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Bose-Einstein Condensation in Trapped Atomic Gases

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We discuss Bose-Einstein condensation in a trapped atomic gas and analyze how the sign of the scattering length a and the ratio η of the interaction between particles to the level spacing in the trap influence the behavior of the condensate wave function ψ_0. We find that for $a < 0$ and $\eta \ll 1$ it is possible to form a metastable Bose condensate, with a long characteristic lifetime with respect to contraction and transitions of particles to excited trap states. For $\eta \gg 1$ a negative scattering length prevents the formation of the condensate. If $a > 0$, then an increase of density is accompanied by the evolution of ψ_0 to a comparatively wide quasihomogeneous distribution.

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One of the main goals in the study of low-temperature atomic gases is to observe Bose-Einstein condensation (BEC) and related macroscopic quantum phenomena. Magnetostatic trapping is a powerful method of achieving BEC, since it provides surface-free confinement and allows efficient evaporative and optical cooling [1–4]. A growing interest in trapped gases is stimulated by recent success in achieving BEC in experiments with trapped rubidium [3], lithium [4] and sodium [5], where densities $n \sim 10^{12}–10^{14}$ cm^{-3} and temperatures $T 1$ μK have been reached.

The character of BEC in trapped atomic gases is influenced by the presence of discrete trap levels. For noninteracting particles, Bose condensation occurs in the ground state of the trapping potential. In a weakly interacting trapped gas ($n_0|a|^3 \ll 1$, with n_0 being the condensate density and a the scattering length) under the condition $|a| \ll l_0$, where l_0 is the amplitude of zero point oscillations in the trap, the interaction between particles introduces a new dimensionless parameter

$$\eta = n_0|\tilde{U}|/\varepsilon_0 \tag{1}$$

($\tilde{U} = 4\pi\hbar^2 a/m$ and m is the atom mass), which is the ratio of the mean interaction energy per particle to the characteristic level spacing $\varepsilon_0 \approx \hbar^2/ml_0^2$. With the one-particle wave function localized in a spatial region of size l_0 one has $n_0 \approx N_0/(4\pi/3)l_0^3$, where N_0 is the number of particles in the condensate. We assume

$$N_0 \gg 1\,, \tag{2}$$

which, due to the condition $|a| \ll l_0$, is compatible with the inequality $n_0|a|^3 \ll 1$.

A question of principal importance concerns the stability of the condensate with respect to elastic interaction between particles. A repulsive interaction ($a > 0$) makes the condensate stable, as in this case the transfer of a particle from the condensate to any other state should lead to increasing energy of the system. The shape of the condensate wave function $\psi_0(\mathbf{r})$ in the trapping field significantly changes with an increasing number of condensate particles, N_0. For sufficiently small N_0 (but $N_0 \gg 1$) the parameter $\eta \ll 1$, and the shape of $\psi_0(\mathbf{r})$ is close to that of one-particle wave function in the ground state of the trapping potential, i.e., BEC can be regarded as macroscopic occupation of this state. By increasing N_0 we arrive at the opposite limiting case $\eta \gg 1$, which can be called quasihomogeneous. In this case the size of the BEC spatial region, $l \gg l_0$, and the structure of trap levels becomes unimportant as the levels will be smeared out by the interaction between particles.

For attractive interaction between particles ($a < 0$) the picture drastically changes. A Bose condensate with $\eta > 1$, for which the discrete structure of trap levels is not important, cannot be formed at all, since in this case the accumulation of particles in one quantum state would be associated with an increase of energy (see below). Moreover, even prepared artificially, such a Bose-condensed state will be absolutely unstable. On the other hand, the case $\eta \ll 1$ is characterized by the presence of an energy gap ε_0 for one-particle excitations. As shown below, in this case it is possible to form a metastable Bose-condensed state. This state is separated by a large energy barrier from lower states, which ensures a long characteristic lifetime of the metastable condensate.

We consider a Bose gas with a fixed number of particles N in a potential well $V(r)$. Under the conditions $|a| \ll l_0$ and $n_0|a|^3 \ll 1$, one can use the potential of pair interaction in the form $U(\mathbf{r}) = \tilde{U}\delta(\mathbf{r})$. Then the Schrödinger equation for the Heisenberg field operator of atoms, $\hat{\psi}(\mathbf{r}, t)$, reads

$$i\hbar(\partial\hat{\psi}/\partial t) = -(\hbar^2/2m)\Delta\hat{\psi} + V(r)\hat{\psi} + \tilde{U}\hat{\psi}^\dagger\hat{\psi}\hat{\psi}\,, \tag{3}$$

where the last term in the right-hand side of Eq. (3) corresponds to the interaction of atoms with each other. The field operator $\hat{\psi}$ can be represented as a sum of the above-condensate part $\hat{\psi}'$ and the condensate wave function which is a c-number (see, e.g., [6]):

$$\hat{\psi} = \psi_0 + \hat{\psi}'. \tag{4}$$

Averaging both sides in Eq. (3) and recalling that in thermal equilibrium $\psi_0 \sim \exp(-i\mu t)$, where μ is the chemical potential [6], we obtain

$$-(\hbar^2/2m)\Delta\psi_0 + V(r)\psi_0 + \tilde{U}\psi_0^3 - \tilde{\mu}\psi_0 = 0\,. \quad (5)$$

Here $\tilde{\mu} = \mu - 2n'\tilde{U}$, and $n'(\mathbf{r}) = \langle \hat{\psi}'^{\dagger}\hat{\psi}' \rangle$ is the density of above-condensate particles in the spatial BEC region. At $a > 0$ and $T \gg n\tilde{U}$ the density n' is coordinate independent and equals the critical BEC density $n_c = 2.6\Lambda_T^{-3}$ [7–10], where $\Lambda_T = (2\pi\hbar^2/mT)^{1/2}$ is the thermal de Broglie wavelength of the atom. For $T \lesssim n\tilde{U}$ we have $n' \ll n_0$, and $\tilde{\mu} \approx \mu$. In Eq. (5), due to the condition $n|a|^3 \ll 1$, we neglected the anomalous average $\langle \hat{\psi}'\hat{\psi}' \rangle$. This equation should be solved using the normalization condition

$$\int \psi_0^2(\mu, \mathbf{r})d^3r = N_0\,, \quad (6)$$

which gives a relation between μ and N_0.

The possibility to turn to representation (4) and introduce ψ_0 as an average of the field operator $\hat{\psi}$ assumes that ψ_0 is a quantity averaged over a volume containing a large number of particles. At the same time, the linear size of this volume should be small compared to a characteristic distance at which ψ_0 changes due to the field inhomogeneity. Therefore, Eq. (5) can be used for finding a unified condensate wave function only if inequality (2) is satisfied.

For $a > 0$ we numerically solved Eq. (5), with the normalization condition (6), in a harmonic potential

$$V(r) = m\omega^2 r^2/2\,, \quad (7)$$

where ω is the trap frequency. The results for $\psi_0(r)$ at various values of the parameter η are presented in Fig. 1. These results show how the structure of the condensate wave function changes under variations of N_0 or η.

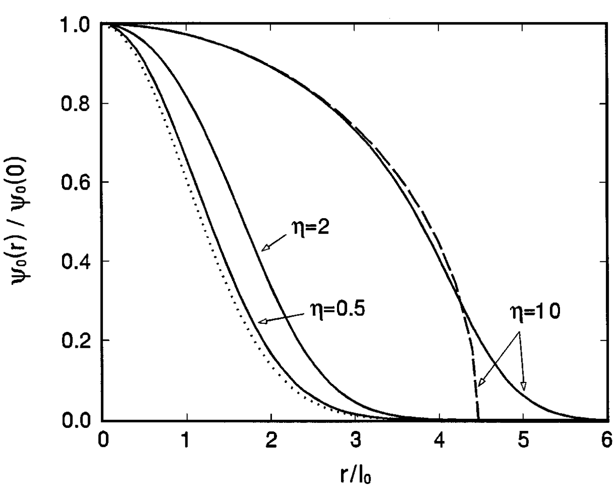

FIG. 1. Condensate wave function $\psi_0(r)$ for potential (7). The parameter $\eta = n_{0\,\max}\tilde{U}/\hbar\omega$, with $n_{0\,\max} = \psi_0^2(0)$ being the maximum condensate density. Solid curves represent numerical solutions of Eq. (5) for $\eta 10(\tilde{\mu} \approx 10\hbar\omega)$, $\eta = 2(\tilde{\mu} \approx 2.5\hbar\omega)$, and $\eta = 0.5(\tilde{\mu} \approx 1.7\hbar\omega)$. The dashed curve corresponds to approximate solution (11) for $\eta = 10$, and the dotted curve to approximate solution (8).

For $\eta \ll 1$ the nonlinear term in Eq. (5) is of minor importance, and the solution is close to

$$\psi_0 = (N_0/\pi^{3/2}l_0^3)^{1/2}\exp(-r^2/2l_0^2)\,. \quad (8)$$

The size of the condensate l is close to the amplitude of zero point oscillations in the trap, $l_0 = (\hbar/m\omega)^{1/2}$, and the condensate density $n_0 \propto N_0$. The parameter η takes the form $\eta \approx (3a/l_0)N_0$, and the inequality $\eta \ll 1$ can be rewritten as

$$1 \ll N_0 \ll l_0/a\,. \quad (9)$$

In fact, under this condition one can consider BEC as macroscopic occupation of the ground state in the trapping field.

In the limiting case $\eta \gg 1$, where the correlation length

$$l_c = \hbar/(2mn_0\tilde{U})^{1/2} \approx l_0/(2\eta)^{1/2} \ll l_0\,, \quad (10)$$

the kinetic energy term in Eq. (5) is unimportant, as well as the discrete structure of trap levels. The solution is close to a well-known result [7,8] following directly from Eq. (5). With $V(r)$ given by Eq. (7), we have

$$\psi_0 \approx \{[\tilde{\mu} - V(r)]/\tilde{U}\}^{1/2} = n_{0\,\max}^{1/2}(1 - r^2/2l_0^2\eta)^{1/2}. \quad (11)$$

We call this case quasihomogeneous, since ψ_0 is a smooth function of r, and, due to inequality (10), spatial correlation properties are governed by the local value of l_c. The quantity $\tilde{\mu} = n_{0\,\max}\tilde{U} \gg \hbar\omega$ and the size of the BEC spatial region, $l \approx l_0(2\eta)^{1/2} \gg l_0$. The parameter $\eta = n_{0\,\max}\tilde{U}/\hbar\omega$, which can be rewritten as $\eta \approx (3al_0^2/l^3)N_0$, takes the value $(3aN_0/l_0)^{2/5}$ and the maximum condensate density $n_{0\,\max} \propto N_0^{2/5}$.

We now turn to the BEC in an inhomogeneous field at $a < 0$ and discuss the possibility of the formation of a long-lived metastable gaseous phase. In this case, for $N \gg 1$ and sufficiently low temperature, the thermodynamic equilibrium corresponds to a condensed phase or a two-phase system. Usually, the condensed phase formation is a first-order phase transition. The kinetics of this transition is determined by the formation of condensation nuclei with a large number of particles. In a low-density gas the probability of such a nucleation is extremely small. Even the formation of dimers, which can stimulate the nucleation, requires three-body collisions and will be suppressed at sufficiently low density. The physical picture is dominated by elastic pair collisions. For $a < 0$ these collisions prevent the formation of a Bose condensate with densities $n_0|\tilde{U}| \gg \hbar\omega$, since in this (quasihomogeneous) case the structure of trap levels is essentially smeared out by interatomic interaction, and there is no gap for the excitation of particles from the condensate. If $a < 0$, the excitation is energetically favorable because the interaction energy per particle in the condensate is $n_0\tilde{U}$, whereas the interaction of the above-condensate particle with the condensate equals $2n_0\tilde{U}$.

In the opposite limiting case, $\eta \ll 1$, the pair collisions, as themselves, do not destroy the quasiequilibrium state formed by N_0 atoms accumulated in the ground state of the trapping potential. From Eq. (5) one can find the wave function ψ_0 for this state, which is again close to Eq. (8). One can also construct a many-particle wave function which, to first approximation, is a product of one-particle wave functions ϕ_0. Each of these functions is the wave function of an atom in the self-consistent field created by the trapping potential and other particles.

It is important that, even in the absence of inelastic processes, the considered state is quasistationary. The attraction between particles enables the existence of a much more dense state of N_0 atoms, with the same total energy $E \approx 0$ ($E \approx \frac{3}{2}N_0\hbar\omega - \frac{1}{2}n_0N_0|\tilde{U}|$). For particles localized in a spatial region of size L_0, we have

$$E \approx \hbar^2 N_0/2mL_0^2 - N_0^2|\tilde{U}|/(8\pi/3)L_0^3 . \qquad (12)$$

This energy is equal to zero at $L_0 = L_*$, where

$$L_* \approx 3|a|N_0 \approx l_0\eta \ll l_0 , \qquad (13)$$

and, hence, the dense state is strongly compressed compared to the initial sate of the trapping potential.

There is a large energy barrier between these two states. From Eq. (12) it follows that, with diminishing L_0, the energy increases and reaches a maximum at $L_0 \approx (9/2)|a|N_0$. Denoting the one-particle wave function of the dense state as $\phi_*(r)$, for the overlap integral between the wave functions of the two states, we obtain

$$I = \left(\int d^3r\,\phi_0(r)\phi_*(r)\right)^{N_0} \approx \left\{-\frac{3}{2}N_0 \ln\frac{l_0}{L_*}\right\}. \qquad (14)$$

For sufficiently large N_0 the factor in the exponent of Eq. (14) is huge. Since in any case the system will live a finite time, one can claim that the considered dense state will not be formed.

However, there can be other states coinciding in energy with the initial state. These are states containing dense clusters of N_1 particles, with

$$1 \ll N_1 \ll N_0 . \qquad (15)$$

With N_0 replaced by N_1 in Eq. (12), one finds the size L_1 or the density at which $E \approx 0$:

$$L_1 \approx 3|a|N_1 . \qquad (16)$$

The many-particle wave function will have an admixture of states with N_1 particles localized in a region of the size L_1. The amplitude of the admixture is [cf. Eq. (14)]

$$C_{N_1} \sim \exp\{-(3/2)N_1 \ln(l_0/L_1)\} . \qquad (17)$$

The local density in these clusters, $n_1 \approx N_1/(4\pi/3)L_1^3$, satisfies the condition

$$n_1|\tilde{U}| \gg \hbar\omega , \qquad (18)$$

and elastic pair collisions can transfer particles to excited trap states, with a simultaneous contraction of the rest of the cluster. In a collisional event leading to the excitation of two particles, the size of the cluster containing the remaining $N_1 - 2$ particles reduces to [cf. Eq. (16)]

$$\tilde{L}_1 \approx 3|a|(N_1 - 2) , \qquad (19)$$

and the cluster energy decreases by an amount $n_1|\tilde{U}|$.

Formation of clusters with smaller $\tilde{L}_1$ and lower energy is not important as the one-particle wave function in such a cluster should oscillate at distances $\lesssim \tilde{L}_1$, which strongly reduces the transition matrix element. The same remark can be made with respect to the quantity L_1 (16). From the very beginning we could consider clusters with smaller L_1 and lower total energy, which would correspond to much smaller amplitude of the admixture in the many-particle wave function than that determined by Eq. (17).

For the system as a whole, the contribution of N_1-particle clusters to the probability of the transition from the initial state to the states corresponding to the excitation of two particles, with the simultaneous decrease of energy of the rest of the atoms, is given by

$$W_{N_1} \approx Q_{N_1}\frac{N_1^2}{2}\frac{2\pi}{\hbar}|\tilde{U}|^2 \int d\varepsilon\, g(\varepsilon)\,\delta(2\varepsilon - n_1|\tilde{U}|) \times \left|\int \phi_1^2(r)\phi_\varepsilon^2(r)d^3r\right|^2 \times \left|\int \phi(r)\tilde{\phi}_1(r)d^3r\right|^{2(N_1-2)} , \qquad (20)$$

where $\phi_1(r)$ and $\tilde{\phi}_1(r)$ are the one-particle wave functions in the initial and contracted clusters, respectively. Owing to Eq. (18), we replaced the summation over the final states $\phi_\varepsilon(r)$ of the excited particles by the integration, with $g(\varepsilon)$ being the density of states at energy ε. The first overlap integral in Eq. (20) comes from the transition matrix element of two particles to the excited state ϕ_ε. For this integral, we have

$$\left|\int \phi_1^2(r)\phi_\varepsilon^2(r)d^3r\right|^2 \approx 1/\Omega_\varepsilon^2, \quad \Omega_\varepsilon = 4\pi l_\varepsilon^3/3 , \qquad (21)$$

where $l_\varepsilon \gg L_1$ is a linear size of the spatial region in which the exited particles are localized. The transitions to states with energies $\varepsilon_1 \neq \varepsilon_2$, being included, do not appreciably change the estimate for W_{N_1} because in this case the transition matrix element strongly decreases due to oscillations of the integrand in the overlap integral. The last factor in Eq. (20) is the overlap integral between the states of $N_1 - 2$ particles before and after the contraction. Using Eqs. (16) and (19), we obtain

$$\int \phi_1(r)\tilde{\phi}_1(r)d^3r \approx (\tilde{L}_1/L_1)^{3/2} = (1 - 2/N_1)^{3/2}, \qquad (22)$$

and for $N_1 \gg 1$ the last factor in Eq. (20) reduces to e^{-6}. The factor Q_{N_1} in Eq. (20) accounts for the number of combinations to select N_1 from N_0 particles. One should also include the number of possible locations of the dense cluster in the spatial region of the initial state $(l_0/L_1)^3$. Together with the square of the amplitude (17), we obtain

$$Q_{N_1} \approx (l_0/L_1)^3 P_{N_1} , \qquad (23)$$

where P_{N_1} is equivalent to the Poisson distribution:

$$P_{N_1} \approx \frac{1}{\sqrt{2\pi N_1}} \exp\left\{-N_1 \ln\left[\left(\frac{l_0}{L_1}\right)^3 \left(\frac{N_1}{eN_0}\right)\right]\right\}. \qquad (24)$$

For the density of states in a harmonic potential (7) at $\varepsilon \gg \hbar\omega$, one has $g(\varepsilon) = \varepsilon^2/2(\hbar\omega)^3$. Then, integrating over $d\varepsilon$ in Eq. (20), with $l_\varepsilon \approx (2\varepsilon/m\omega^2)^{1/2}$ we find

$$W_{N_1} \approx P_{N_1}(2e)^{-6} N_1 |\tilde{U}|/\hbar l_0^3 . \qquad (25)$$

Equation (25) is valid for $N_1 \gg 1$. But even for rather moderate values of N_1 the factor P_{N_1} predetermines a very long kinetic time: The argument of the logarithm in Eq. (24), $(l_0/L_1)^3(N_1/eN_0) \approx (N_0/N_1)^2/\eta^3$, is very large $(\eta \ll 1)$. The sum of Eq. (25) over N_1 is practically determined by the terms with minimum possible value of N_1, and this does not change the above statement.

Thus for $\eta \ll 1$ the initial state is practically stable at $a < 0$ with respect to collapse and "evaporation" induced by elastic interaction between particles. This statement is also valid at finite temperatures, since for $\eta \ll 1$ characteristic excitation energies ε are much larger than the gas temperature even at T close to the BEC transition point, and, hence, W_{N_1} (25) is temperature independent. The excitation of condensate particles induced by their interaction with above condensate ones can also be neglected as the thermal size of the sample greatly exceeds L_1.

Let us consider how quantum fluctuations leading to the virtual formation of dense clusters in the considered initial state of a trapped gas influence the rates of intrinsic inelastic processes. For the process of three-body recombination the virtual formation of clusters containing N_1 atoms gives the recombination rate

$$R_{N_1}^{(3)} \approx Q_{N_1}(\alpha n_1^2 N_1) . \qquad (26)$$

The term in parenthesis represents the number of recombination events per unit time for N_1 atoms localized in a spatial region of linear size L_1 (16), α being the recombination rate constant. Again, the smaller is N_1, the larger is the rate. Putting formally $N_1 = 3$ and using Eqs. (23) and (24), we obtain $R_{N_1}^{(3)} \approx \alpha N_0^3/\Omega_0^2$, where $\Omega_0 = (4\pi/3)l_0^3$. Hence we arrived at the recombination rate which, independent of the sign of a, is characteristic for N_0 particles localized in the ground state of the potential well. Similar considerations apply to the two-body relaxation rate or the rate of the formation of a N-particle bound state: The maximum rate coincides with that in the absence of virtual formation of clusters.

So we come to the conclusion that the quantum fluctuations characteristic for the case $a < 0$ at $\eta \ll 1$ do not influence the rate of intrinsic inelastic processes. Together with the result of the previous section, this ensures the existence of a long-lived metastable Bose-condensed state in trapped gases with negative scattering length, provided the parameter $\eta \ll 1$.

We can now sketch the scenario of BEC in a trapped gas with $a < 0$. Once the temperature gets lower than the BEC transition point, the particles start to accumulate in the ground state of the trap. For the maximum number of particles N_0 still satisfying the condition $\eta \ll 1$, the rate of inelastic processes will be sufficiently low to allow a metastable Bose condensate. If N_0 takes the value corresponding to the condition $n_0|\tilde{U}| \gg \hbar\omega$, then the major part of particles will be in the excited states. Only a small fraction will remain in the Bose-condense state, the parameter η for this particular fraction being smaller than unity.

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Note added.—After this paper was finished, we got Ref. [11], where, on the basis of time-dependent nonlinear Schrödinger equation for the condensate wave function, the authors found a ground-state solution at $a < 0$ and made a conclusion on its stability. The physical picture presented in our paper is completely different. Our analysis shows that for $a < 0$, due to quantum fluctuations leading to the virtual formation of dense clusters, there is a large set of states with the same energy for fixed N_0. These fluctuations, with subsequent transitions of condensate particles to excited trap states, open the decay channels of the condensate. For sufficiently small η, the characteristic decay time is found to be rather large, and it is this result that predetermines the existence of a metastable Bose-condensed state.

[1] D. M. Doyle, J. C. Sandberg, I. A. Yu, C. L. Cesar, D. Kleppner, and T. J. Greytak, Phys. Rev. Lett. **67**, 603 (1991).
[2] I. D. Setija, H. G. C. Werij, O. J. Luiten, M. W. Reynolds, T. W. Hijmans, and J. T. M. Walraven, Phys. Rev. Lett. **70**, 2257 (1993).
[3] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science **269**, 198 (1995).
[4] C. C. Bradley, C. A. Sackett, J. J. Tolett, and R. G. Hulet, Phys. Rev. Lett. **75**, 1687 (1995).
[5] K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druiten, D. S. Durfee, D. M. Kurn, and W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995).
[6] L. D. Landau and E. M. Lifshitz, *Statistical Physics, Part 2* (Pergamon Press, Oxford, 1980).
[7] V. V. Goldman, I. F. Silvera, and A. J. Leggett, Phys. Rev. B **24**, 2870 (1981).
[8] D. A. Huse and E. D. Siggia, J. Low Temp. Phys. **46**, 137 (1982).
[9] Yu. Kagan and G. V. Shlyapnikov, Phys. Lett. A **130**, 483 (1988).
[10] T. W. Hijmans, Yu. Kagan, G. V. Shlyapnikov, and J. T. M. Walraven, Phys. Rev. B **48**, 12 866 (1993).
[11] P. A. Ruprecht, M. J. Holland, K. Burnett, and M. Edwards, Phys. Rev. A **51**, 4704 (1995).