gg \hbar \sqrt{1-\zeta}/\Lambda$. Hence, our procedure for calculating $S^{(+)}(0;t)$ turns out to be self-consistent. In addi-

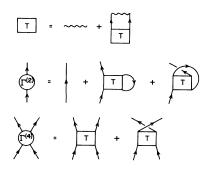


FIG. 1. Diagrammatic representation of the T matrix or ladder approximation. The wavy line corresponds to the interaction V and the straight line to the propagator G_0 .

tion, Eq. (28) can essentially also be obtained by the following simple argument: Calculating the average number of particles in the zero-momentum state $|\mathbf{k}=0\rangle$, using second-order perturbation theory for a system in a finite volume V, we find

$$\begin{split} \left< N_0 \right>_{\zeta \nearrow 1} \frac{1}{1 - \zeta} \left\{ 1 + \frac{2}{V^2} \sum_{\mathbf{k}, \mathbf{k}'} \left[\frac{T^{(+)}(\mathbf{0}, \mathbf{0}; \mathbf{0})}{\hbar \mathbf{k} \cdot \mathbf{k}' / m} \right]^2 \\ \times \left[N_{\mathbf{k}} N_{\mathbf{k}'} - N_{\mathbf{k} + \mathbf{k}'} \right] \right\}, \end{split}$$

which formally diverges, due to the integration over the angle between k and k'. However, this is an artifact since the terms with $\mathbf{k} \cdot \mathbf{k}' = 0$ in the above sum should be treated by degenerate perturbation theory and are expected to be unimportant in the thermodynamic limit. Therefore, we can replace the angular integration by some constant C of O(1). Neglecting inside the curly brackets the term involving $N_{\mathbf{k}+\mathbf{k}'}$, because it remains finite if $\zeta \nearrow 1$, we perform the momentum integrations and obtain

$$\langle N_0 \rangle_{\zeta \neq 1} \frac{1}{1-\zeta} \left\{ 1 + 4C \left[\frac{a}{\Lambda} \right]^2 g_{1/2}^2(\zeta) + O((a/\Lambda)^4) \right\}.$$

Summing all orders of perturbation theory, we then conclude that

$$\langle N_0 \rangle_{\zeta \nearrow 1} \frac{1}{1-\zeta} \frac{1}{1-4C(a/\Lambda)^2 g_{1/2}^2(\zeta)}$$

which diverges for $T_c = T_0[1+O(a/\Lambda)]$, in agreement with the more rigorous result found before. Finally, we note that Eq. (28) disagrees with the estimate $T_c = T_0[1+O((a/\Lambda)^{2/3})]$ found in Ref. [5]. In that paper we concentrated on the condensation time and used an approximation for $\Xi(\mathbf{p}+\mathbf{p}')$ that, although brings out the essential physics of the condensation process, is not adequate for the calculation of the critical temperature.

C. Bose-Einstein condensation

We now turn to the full time-dependent problem and assume that during the kinetic state of the phase transition the system is quenched into the critical region $T_0 < T < T_c$, where $S^{(+)}(0; \infty) < 0$. Our previous discussion shows that in this case $S^{(+)}(0;t)$, starting from the positive value $2nT^{(+)}(0,0;0)$ at $t=t_0$, passes through zero at

(26)

$$t \equiv t_c = t_0 + O\left[\frac{a}{\Lambda_c}\frac{\hbar}{k_B(T_c - T)}\right]$$

implying that the typical time scale for the onset of the instability is generally of $O(\hbar/k_B T_c)$ except for temperatures very close to the critical temperature, where $(T_c - T)/T_c \ll a/\Lambda_c$.

To calculate the condensate density $\rho_0(t)$ we must solve the equations of motion $\delta S[\phi^*,\phi]/\delta\phi^* = \delta S[\phi^*,\phi]/\delta\phi=0$ for the order parameter. Introducing a time-dependent chemical potential $\mu(t)$ by means of

$$\langle \psi_H(\mathbf{x},t) \rangle \equiv \sqrt{\rho_0(t)} \exp\left\{ i \chi_0 - \frac{i}{\hbar} \int_{t_0}^t dt' \mu(t') \right\},$$
 (29)

they lead to $\chi_0 = 0$ and

$$\sqrt{\rho_0(t)} \{ \mu(t) - S^{(+)}(\mathbf{0}; t) - T^{(+)}(\mathbf{0}, \mathbf{0}; \mathbf{0}; \mathbf{0}) \rho_0(t) \} = 0 ,$$
(30)

which for $t \le t_c$ has only the trivial solution $\rho_0(t)=0$. However, for $t > t_c$ this solution becomes metastable and we find in addition

$$\rho_0(t) = \frac{-S^{(+)}(0;t) + \mu(t)}{T^{(+)}(0,0,0;0)} , \qquad (31)$$

describing the buildup of the condensate.

For the determination of the chemical potential also the fluctuations around $\rho_0(t)$ need to be considered. In Nambu-space their effect is determined by the Green's function

$$\hbar G^{-1}(\mathbf{x},t;\mathbf{x}',t') = \begin{vmatrix} i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 + \mu - \hbar \Sigma_{11} & -\hbar \Sigma_{12} \\ -\hbar \Sigma_{21} & -i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla^2 + \mu - \hbar \Sigma_{22} \end{vmatrix} \delta(\mathbf{x} - \mathbf{x}') \delta(t - t') , \qquad (32a)$$

and the self-energy matrix

$$\hbar\Sigma(t) = \begin{bmatrix} S^{(+)}(0;t) + 2\rho_0(t)T^{(+)}(0,0,0;0) & \rho_0(t)T^{(+)}(0,0,0;0) \\ \rho_0(t)T^{(+)}(0,0,0;0) & S^{(+)}(0;t) + 2\rho_0(t)T^{(+)}(0,0,0;0) \end{bmatrix}.$$
(32b)

In terms of the normal and anomalous self-energies Eq. (31) can thus be written as $\mu(t) - \hbar \Sigma_{11}(t) + \hbar \Sigma_{12}(t) = 0$, which is just our nonequilibrium version of the celebrated Hugenholtz-Pines theorem [18]. Performing the integration over the fluctuations $\phi'(\mathbf{x},t) \equiv \exp\{i/\hbar \int dt' \mu(t')\}\phi(\mathbf{x},t) - \sqrt{\rho_0(t)}$ we easily find that

$$S[\mu] = \int dt \int d\mathbf{x} \left\{ \mu(t)(\rho_0(t) - n) - \frac{T^{(+)}(\mathbf{0}, \mathbf{0}, \mathbf{0}; \mathbf{0})}{2} \rho_0^2(t) \right\} + \frac{i\hbar}{2} \operatorname{Tr}[\ln G^{-1}], \qquad (33)$$

where the second term represents the usual contribution from the fluctuation determinant [14]. Making this action stationary with respect to variations in $\mu(t)$ then leads to the expected equation

$$n = \rho_0(t) + \frac{1}{V} \int d\mathbf{x} \langle \psi_H^{\dagger}(\mathbf{x}, t) \psi_H^{\dagger}(\mathbf{x}, t) \rangle , \qquad (34)$$

enforcing the conservation of particle number at all times.

We are left with the task of solving Eqs. (31) and (34) for $\rho_0(t)$ and $\mu(t)$. If $t \le t_c$ the solution is evidently $\rho_0(t) = \mu(t) = 0$ and we are in the symmetric phase. If t is slightly larger than t_c , more quantitatively such that $t_c < t < O((a/\Lambda_c)^2\hbar/k_BT_c)$, we still have $\mu(t) \simeq 0$ and therefore that $\rho_0(t) = -S^{(+)}(0;t)/T^{(+)}(0,0,0;0)$. In this interval the actual nucleation of the condensation takes place by means of a coherent population of the one-particle ground state. However, by this mechanism only a small condensate density of order $O(n(a/\Lambda_c)^2)$ is formed and a different mechanism is needed to cause the growth of the condensate for larger times $t > O((a/\Lambda_c)^2\hbar/k_BT_c)$. The nature of the latter is most conveniently discussed by considering the time evolution of the operator $\psi'_H(\mathbf{x}, t)$. At the quadratic level we obtain from Eq. (32)

$$i\hbar\frac{\partial}{\partial t}\begin{bmatrix}\psi'_{H}(\mathbf{x},t)\\\psi'_{H}^{\dagger}(\mathbf{x},t)\end{bmatrix} = \begin{bmatrix} -\frac{\hbar^{2}}{2m}\nabla^{2} + \rho_{0}T^{(+)} & \rho_{0}T^{(+)}\\ -\rho_{0}T^{(+)} & \frac{\hbar^{2}}{2m}\nabla^{2} - \rho_{0}T^{(+)} \end{bmatrix} \begin{bmatrix}\psi'_{H}(\mathbf{x},t)\\\psi'_{H}^{\dagger}(\mathbf{x},t)\end{bmatrix}.$$
(35)

For time independent ρ_0 this leads of course to the Bogoliubov dispersion relation [19]

 $\hbar\omega(\mathbf{k}) = \epsilon(\mathbf{k}) [1 + 2\rho_0 T^{(+)} / \epsilon(\mathbf{k})]^{1/2},$

which shows that the quadratic part in $\psi'_{H}(\mathbf{x},t)$ describes a gas of noninteracting quasiparticles.

However, from the work of Lee and Yang [20] we know that near the critical temperature the interaction

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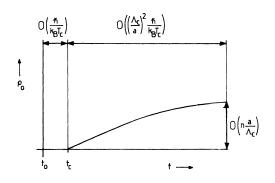


FIG. 2. Time evolution of the condensate density during the coherent stage of the phase transition for a dilute Bose gas.

between the quasiparticles is very important and cannot be neglected. Taking it into account in a mean-field-like manner gives

$$i\hbar\frac{\partial}{\partial t}\begin{bmatrix}\psi'_{H}(\mathbf{x},t)\\\psi'_{H}^{\dagger}(\mathbf{x},t)\end{bmatrix} = \begin{bmatrix}-\frac{\hbar^{2}}{2m}\nabla^{2} & \rho_{0}T^{(+)}\\-\rho_{0}T^{(+)} & \frac{\hbar^{2}}{2m}\nabla^{2}\end{bmatrix}\begin{bmatrix}\psi'_{H}(\mathbf{x},t)\\\psi'_{H}^{\dagger}(\mathbf{x},t)\end{bmatrix}.$$
(36)

Contrary to Eq. (35) the dispersion relation is now $\hbar\omega(\mathbf{k}) = [\epsilon^{2}(\mathbf{k}) - (\rho_{0}T^{(+)})^{2}]^{1/2}$ and we conclude that the modes with $\epsilon(\mathbf{k}) < \rho_{0}T^{(+)}$ are unstable and show an exponential decay of their population, resulting in a buildup of the condensate. Although the above set of equations cannot be solved analytically, it is clear that the time scale for the further increase of the condensate is of $O(\hbar/\rho_{0}T^{(+)})$ or equivalently of $O((\hbar/k_{B}T_{c})(1/\rho_{0}a\Lambda_{c}^{2}))$, which is much larger than the time scale for the onset of the phase transition. Moreover, the final order of magnitude of the condensate density can be estimated from

$$ho_0 \simeq \int_0^{\sqrt{
ho_0 a}} \frac{4\pi k^2 dk}{(2\pi)^3} N(k) ,$$

with the result that in the limit $t \to \infty$, ρ_0 is of $O(na / \Lambda_c)$. The various estimates obtained above are summarized in Fig. 2, which gives a complete picture of the coherent stage of the condensation process for a weakly interacting Bose gas. Note that the effect of the subsequent kinetic stage of the transition, during which the condensate and the quasiparticles equilibrate, is not included in this figure.

IV. CONCLUSIONS

We study the nucleation of the Bose-Einstein condensation process, by developing a functional approach to the Keldysh formalism. In this manner we derive a time-dependent Landau-Ginzburg theory for the longwavelength dynamics of a weakly interacting Bose gas and use this to obtain first of all the critical region and, in particular, the critical temperature of the system. Secondly, we consider the nonequilibrium dynamics of the gas by concentrating on the time evolution of the condensate density after a quench into the critical region. The preceding and ensuing kinetic stages of the phase transition have been published elsewhere [6-8] and are not treated here.

We show that the actual nucleation of the condensation takes place on a short time scale of $O(\hbar/k_B T_c)$, in contrast with previous claims in the literature [6], predicting that an infinite time is needed for the nucleation, i.e., Bose-Einstein condensation will never take place in a realistic system. Therefore, the phase transition is not impeded by the nucleation but by the way in which the gas is quenched into the critical region. This can be studied by a quantum Boltzmann equation and leads to the conclusion that from an experimental point of view the dominant time scale is set by (incoherent) elastic collisions between the particles and thus of $O((\Lambda_c/a)^2\hbar/a)$ $k_B T_c$). Since this is a much shorter time than the lifetime of spin-polarized atomic hydrogen or cesium samples, due to inelastic collisions that flip a spin, there is no fundamental reason to believe that Bose-Einstein condensation cannot be obtained in these experiments.

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