PHYSICAL REVIEW A VOLUME 54, NUMBER 6 DECEMBER 1996

Condensate fraction and critical temperature of a trapped interacting Bose gas

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(Received 16 July 1996)

By using a mean-field approach, based on the Popov approximation, we calculate the temperature dependence of the condensate fraction of an interacting Bose gas of N atoms confined in an anisotropic harmonic trap. For systems interacting with repulsive forces we find a significant decrease of the condensate fraction and of the critical temperature with respect to the predictions of the noninteracting model with the same value of N. An analytic result for the shift of the critical temperature holding to first order in the scattering length is also derived. [S1050-2947(96)51212-6]

PACS number(s): 03.75.Fi, 02.70.Lq, 67.40.Db

The recent experiments on Bose-Einstein condensation (BEC) in magnetically trapped atomic vapors [1] have stimulated a new interest in the theoretical study of inhomogeneous Bose gases. Although the atom clouds realized in these experiments are very dilute, the effects due to the interatomic forces are known to be important at low temperature. In particular, the shape and the energy of the condensate cloud [2,3] as well as the dispersion law of the elementary excitations [4] are strongly affected by the interaction. In the very recent experiments by Mewes *et al.* [5], Jin *et al.* [6], and Mewes *et al.* [7], the measured release energy and excitation frequencies of the collective modes have been found to be in good agreement with the theoretical predictions, thereby revealing important features of the trapped Bose condensed gases that are undoubtedly connected to the interparticle interaction. The question of how two-body forces affect the thermodynamic properties of these systems has also been the object of several theoretical investigations [8]. The critical temperature of the BEC transition in a homogeneous dilute gas has been recently calculated [9] using the renormalization-group theory. The result is a shift towards higher temperatures, with respect to the prediction of the ideal Bose gas. Similar results have also been obtained with path integral Monte Carlo simulations [10]; however, no definitive conclusions have so far been drawn on the behavior of the condensate fraction, nor of the critical temperature in the presence of a confining potential [11]. The first experimental data on these relevant quantities are now becoming available [5,12].

Finite-size effects on the temperature dependence of the condensate fraction and on the critical temperature in the presence of an external trap have recently been investigated by several authors within the noninteracting model [13,14]. In the presence of an anisotropic harmonic potential of the form $V_{ext}=m(\omega_x^2x^2+\omega_y^2y^2+\omega_z^2z^2)/2$ this model predicts, in the large-N limit, the well known results [8] for the critical temperature

$$T_c^0=\frac{\hbar\omega}{k_B}\left(\frac{N}{\zeta(3)}\right)^{1/3}\simeq 0.94\frac{\hbar\omega}{k_B}N^{1/3}, \tag{1}$$

where $\omega=(\omega_x\omega_y\omega_z)^{1/3}$ is the geometrical average of the oscillator frequencies, and for the temperature dependence of the number of atoms in the condensate

$$\frac{N_0(T)}{N}=1-\left(\frac{T}{T_c^0}\right)^3. \tag{2}$$

Results (1) and (2) are obtained using the semiclassical approximation for the excited states and setting the chemical potential equal to zero at the transition. The first correction to the critical temperature (1) due to the finite number of atoms in the trap has recently been shown [14] to obey the law

$$\frac{\delta T_c^0}{T_c^0}=-\frac{\zeta(2)}{2\zeta(3)^{2/3}}\frac{\overline{\omega}}{\omega}N^{-1/3}\simeq -0.73\frac{\overline{\omega}}{\omega}N^{-1/3}, \tag{3}$$

where $\overline{\omega}=(\omega_x+\omega_y+\omega_z)/3$ is the mean frequency. This result can be obtained by still employing the semiclassical description for the excited states, while keeping the quantum value $\mu=3\hbar\overline{\omega}/2$ for the chemical potential at the transition. The discretization of the excited energy levels gives rise to higher-order corrections to δT_c^0

In this Rapid Communication we present results for the temperature dependence of the condensate fraction and for the critical temperature of a dilute Bose gas interacting with repulsive forces and confined in a harmonic potential. We use a mean-field approach and the semiclassical approximation for the excited states. This approximation is expected to be accurate for temperatures significantly larger than the oscillator temperature $\hbar\omega/k_B$. This condition is satisfied well in a useful range of temperatures, provided N is sufficiently large. In the presence of repulsive interactions we find that the thermal depletion of the condensate is enhanced and the critical temperature is shifted towards lower temperatures. These results go in the opposite direction compared to the homogeneous case, revealing an interesting behavior exhibited by a confined Bose gas.

Our starting point is the finite-temperature generalization of the Gross-Pitaevskii equation within the Popov approximation [15,16]

$$-\frac{\hbar^2\nabla^2}{2m}\Phi(\mathbf{r})+[V_{ext}(\mathbf{r})-\mu+g(n_0(\mathbf{r})+2n_T(\mathbf{r}))]\Phi(\mathbf{r})=0, \tag{4}$$

and

$$i\hbar\frac{\partial\Phi'(\mathbf{r},t)}{\partial t}=-\frac{\hbar^2\nabla^2}{2m}\Phi'(\mathbf{r},t)+[V_{ext}(\mathbf{r})-\mu+2gn(\mathbf{r})]\Phi'(\mathbf{r},t)+gn_0(\mathbf{r})\Phi'^*(\mathbf{r},t). \tag{5}$$

The first equation describes the space variations of the condensate wave function $\Phi(\mathbf{r})=\langle\psi(\mathbf{r})\rangle$ at statistical equilibrium, where $\psi(\mathbf{r})$ is the particle field operator. The second one is the equation for the fluctuations of the condensate $\Phi'(\mathbf{r},t)=\langle\psi(\mathbf{r},t)\rangle-\Phi(\mathbf{r})$, which give the elementary excitations of the system. In Eqs. (4) and (5), V_{ext} is the external potential, μ is the chemical potential, $g=4\pi\hbar^2a/m$ is the interaction coupling constant fixed by the s-wave scattering length a, n_0 is the equilibrium condensate density $n_0(\mathbf{r})=|\Phi(\mathbf{r})|^2$, $n(\mathbf{r})=\langle\psi^\dagger(\mathbf{r})\psi(\mathbf{r})\rangle$ is the particle density, and finally n_T is the density of the thermally excited particles $n_T(\mathbf{r})=n(\mathbf{r})-n_0(\mathbf{r})$. Equations (4) and (5) are obtained from the equation of motion for the particle field operator $\psi(\mathbf{r},t)$, by treating the cubic interaction term $g\psi^\dagger(\mathbf{r},t)\psi(\mathbf{r},t)\psi(\mathbf{r},t)$ in the mean-field scheme. The Popov approximation consists in neglecting the anomalous density $m_T(\mathbf{r})=\langle\psi(\mathbf{r})\psi(\mathbf{r})\rangle-\Phi(\mathbf{r})^2$ entering the interaction term. As discussed in Ref. [16] this approximation is expected to be good for high temperatures where $m_T\ll n_T$ and also in the low-temperature regime where n_T and m_T are of the same order but both are negligible. The present mean-field approach is expected to provide correctly the thermodynamic properties of the system, apart from the critical behavior near T_c where the mean-field approach is known to fail.

The energies of the elementary excitations can be explicitly obtained from Eq. (5) using the semiclassical WKB approximation. Let us write the fluctuations of the condensate in the form $\Phi'(\mathbf{r},t)=A\exp[i\varphi(\mathbf{r},t)]+B\exp[-i\varphi(\mathbf{r},t)]$. In the WKB approximation the coupled equations for $\Phi'(\mathbf{r},t)$ and $\Phi'^*(\mathbf{r},t)$, given by Eq. (5) and its complex conjugate, can be solved in an explicit way, yielding the semiclassical excitation spectrum

$$\epsilon(\mathbf{p},\mathbf{r})=\sqrt{\left(\frac{p^2}{2m}+V_{ext}(\mathbf{r})-\mu+2gn(\mathbf{r})\right)^2-g^2n_0^2(\mathbf{r})}, \tag{6}$$

where $p=\hbar\nabla\varphi$ and $\epsilon=-\hbar\partial\varphi/\partial t$ are, respectively, the impulse and the energy of the excitation. For a homogeneous system at low temperatures, where n_T can be neglected, the above excitations coincide with the usual Bogoliubov spectrum. The quasiparticles with energies $\epsilon(\mathbf{p},\mathbf{r})$ are distributed according to the Bose distribution function

$$f(\mathbf{p},\mathbf{r})=\frac{1}{\exp[\epsilon(\mathbf{p},\mathbf{r})/k_BT]-1}, \tag{7}$$

whereas the particle distribution function can be obtained from the Bogoliubov canonical transformations and is given by

$$F(\mathbf{p},\mathbf{r})=-\left(\frac{\partial\epsilon}{\partial\mu}\right)_{n_0}f(\mathbf{p},\mathbf{r}), \tag{8}$$

where the partial derivative is taken at constant condensate density n_0. The noncondensate density is then obtained by integrating $F(\mathbf{p},\mathbf{r})$ in momentum space

$$n_T(\mathbf{r})=\int\frac{d^3\mathbf{p}}{(2\pi\hbar)^3}F(\mathbf{p},\mathbf{r}), \tag{9}$$

and the total number of atoms out of the condensate is given by

$$N_T=\int d^3\mathbf{r}\,n_T(\mathbf{r}). \tag{10}$$

In the above equations the chemical potential μ is fixed by the normalization condition

$$N=N_0(T)+N_T, \tag{11}$$

where $N_0(T)=\int d^3\mathbf{r}n_0(\mathbf{r})$ is the number of atoms in the condensate, with $n_0(\mathbf{r})$ fixed by the solution of Eq. (4).

We have solved Eqs. (4)–(11) in a self-consistent way employing the following procedure:

(i) Equation (4) is solved, using the method described in Ref. [3] for the condensate density $n_0(\mathbf{r})$ and the chemical potential μ, by keeping fixed the number $N_0(T)$ of particles in the condensate and the density $n_T(\mathbf{r})$ of thermally excited atoms.

(ii) The condensate density and chemical potential found in step (i) are used to calculate the excitation energies from Eq. (6). A new density n_T is then obtained from Eq. (9), and new values for the number of atoms out of the condensate, N_T, and in the condensate, $N_0(T)$, are derived from Eqs. (10) and (11).

(iii) Steps (i) and step (ii) are repeated until convergence is reached.

It is worth noting that the present method accounts for finite-size effects because of the quantum nature of Eq. (4) for the order parameter and of the corresponding value of the chemical potential. In particular, in the absence of interactions, it reproduces result (3) for the shift of the critical temperature.

In Fig. 1 we present our results for the temperature dependence of the condensate fraction $N_0(T)/N$ for a system of 5000 Rb atoms interacting with scattering length $a=110a_0$, where a_0 is the Bohr radius, which is trapped in a deformed harmonic potential fixed by $a_{HO}=(\hbar/m\omega)^{1/2}=7.92\times10^{-5}$ cm with the deformation parameter $\lambda=\omega_z/\omega_x=\omega_z/\omega_y$ equal to $\sqrt{8}$, according to the experimental conditions of Ref. [6]. We have also considered the case of a spherical trap (dotted lines). As clearly emerges from the figure, finite-size effects are not negligible for this value of N; however, interaction effects are more important and result in a sizable quenching of the condensate fraction. Contrarily the effects of the deformation of the trap are always very small. The sizable enhancement of the thermal depletion predicted by our calculation follows from the fact that in the presence of the harmonic trap the overlap between the condensed and noncondensed densities is small. As a consequence it is energetically favorable for the atoms to leave the condensate

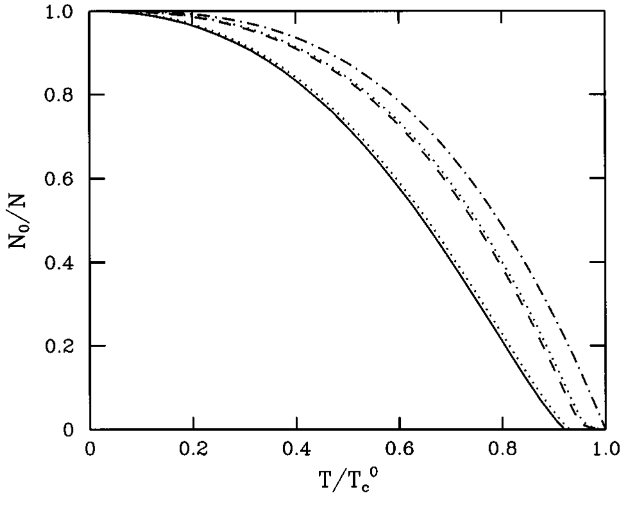

FIG. 1. Temperature dependence of the condensate fraction for a system of 5000 Rb atoms in a deformed harmonic trap ($\lambda=\sqrt{8}$). The solid line is the result for the interacting case, the dashed line is the exact result for the noninteracting case, and the dot-dashed line corresponds to the noninteracting case in the thermodynamic limit [Eq. (2)]. The dotted lines correspond to the spherical case ($\lambda=1$) for the same number of atoms.

where the density is higher and the effects of repulsion are stronger. This behavior differs from the one exhibited by a homogeneous dilute Bose gas at fixed density where the same mean-field approach predicts a reduction of the thermal depletion with respect to the prediction of the noninteracting model.

When the number of atoms in the trap increases, the effects due to the interaction become more and more important, as explicitly shown in Fig. 2, where we report results for $N_0(T)$ corresponding to three values of N ($N=10^5$, 10^6, 10^7). The calculations of Fig. 2 have been carried out using the value 2.56×10^{-3} for the ratio a/a_{HO} and $\lambda=18/320$. This choice corresponds to the experimental situation of Ref. [5] for Na atoms. We have checked that for such large values of N the results for $N_0(T)$ are practically indistinguishable from the ones with a spherical trap ($\lambda=1$) and the same value of a/a_{HO}. Notice that the quenching effects shown in Fig. 2 are quantitatively similar to the ones of Fig. 1, despite the much larger values of N contained in the trap. This is due to the fact that in the trap of Fig. 2 (MIT-type trap) the ratio a/a_{H0} is a factor of 3 smaller than in the trap of Fig. 1 (JILA-type trap).

The shift δT_c in the critical temperature can be estimated analytically to the lowest order in the coupling constant g by studying the behavior of the trapped gas for temperatures $T\geqslant T_c$. In this case the order parameter $\Phi(\mathbf{r})$ vanishes and the dispersion of the elementary excitations takes the simple Hartree-Fock form

$$\epsilon(\mathbf{p},\mathbf{r})=\frac{p^2}{2m}+V_{ext}(\mathbf{r})+2gn_T(\mathbf{r})-\mu. \tag{12}$$

To the lowest order in g the total number of particles above T_c can be written, as a function of the chemical potential, in the following form:

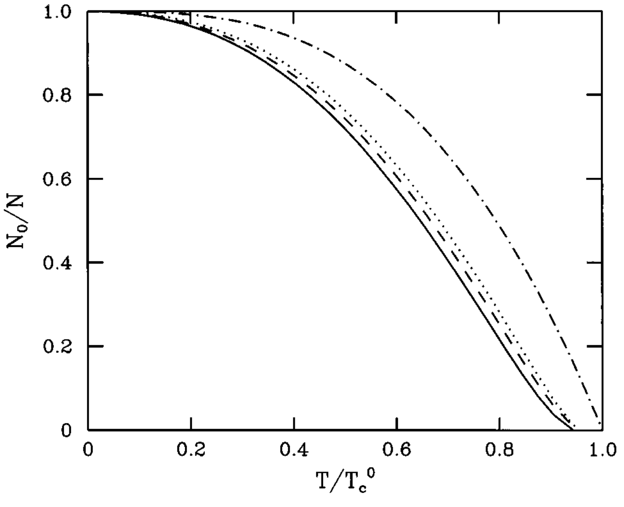

FIG. 2. Temperature dependence of the condensate fraction for interacting Na atoms. The solid line corresponds to $N=10^7$, the dashed line corresponds to $N=10^6$, and the dotted line to $N=10^5$. The dot-dashed line is the result for the noninteracting case in the thermodynamic limit [Eq. (2)].

$$N=N_T^0(\mu)-2g\int d^3\mathbf{r}\frac{\partial n_T^0}{\partial\mu}n_T^0(\mathbf{r},\mu), \tag{13}$$

where we have used Eqs. (7)–(10) with $\epsilon(\mathbf{p},\mathbf{r})$ given by Eq. (12). The quantity $N_T^0(\mu)$ is the integral of the noncondensed density $n_T^0(\mathbf{r},\mu)$ given by the noninteracting model

$$n_T^0(\mathbf{r},\mu)=\lambda_T^{-3}g_{3/2}(\exp\{-[V_{ext}(\mathbf{r})-\mu]/k_BT\}), \tag{14}$$

where $\lambda_T=\hbar(2\pi/mk_BT)^{1/2}$ is the thermal wavelength and $g_{3/2}(x)=\Sigma_{n=1}^{\infty}x^n/n^{3/2}$.

Bose-Einstein condensation starts at the temperature T_c at which the chemical potential reaches the energy of the lowest solution of the Schrödinger equation corresponding to the Hamiltonian (12). To the lowest order in g and for large values of N one finds

$$\mu=\frac{3\hbar\overline{\omega}}{2}+2gn_T^0(\mathbf{r}=0,\ \mu=0). \tag{15}$$

By expanding the right-hand side (rhs) of Eq. (13) around $\mu=0$ and $T=T_c^0$, we obtain the following relationship for the shift $\delta T_c=T_c-T_c^0$ of the critical temperature:

$$\delta T_c\int d^3\mathbf{r}\frac{\partial n_T^0}{\partial T}=-\frac{3\hbar\overline{\omega}}{2}\int d^3\mathbf{r}\frac{\partial n_T^0}{\partial\mu}-2g\int d^3\mathbf{r}\frac{\partial n_T^0}{\partial\mu}[n_T^0(\mathbf{r}=0)-n_T^0(\mathbf{r})], \tag{16}$$

where, for simplicity, we have dropped the argument $\mu=0$ from the n_T^0 functions, evaluated here at $T=T_c^0$. The shift δT_c of the critical temperature is hence the sum of two distinct effects given by the two terms on the rhs of Eq. (16). The first contribution is due to the finite number of particles present in the trap and after a straightforward integration gives exactly result (iii) for the shift $\delta T_c^0/T_c^0$. The second contribution arises instead from interaction effects and takes the form

$$\frac{\delta T_c^{int}}{T_c^0}=-\frac{2g}{T_c^0}\frac{\int d^3\mathbf{r}\partial n_T^0/\partial\mu[n_T^0(\mathbf{r}=0)-n_T^0(\mathbf{r})]}{\int d^3\mathbf{r}\partial n_T^0/\partial T}$$

$$=-\frac{a}{a_{HO}}N^{1/6}\frac{2^{3/2}\zeta(3/2)\zeta(2)}{3\sqrt{\pi}\zeta(3)^{7/6}}(1-S) \qquad (17)$$

where $S=\Sigma_{n,m=1}^{\infty}(1/n^{1/2}m^{3/2})[1/(n+m)^{3/2}]/\zeta(3/2)\zeta(2)\simeq 0.281$. By evaluating explicitly the numerical factors one gets the relevant result

$$\frac{\delta T_c^{int}}{T_c^0}\simeq -1.33\frac{a}{a_{HO}}N^{1/6}. \qquad (18)$$

The shift δT_c^0 originating from finite-size effects is always negative and vanishes in the large-N limit. For an axially deformed trap it depends on the deformation parameter $\lambda=\omega_z/\omega_x=\omega_z/\omega_y$ through the ratio $\overline{\omega}/\omega=(\lambda+2)/3\lambda^{1/3}$ and is minimum for an isotropic trap. Contrarily, the shift δT_c^{int} due to interactions can be either negative or positive; depending on the sign of a, it increases as $N^{1/6}$ and does not depend on the deformation parameter λ, but only on the geometrical average ω. Furthermore it vanishes for a homogeneous system [see Eq. (17)]. This result is due to the fact that, according to Eq. (12), in a homogeneous system the effects of the interaction above T_c consist of a simple renormalization of the chemical potential. It is also important to note that in the present mean-field approach the relationship between the critical temperature and the corresponding value of the density in the center of the trap is unaffected by the interaction. The shift (18) is hence always associated with a change in the central density produced by the interparticle forces and differs from the one exhibited by an interacting homogeneous gas at fixed density. The prediction $\delta T_c=\delta T_c^0+\delta T_c^{int}$, obtained from Eqs. (3) and (18), agrees well with the numerical values obtained in the self-consistent calculation discussed above and reported in Figs. 1 and 2. The relative importance of the two effects depends on the value of N. Notice however that the interaction effects depend very weakly on N and scale as $N^{1/6}a/a_{HO}$. This behavior should be compared with the effects of the interactions on the low-temperature properties of the system (e.g., the size and the energy of the condensate), which instead scale [3] as Na/a_{HO}.

We finally note that according to the Ginzburg criterion critical fluctuations violate the mean-field result in the region

$$\delta\mu=|\mu-\mu_c|\leqslant\frac{m^3g^2T_c^{02}}{\hbar^6}, \qquad (19)$$

where μ_c is the value of the chemical potential at the critical point. These fluctuations can affect the shift in the chemical potential at the critical point only to order g^2. It means that the mean-field approach can provide a reliable prediction of the shift of the critical temperature up to terms linear in the scattering length. Higher-order effects should be investigated using alternative methods, such as renormalization-group theory [9] or numerical simulations [10]. A more systematic discussion of the thermodynamic behavior of a trapped Bose gas, including the temperature dependence of the density profiles, the specific heat, and the superfluid density will be the object of a future paper.

Useful discussions with Franco Dalfovo are acknowledged.

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