Formation of the Condensate in a Dilute Bose Gas

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We examine the time evolution of a weakly interacting Bose gas in the course of the Bose-Einstein phase transition and show that, in contrast with previous claims in the literature, the relevant time scale for the appearance of the condensate is finite and, under the conditions we consider, of $O(\hbar/k_B T_c)$, which is very small compared to the characteristic lifetime of the system due to inelastic collisions in the gas.

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The remarkable progress made in the last few years in manipulating neutral atoms by means of electromagnetic fields[1,2] has led to the exciting possibility of studying very cold atomic samples in a density regime where the Bose-Einstein phase transition is expected to occur in an almost ideal fashion. The most promising candidate in this respect is spin-polarized atomic hydrogen in a magnetic trap,[3,4] although it has recently been proposed that a combination of optical cooling and magnetic trapping may also lead to Bose condensation in alkali-metal vapors, such as sodium and cesium.[5]

In both cases the gas is effectively isolated from its surroundings and has no interaction with a "thermal heat bath," which is essential for a thermodynamic description to be valid. In these circumstances the question of the time scale for the formation of a condensate becomes a very urgent one, because for experiments to be successful it is evident that this time scale should be short compared to the lifetime of the sample. However, both scales are due to the interaction between the atoms and it is *a priori* not clear that this condition is satisfied in general. Indeed, work by Levich and Yakhot[6] indicates that in an isolated situation the condensation time is infinite.

The argument is essentially as follows: Assuming a homogeneous system of N atoms in a volume V and treating the collisions in the gas with a Boltzmann equation, phase-space arguments show that the production rate of the condensate fraction is given by $d/dt(N_0/N)=C\langle v\sigma\rangle(1+N_0)/V$, where N_0 is the number of particles in the $|\mathbf{k}=\mathbf{0}\rangle$ ground state, σ is the cross section for elastic collisions with initial relative velocity v, $\langle\cdot\rangle$ denotes the appropriate average over the relative motion, and C is a constant of the order of 1. This shows explicitly that in the thermodynamic limit ($N,V\rightarrow\infty$, with fixed density $n=N/V$) the production rate is nonzero only if a condensate already exists. Notice that the above argument is independent of the number of particles involved in the collision and applies also, with an appropriate redefinition of $\langle v\sigma\rangle$, to three-body processes. Therefore, the suggestion made by Snoke and Wolfe,[7] that three-body processes will nucleate the formation of the condensate, offers no solution.

Moreover, the same reasoning is also valid for the interactions of the gas with a thermodynamic heat bath if treated with a Boltzmann equation. This was already shown by Levich and Yakhot[6] and more recently by Tikhodeev.[8] Therefore, the results obtained below are also relevant to the Bose condensation of excitons in Cu_2O (Ref. 9) and the proposed experiments with positronium inside crystal vacancies,[10] although we consider only the isolated case, with particularly spin-aligned atomic hydrogen in mind.

We obtain a clue to the solution of this nucleation problem by realizing that a Boltzmann equation is unable to treat the buildup of coherence, which is crucial for the phase transition to occur. In this Letter we briefly outline how to formulate a theory that takes the existence of coherences into account and by which we can actually study the time evolution of the condensate fraction. The formalism is general enough to discuss, for example, the final distribution of Bogoliubov quasiparticles after the condensation has taken place and the moment when the property of superfluidity appears. Although these are important issues in their own right we defer them and various technical details to a following paper and focus here on the condensation time.

To address this nonequilibrium problem we express the Keldysh formalism[11] in a functional form. Taking the Hamiltonian of the interacting gas equal to

$$H=\int d\mathbf{x}\,\psi_H^\dagger(\mathbf{x},t)\frac{-\hbar^2\nabla^2}{2m}\psi_H(\mathbf{x},t)+\tfrac{1}{2}\int d\mathbf{x}\int d\mathbf{x}'\,\psi_H^\dagger(\mathbf{x},t)\psi_H^\dagger(\mathbf{x}',t)V(\mathbf{x}-\mathbf{x}')\psi_H(\mathbf{x}',t)\psi_H(\mathbf{x},t)\,, \tag{1}$$

with $V(\mathbf{x}-\mathbf{x}')$ the predominantly repulsive two-body interaction potential and m the mass of the particles, the generating functional of all Green's functions is given by

$$Z[J,J^*]=\left\langle T\left[\exp\left\{i\int_C dt\int d\mathbf{x}[J^*(\mathbf{x},t)\psi_H(\mathbf{x},t)+J(\mathbf{x},t)\psi_H^\dagger(\mathbf{x},t)]\right\}\right]\right\rangle. \tag{2}$$

Here T is the time-ordering operator along the Keldysh contour C shown in Fig. 1, $\psi_H(\mathbf{x},t)$ and $\psi_H^\dagger(\mathbf{x},t)$ are the (Bose) annihilation and creation operators in the Heisenberg picture, $J^*(\mathbf{x},t)$ and $J(\mathbf{x},t)$ are c-number sources, and $\langle\cdot\rangle$ is the average with respect to an initial density matrix $\rho(t_0)$. For physical reasons we take $\rho(t_0)$ to be the noninteracting (grand canonical) equilibrium density matrix, although more complex initial conditions, depending on the precise experimental circumstances, are possible as long as they allow for a Wick decomposition. The generating functional of the connected Green's functions $iW[J,J^*]$ is obtained by taking the logarithm of $Z[J,J^*]$.

To arrive at a description in terms of the order parameter $\langle\psi_H(\mathbf{x},t)\rangle$ of the phase transition we need the Legendre transform of $W[J,J^*]$, defined by the relations

$$\Gamma[\phi^*,\phi]=\int_C dt\int d\mathbf{x}[J(\mathbf{x},t)\phi^*(\mathbf{x},t)+J^*(\mathbf{x},t)\phi(\mathbf{x},t)]-W[J,J^*]\,, \tag{3a}$$

$$\phi^*(\mathbf{x},t)\equiv\frac{\delta W[J,J^*]}{\delta J(\mathbf{x},t)},\quad \phi(\mathbf{x},t)\equiv\frac{\delta W[J,J^*]}{\delta J^*(\mathbf{x},t)}\,, \tag{3b}$$

assuming that Eqs. (3b) are inverted to eliminate the sources J,J^* in Eq. (3a). $\Gamma[\phi^*,\phi]$ is the generating functional of the one-particle irreducible diagrams (or vertex functions) and its importance for the discussion of a broken symmetry follows from $\delta\Gamma[\phi^*,\phi]/\delta\phi=J$, showing that in the limit of vanishing sources we have a broken symmetry if $\delta\Gamma[\phi^*,\phi]/\delta\phi=0$ for $\phi=\langle\psi_H\rangle\neq0$. Note that in thermal equilibrium $\Gamma[\phi^*,\phi]/(-i\beta)$ reduces to the free energy of the system and the condition $\delta\Gamma[\phi^*,\phi]/\delta\phi=0$ to the requirement that the free energy is a minimum.[12]

More important for our purposes is the interpretation of $-\hbar\Gamma[\phi^*,\phi]$ as an effective action $S[\phi^*,\phi]$ for the time evolution of the gas, since using the definition of $\Gamma[\phi^*,\phi]$, $Z[J,J^*]$ can be written as a functional integral:

$$Z[J,J^*]=\text{“}\lim_{\hbar\to0}\text{”}\int d[\phi^*]d[\phi]\exp\left\{\frac{i}{\hbar}S[\phi^*,\phi]+i\int_C dt\int d\mathbf{x}[J(\mathbf{x},t)\phi^*(\mathbf{x},t)+J^*(\mathbf{x},t)\phi(\mathbf{x},t)]\right\}, \tag{4}$$

where "$\lim_{\hbar\to0}$" means that we include only the tree (no-loop) diagrams. This restriction is necessary because $\Gamma[\phi^*,\phi]$ already contains all diagrams of the theory.

To calculate the action we must specialize to the case of interest. A considerable simplification occurs because we are dealing with a weakly interacting gas. Denoting the scattering length by a this implies $na^3\ll1$. Therefore, three-body processes in the gas can be neglected and we only need to evaluate the two- and four-point vertex functions in the T-matrix approximation.[11] Performing the calculation we find that the action can be expressed in terms of the (initial) particle distribution $N(\mathbf{k})$ and the retarded (advanced) T matrices $T^{(\pm)}(\mathbf{p},\mathbf{p}',\mathbf{P};E)$. For a Bose gas at low temperatures, well inside the quantum regime we also have a small parameter a/Λ, where $\Lambda=(2\pi\hbar^2/mk_BT)^{1/2}$ is the thermal de Broglie wavelength. As a result we can completely neglect the dependence of $T^{(\pm)}$ on the relative momenta $\mathbf{p}$ and $\mathbf{p}'$. However, the dependence on the center-of-mass momentum $\mathbf{P}$ and thus on the total energy E of the scattering process is due to the presence of a surrounding gas and cannot be neglected in general. From the T-matrix equation for $T^{(\pm)}$ we can show that

$$T^{(\pm)}(\mathbf{0},\mathbf{0},\mathbf{P};\hbar^2\mathbf{P}^2/4m)=T^{(\pm)}(\mathbf{0},\mathbf{0};0)/[1+T^{(\pm)}(\mathbf{0},\mathbf{0};0)\Xi(\mathbf{P})]\,,$$

with $T^{(\pm)}(\mathbf{p},\mathbf{p}';E)$ the genuine two-body T-matrix without the many-body aspect and $\Xi(\mathbf{P})$ given by

$$\Xi(\mathbf{P})=\int\frac{d\mathbf{p}}{(2\pi)^3}\frac{m}{\hbar^2p^2}[N(\mathbf{P}/2+\mathbf{p})+N(\mathbf{P}/2-\mathbf{p})]\,. \tag{5}$$

For the Bose distribution $N(\mathbf{k})=(\zeta^{-1}e^{\beta\epsilon(\mathbf{k})}-1)^{-1}$, with $\epsilon(\mathbf{k})=\hbar^2\mathbf{k}^2/2m$ and $\zeta\equiv e^{\beta\mu}$, the influence of the surrounding gas is maximal when $\mathbf{P}=\mathbf{0}$. In that case

$$T^{(\pm)}(\mathbf{0},\mathbf{0};0)\Xi(\mathbf{0})=4(a/\Lambda)g_{1/2}(\zeta)\underset{\zeta\uparrow1}{\sim}4(a/\Lambda)\sqrt{\pi/1-\zeta}\,,$$

using $T^{(\pm)}(\mathbf{0},\mathbf{0};0)=4\pi\hbar^2a/m$ and the properties of the Bose functions $g_n(\zeta)$.[13] Below we show that this quantity is indeed small for all practical purposes. In particular, at the critical point, $1-\zeta_c$ turns out to be $O((a/\Lambda)^{4/3})$ and therefore $T^{(\pm)}(\mathbf{0},\mathbf{0};0)\Xi(\mathbf{0})=O((a/\Lambda)^{1/3})$.

Bearing the latter remark in mind, we find that the effective action is, to a very good approximation, given by

$$S[\phi^*,\phi]=\int dt\int d\mathbf{x}\,\phi^*(\mathbf{x},t)\left\{i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2\nabla^2}{2m}-S^{(+)}(0;t)-\frac{T^{(+)}(\mathbf{0},\mathbf{0};0)}{2}|\phi(\mathbf{x},t)|^2\right\}\phi(\mathbf{x},t)\,, \tag{6a}$$

$$S^{(+)}(0;t)=2nT^{(+)}(\mathbf{0},\mathbf{0};0)-2[T^{(+)}(\mathbf{0},\mathbf{0};0)]^3\int\frac{d\mathbf{p}}{(2\pi)^3}\int\frac{2\mathbf{p}'}{(2\pi)^3}N(\mathbf{p})N(\mathbf{p}')\times\frac{1-\cos(\hbar\mathbf{p}\cdot\mathbf{p}'t/m)}{\hbar^2\mathbf{p}\cdot\mathbf{p}'/m}[\Xi(\mathbf{0})-\Xi(\mathbf{p}+\mathbf{p}')]\,, \tag{6b}$$

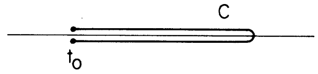

FIG. 1. The Keldysh contour in the complex time plane.

where $S^{(+)}(\mathbf{0};t)$ corresponds to a local approximation of the retarded self-energy. Although this is not justified at this point, it can be shown *a posteriori* that the corrections due to memory effects are $O((na\Lambda^2)^2)$ and negligible, making the assumption self-consistent. Furthermore, the imaginary part of the self-energy is not included, since it is in general a factor of $O(na\Lambda^2)$ smaller than the real part. Because of the form of the action, defining a time-dependent Landau-Ginzburg theory, we conclude that we are dealing with a second-order phase transition and a critical point if $S^{(+)}(\mathbf{0};\infty)=0$. Looking at the divergence of the second term in Eq. (6b) as $\zeta \uparrow 1$ we can express the critical temperature $T_c = T_0[1 + O((a/\Lambda_0)^{2/3})]$ in terms of the critical temperature T_0 of an ideal Bose gas. Note that in contrast with ^{4}He the critical temperature is enhanced. The difference is that in liquid helium the renormalized mass is larger than the bare one, resulting in a lower critical temperature, whereas for a weakly interacting gas this effect is essentially absent.

In discussing the physical content of the field theory given by the action $S[\phi^*,\phi]$ we have to distinguish between two cases. If $S^{(+)}>0$ the ground state of the system is $\phi(\mathbf{x},t)=0$ and we are in the symmetric state. The action describes a gas of particles interacting via the pseudopotential $V(\mathbf{x}-\mathbf{x}')=T^{(+)}(\mathbf{0},\mathbf{0};0)\delta(\mathbf{x}-\mathbf{x}')$. The dispersion is slightly changed due to the presence of the $S^{(+)}|\phi(\mathbf{x},t)|^2$ term, but for a thermal particle the correction is $O(na\Lambda^2)$ and unimportant. This is indeed a valid description of a weakly interacting Bose gas above the critical temperature.[14] More interesting is the case $S^{(+)}<0$, when the U(1) gauge symmetry is spontaneously broken. To find the particle content of the theory we transform to the new variables $\rho(\mathbf{x},t)$ and $\chi(\mathbf{x},t)$ corresponding to the (squared) magnitude and the phase of $\phi(\mathbf{x},t)$, respectively. The action becomes

$$S[\rho,\chi]=\int dt \int d\mathbf{x} \left\{ \hbar\chi(\mathbf{x},t)\frac{\partial\rho(\mathbf{x},t)}{\partial t} - S^{(+)}(\mathbf{0};t)\rho(\mathbf{x},t) - \frac{T^{(+)}(\mathbf{0},\mathbf{0};0)}{2}\rho^2(\mathbf{x},t) - \frac{\hbar^2\rho(\mathbf{x},t)}{2m}[\nabla\chi(\mathbf{x},t)]^2 - \frac{\hbar^2}{8m}\frac{[\nabla\rho(\mathbf{x},t)]^2}{\rho(\mathbf{x},t)} \right\}. \tag{7}$$

Replacing $\rho(\mathbf{x},t)$ by $\rho_0(t)+\delta\rho(\mathbf{x},t)$ in the last two interaction terms, with $\rho_0(t)$ having the physical significance of the condensate density, and neglecting terms of $O(\delta\rho/\rho_0)$ which are expected to be small,[14] we arrive at a quadratic action. Going over to momentum space and integrating out the phase field $\chi(\mathbf{x},t)$ by taking only tree diagrams [cf. Eq. (4)] into account, we find the equation of motion of the condensate fraction, $\rho(\mathbf{0},t)=\rho_0(t)V=-S^{(+)}(\mathbf{0};t)V/T^{(+)}(\mathbf{0},\mathbf{0};0)$, and the effective Lagrangian density

$$\mathcal{L}(\rho,\partial\rho/\partial t)=\frac{1}{V}\sum_{\mathbf{k}\neq\mathbf{0}}\left\{ \frac{m}{2\mathbf{k}^2\rho_0(t)}\left|\frac{\partial\rho(\mathbf{k},t)}{\partial t}\right|^2 - \left[\frac{\hbar^2\mathbf{k}^2}{8m}\frac{1}{\rho_0(t)}+\frac{T^{(+)}(\mathbf{0},\mathbf{0};0)}{2}\right]|\rho(\mathbf{k},t)|^2\right\}. \tag{8}$$

From the equations of motion, in the case of constant ρ_0, we obtain the famous Bogoliubov dispersion relation:[14] $\hbar\omega(\mathbf{k})=\epsilon(\mathbf{k})[1+2\rho_0 T^{(+)}/\epsilon(\mathbf{k})]^{1/2}$, which shows that $\mathcal{L}(\rho,\partial\rho/\partial t)$ describes a gas of noninteracting (Bogoliubov) quasiparticles, as we expect for a Bose gas below the critical temperature. Note that the terms of $O(\delta\rho/\rho_0)$, which we neglected so far, describe the interactions between the quasiparticles and are indeed of no importance in general. If necessary for a specific problem they can be treated in perturbation theory. Furthermore, Eq. (8) offers the possibility of studying the time evolution of the dispersion relation and therefore the appearance of superfluidity.

Most important for the purpose of this Letter is the expression for ρ_0. It shows that the time scale for the formation of a condensate is equal to the time scale associated with the change of $S^{(+)}(\mathbf{0};t)$. A careful examination of Eq. (6b) gives a condensation time of $O((a/\Lambda_c)^{2/3}\hbar/k_B(T_c-T))$, which is $O(\hbar/k_BT_c)$ except in a small critical region where $(T_c-T)/T_c \ll (a/\Lambda_c)^{2/3}$.

As an illustration, we calculate $S^{(+)}(\mathbf{0};t)$ for three densities of the gas. For densities $n\ll n_c$, $S^{(+)}(\mathbf{0};t)$ is essentially constant and equal to $2nT^{(+)}(\mathbf{0},\mathbf{0};0)$, implying a correlation length ξ of $O(1/\sqrt{na})$. This is the density regime where a Boltzmann equation is valid. However, if $n \lesssim n_c$ we see in Fig. 2 clearly a buildup of correlations in the gas as time evolves. For $n=n_c$, ξ diverges in the time $t\rightarrow\infty$ and we are at the critical point. Increasing the density beyond n_c we actually see the phase transition taking place as $S^{(+)}(\mathbf{0};t)$ becomes negative.

In conclusion, we have shown that a dilute Bose gas will, under suitable experimental conditions, show a second-order phase transition and form a condensate in a finite time of $O(\hbar/k_BT_c)=O(m/\hbar n^{2/3})$. Because a typical time between collisions is $O(m\Lambda/\hbar na^2)$, their ratio is $O(na^2\Lambda)$ and very small compared to 1, implying that the condensation will take place well within the lifetime of the sample. At first sight it is surprising that the condensation time is insensitive to the interaction. Phys-

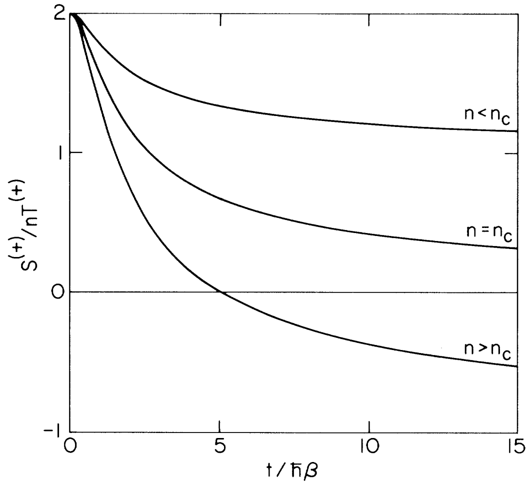

FIG. 2. The time evolution of the condensate fraction for three densities of the Bose gas. See text for more details.

ically this is due to a coherent, in contrast to incoherent, population of the zero-momentum state. Subsequently, the buildup of coherence being determined by the Hamiltonian and for a weakly interacting gas by the kinetic energy, the typical time scale for the appearance of the condensate is set by the temperature of the gas. Of course, the experimental realization of the required densities and temperatures is still a difficult task and poses an important challenge for the future.

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