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Citation: Low Temperature Physics **27**, 873 (2001); doi: 10.1063/1.1414580
View online: http://dx.doi.org/10.1063/1.1414580
View Table of Contents: http://aip.scitation.org/toc/ltp/27/9
Published by the American Institute of Physics

Real-space condensation in a dilute Bose gas at low temperature

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(Submitted May 16, 2001)
Fiz. Nizk. Temp. **27**, 1179–1182 (September–October 2001)

We show with a direct numerical analysis that a dilute Bose gas in an external potential—which is chosen for simplicity as a radial parabolic well—undergoes at a certain temperature T_c a phase transition to a state supporting a macroscopic fraction of particles at the origin of the phase space ($\mathbf{r}=0$, $\mathbf{p}=0$). Quantization of particle motion in a well wipes out the sharp transition but supports a distribution of a radial particle density $\rho(r)$ peaked at $r=0$ (a real-space condensate) as well as a phase-space Wigner distribution density $W(\mathbf{r,p})$ peaked at $\mathbf{r}=0$ and $\mathbf{p}=0$ below a crossover temperature T_c^* of order of T_c. A fixed-particle-number canonical ensemble, which is a combination of the fixed-N condensate part and the fixed-μ excitation part, is suggested to resolve the difficulty of large fluctuation of the particle number ($\delta N \sim N$) in the Bose-Einstein condensation problem treated within the orthodox grand canonical ensemble formalism. [DOI: 10.1063/1.1414580]

The phenomenon of Bose-Einstein (BE) condensation (see textbooks, e.g., Refs. 1–3) manifests itself in the formation of macroscopic fraction of zero-momentum particles uniformly distributed in a coordinate space. Such transition was recently observed in laser-trapped, evaporation-cooled atomic vapors[4–6] in magnetic traps (see recent reviews[7–9]). We will show by a direct numerical analysis, partly similar to and sometimes overlapping with the previous theoretical works on the subject,[10–13] that a Bose gas in an external confining potential condenses at low temperature to a position of minimum potential energy; the particles of that "condensate" also have zero kinetic energy. Quantization of particle states in a well makes the real-space condensation a continuous transition rather than a phase transition but still supports a macroscopic fraction of particles near the origin of the coordinate space below a crossover temperature T_c^* which is of the order of Bose-condensation temperature T_c.

Experimental realization of BE condensation implies confinement of a dilute gas within some region of space in a "trap" cooled by its interaction with an "optical molasses" created by laser irradiation[14] and finally cooled to microwave-range temperature by evaporative cooling.[11] Bose gas in a trap may be considered to be interacting with two thermal reservoirs, the first one representing the thermal environment (walls, blackbody radiation at temperature T_1) and the second one the optical molasses at temperature $T_2 \ll T_1$. The equilibrium distribution of particles $f(\mathbf{p},\mathbf{r},t)$ can be obtained by solving the Boltzmann kinetic equation

$$\frac{df}{dt}=\hat{I}_1\{f\}+\hat{I}_2\{f\}, \tag{1}$$

where $\hat{I}_1$ is the interaction term (Stoss integral) corresponding to coupling with a media 1, and $\hat{I}_2$, respectively, with media 2. If we choose for simplicity the relaxation time approximation for $\hat{I}_{1,2}$,

$$\hat{I}_i=-\frac{f-f_i}{\tau_i}, \tag{2}$$

then the solution for the equilibrium state will be

$$f=\frac{\tau_1^{-1}f_1^0+\tau_2^{-1}f_2^0}{\tau_1^{-1}+\tau_2^{-1}}. \tag{3}$$

The relaxation rate τ_2^{-1} is proportional to the laser intensity P. At large intensity, assuming $\tau_2^{-1} \gg \tau_1^{-1}$, Eq. (3) gives $f \simeq f_2^0$.

In a semiclassical approximation, the particle energy is

$$\varepsilon=\frac{\mathbf{p}^2}{2m}+\frac{1}{2}m\Omega^2\mathbf{r}^2, \tag{4}$$

where the thermodynamic potential $\Omega=-T\ln Z$, Z is the grand partition function (assuming zero spin of particles)

$$Z=\int\frac{d\mathbf{p}d\mathbf{r}}{(2\pi\hbar)^3}\ln(1-e^{(\mu-\varepsilon)/T}), \tag{5}$$

where $\hbar$ is Planck's constant. The chemical potential μ is determined from (5) to satisfy an equation

$$N=\int\frac{d\mathbf{p}d\mathbf{r}}{(2\pi\hbar)^3}\frac{1}{e^{(\varepsilon-\mu)/T}-1}, \tag{6}$$

where N is the number of particles. After integration over the directions of $\mathbf{r}$ and $\mathbf{p}$ we obtain

$$N=\frac{(4\pi)^2}{(2\pi\hbar)^3}(2mT)^{3/2}\left(\frac{2T}{m\Omega^2}\right)^{3/2}\times\int_0^\infty x^2dx\int_0^\infty y^2dy\,\frac{1}{e^{x^2+y^2-\zeta}-1}, \tag{7}$$

where $\zeta<0$ is the chemical potential in appropriate dimensionless units.

At low temperature, no nonzero value of ζ can satisfy Eq. (7). It therefore vanishes at a temperature $T=T_{c0}$ determined from the condition $\zeta=0$, thus giving

$$T_{c0}=\hbar\Omega(N/\zeta(3))^{1/3}=0.94\hbar\Omega N^{1/3}, \tag{8}$$

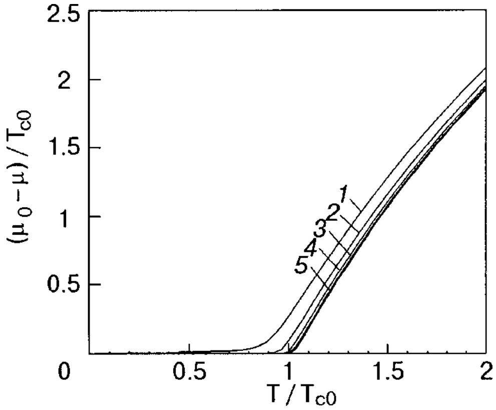

FIG. 1. Chemical potential versus temperature for various values of N:10^2 (1), 10^3 (2), 10^4 (3), 10^5 (4), 10^6 (5).

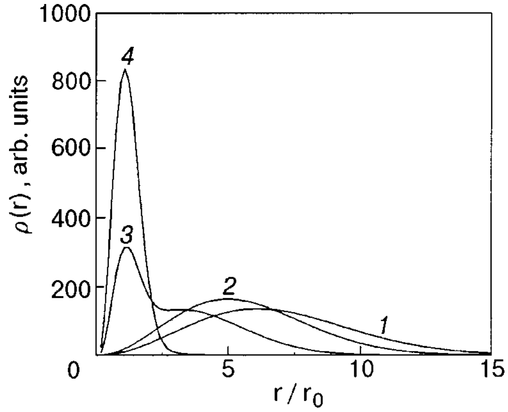

FIG. 2. Radial density distribution $\rho(r)=4\pi r^2 n(r)$ for $N=1000$ and various temperatures: $T/T_{c0}=0.2$ (1), 0.8 (2), 1.4 (3), 2.0 (4).

where $\zeta(z)$ is the Riemann zeta function. Below T_{c0}, ζ remains equal to zero with the total number of particles N_0 having both $\mathbf{r}=0$ and $\mathbf{p}=0$ values, determined from

$$N_0=\left(1-\frac{T^3}{T_{c0}^3}\right)N. \tag{9}$$

Of course, the $\mathbf{r}=0$, $\mathbf{p}=0$ state is not allowed quantum-mechanically, and the derivation leading to Eqs. (6), (7) needs modification. The energy of a particle in a parabolic well, Eq. (4), is

$$\varepsilon=\hbar\Omega(n_1+n_2+n_3+3/2),\quad n_i=0,1\ldots .$$

Then the normalization condition, Eq. (6), reduces to

$$N=\sum_{n=0}^{\infty}\frac{S_n}{\eta e^{nx}-1} \tag{10}$$

with

$$S_n=\sum_{n_1,n_2,n_3=0}^{n}\delta_{n_1+n_2+n_3,n}=\frac{1}{2}(n+1)(n+2)$$

and $\eta=\exp((\mu_0-\mu)/T)$, $x=\hbar\Omega/T$; μ_0 is the value of the chemical potential at $T=0$ ($\mu_0=3/2\hbar\Omega$).

The solution of Eq. (10) shows the dependence $\mu(T)$ (Fig. 1) with a crossover between almost linear dependence above the crossover temperature T_c^* and a practically zero value below that temperature. The value of T_c^* is very near to T_{c0} at large number of particles, $N\gg 1$.

The particle density distribution is expressed through the sum of Hermite polynomials.[15] Employing the identity for these polynomials

$$\sum_{n_1+n_2+\ldots+n_r=n}\prod_{k=1}^{r}\frac{H_{n_k}^2(x_k)}{2^{n_k}n_k!}$$
$$=\sum_{m=0}^{n}r_{n-m}\frac{1}{2^m m!}H_m^2\left(\left(\sum_{k=1}^{r}x_k^2\right)^{1/2}\right), \tag{11}$$

where $r_m=1$ for m even and $r_m=0$ for m odd, we receive by putting $r=3$

$$n(\mathbf{r})=\frac{e^{-r^2}}{\pi^{3/2}}\sum_{m=0}^{\infty}\frac{H_m^2(r)}{2^m m!}\sum_{k=0}^{\infty}\frac{1}{\eta e^{(m+2k)x}-1}. \tag{12}$$

Figure 2 shows the radial density distribution $\rho(r)=4\pi r^2 n(r)$ at various temperatures. Below T_c^*, $\rho(r)$ displays a second maximum at small r, which grows in amplitude as the temperature decreases: the real-space condensate. The formation of such a condensate is even more explicit in the evolution of the z-projected density distribution, Fig. 3, as the temperature is decreased from above to below T_{c0}.

At zero temperature, all excited particles above the condensate vanish. The joint momentum–coordinate distribution function (the Wigner distribution function[16]) takes a value

$$W(\mathbf{p},\mathbf{r})=\frac{N_0}{\pi r_0}e^{-p^2r_0^2}e^{-r^2/r_0^2}, \tag{13}$$

where $r_0=(\hbar/m\Omega)^{1/2}$ is the zero-point oscillation amplitude in a parabolic well.

The question remains, how to reconcile the above results with the free-space Bose-Einstein condensation. The BE condensation temperature equals[1]

$$T_0=3.31\frac{\hbar^2}{m}n^{2/3}. \tag{14}$$

The average density of particles in a well above the condensation temperature is

$$\overline{n}\sim N/T^3,\quad\text{where}\quad\overline{r}=\left(\frac{T}{m\Omega}\right)^{1/2}\sim r_0N^{1/6}(T/T_0)^{1/2}, \tag{15}$$

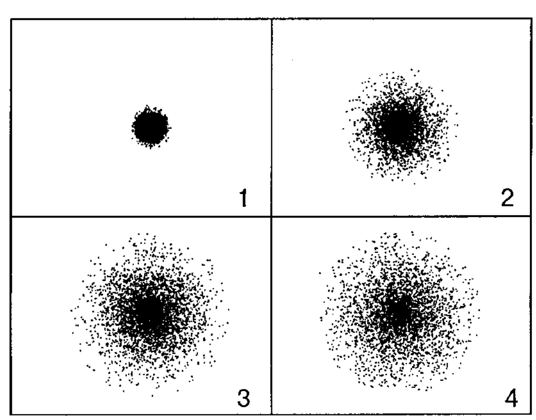

FIG. 3. Side view of particle distribution: *1*—$T=0.2T_{c0}$, *2*—$T=0.8T_{c0}$, *3*—$T=1.4T_{c0}$, *4*—$T=2.0T_{c0}$.

where $\overline{r}$ is a confinement radius (mean radius of the gaseous cloud). It is related to the minimal quantum radius r_0 as $\overline{r} \sim r_0 N^{1/6}(T/T_c)^{1/2}$. By putting $T \sim T_c^*$ as defined above, we obtain T of the order of the BE condensation temperature (14). Therefore, the phenomenon we discussed is just the BE condensation mechanism,[1] except that in a trap the condensation occurs in both the momentum and coordinate spaces or, if we choose to explore the behavior of a dilute low-temperature Bose gas in real space, it will condense there, making up a high-density globular fraction coexisting with the spatially dispersed ''excitations'' in a region of size comparable to the thermal confinement radius $\overline{r}$.

In the grand canonical ensemble which we so far have been considering, the number of particles is not fixed. The mean square fluctuation of particle number in a state α is $\langle \delta n_\alpha^2 \rangle = n_\alpha(n_\alpha + 1)$. In a condensate, by putting $\langle n_{\alpha=0} \rangle = N_0$ we get $\mu \simeq \varepsilon_0 - T/N_0$ and $\langle \delta n_0^2 \rangle^{1/2} \simeq N_0$. This means a huge fluctuation of particle number $\delta N \sim N$ at $T \ll T_0$, an unrealistic property of the model.[17]

In a canonical ensemble, which better fits to experiments with dilute gases in traps, the average value of the condensate population is given by

$$\langle n_0 \rangle = \frac{\sum_{n_0=0}^{N} n_0 \sum_{\{n_\alpha\}'} e^{-\beta \sum_{\alpha>0}(\varepsilon_\alpha - \varepsilon_0) n_\alpha} \delta_{\sum_{\alpha>0} n_\alpha,\ N-n_0}}{\sum_{n_0=0}^{N} \sum_{\{n_\alpha\}'} e^{-\beta \sum_{\alpha>0}(\varepsilon_\alpha - \varepsilon_0) n_\alpha} \delta_{\sum_{\alpha>0} n_\alpha,\ N-n_0}}, \quad (16)$$

where $\{n_\alpha\}'$ stands for a collection of all state numbers except n_0, and $\beta = 1/T$. The average over such states does not fluctuate strongly and therefore can be replaced by its grand canonical value corresponding to an appropriate choice of chemical potential $\mu = \mu_{N-n_0}$. We thus get

$$\langle n_0 \rangle \cong \frac{\sum_{n_0=0}^{N} n_0 Z_{N-n_0}}{\sum_{n_0=0}^{N} Z_{N-n_0}}, \quad (17)$$

where $Z_n = e^{-\beta \Omega_n}$, and Ω_n is the thermodynamic potential of the grand canonical ensemble.[1]

The quantity $Z_n = e^{-\beta N}$ is not exponentially small for a number of particles n smaller than the Bose-condensate fraction, $n < N_0$. Therefore, we can change expression (17) to

$$\langle n_0 \rangle \cong \frac{\sum_{n_0=N_0}^{N} n_0 e^{-\beta \Omega_{N-n_0}}}{\sum_{n_0=N_0}^{N} e^{-\beta \Omega_{N-n_0}}}. \quad (18)$$

The quantity Ω_n is strongly peaked at $n = N_0$, thus giving $\langle n_0 \rangle \simeq N_0$ and, similarly, $\langle \delta n_0^2 \rangle^{1/2} \sim \sqrt{N_0}$ rather than $\langle \delta n_0^2 \rangle^{1/2} \sim N_0$ as in the orthodox grand canonical ensemble. Indeed, at $N \ll N_0$ (corresponding to $T \gg T_0$) we obtain for the thermodynamic potential Ω_N a value $\Omega_N \simeq -NT$, and $Z_N \simeq e^N$. This agrees with the conclusion, reached in a different way in Ref. 12, that the thermodynamic properties of a Bose condensate in a trap with fixed total number of particles are very similar to those in the orthodox grand canonical ensemble with a fixed average number of particles. The above results are consistent with a known statement that the Bose-Einstein condensation temperature T_0 is the same in the canonical and in the grand canonical ensembles.[2]

In conclusion, I hope I have met the goal of elucidating in a direct way the properties of the low-temperature state of an ideal Bose gas of finite-size, finite-particle-number systems. I express my deep gratitude to Prof. B. Tanatar for stimulating discussions and help.

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[1] L. D. Landau and E. M. Lifshitz, *Statistical Physics*, Vol. 1, Pergamon, New York (1987).
[2] K. Huang, *Statistical Mechanics*, Wiley, New York (1987).
[3] A. H. Carter, *Classical and Statistical Thermodynamics*, Prentice Hall, New Jersey (2001).
[4] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science **269**, 198 (1995).
[5] K. B. Davis, M. O. Mewes, M. A. Joffe, M. R. Andrews, and W. Keterle, Phys. Rev. Lett. **74**, 5202 (1995).
[6] W. Petrich, M. H. Anderson, J. R. Ensher, and E. A. Cornell, Phys. Rev. Lett. **74**, 3352 (1995).
[7] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringati, Rev. Mod. Phys. **71**, 463 (1999).
[8] W. Ketterle, D. S. Dufree, and D. M. Stamper-Kurn, *Making, Probing and Understanding Bose-Einstein Condensates*, Preprint xxx.lanl.gov/abs/cond-mat/9904034 (1999).
[9] E. A. Cornell, J. R. Ensler, and C. E. Wieman, *Experiments in Dilute Atomic Bose-Einstein Condensation*, Preprint xxx.lanl.gov/abs/cond-mat/9903109 (1999).
[10] N. L. Balazs and T. Bergeman, Phys. Rev. A **58**, 2359 (1998).
[11] W. Ketterle and N. J. van Druten, Phys. Rev. A **54**, 656 (1996).
[12] P. Navez, D. Bitouk, M. Gajda, Z. Idziaszek, and K. Rzazewski, Phys. Rev. Lett. **79**, 1789 (1997).
[13] F. Brosens, J. T. Devreese, and L. F. Lemmens, Phys. Rev. E **55**, 6795 (1997).
[14] Y. Castin, J. Dalibard, and C. Cohen-Tannoudji, *Laser Cooling and Trapping of Neutral Atoms*, in *Atoms in Electromagnetic Fields*, edited by C. Cohen-Tannoudji, World Scientific, Singapore (1994).
[15] I. S. Gradsteyn and I. M. Ryzhik, *Tables of Integrals, Sums and Products*, edited by A. Jeffrey, Acad. Press, New York (1994).
[16] E. P. Wigner, Phys. Rev. **40**, 749 (1932).
[17] M. Fierz, Helv. Phys. Acta **29**, 47 (1995).

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