Fizika Nizkikh Temperatur, 2001, v. 27, Nos. 9/10, p. 1179–1182

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

I. O. Kulik*

Department of Physics, Bilkent University, Bilkent, Ankara 06533, Turkey
E-mail: kulik@fen.bilkent.edu.tr

Received May 16, 2001

We show with a direct numerical analysis that a dilute Bose gas in an external potential — which is choosen for simplicity as a radial parabolic well — undergoes at certain temperature T_c a phase transition to a state supporting 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 sharp transition but supports a distribution of radial particle density $\rho(r)$ peacked at $r = 0$ (a real-space condensate) as well as the phase-space Wigner distribution density $W(\mathbf{r}, \mathbf{p})$ peaked at $\mathbf{r} = 0$ and $\mathbf{p} = 0$ below the crossover temperature T_c^* of order of T_c. 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.

PACS: **64.60.–i**

The phenomenon of a Bose–Einstein (BE) condensation (see textbooks, e.g., [1–3]) is manifesting itself in the formation of macroscopic fraction of zero-momentum particles uniformly distributed in a coordinate space. Such transition was recently observed in a 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 and sometimes overlapping with the previous theoretical works on the subject [10–13] that Bose gas in an external confining potential condenses at low temperature to the position of minimum of the potential energy; the particles of that «condensate» have also zero kinetic energy. Quantization of particle states in a well makes the real-space condensation a continuous transition rather than the phase transition but still supports macroscopic fraction of particles near the origin of the coordinate space below the 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 an evaporative cooling [11]. Bose gas in a trap may be considered interacting with two thermal reservoirs, the first one representing the thermal environement (walls, blackbody radiation at temperature T_1) and second one the optical molasses at temperature $T_2 << T_1$. 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

* Also at: B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, 47 Lenin. Ave., Kharkov 61103, Ukraine

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

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

In a semiclassical approximation, particle energy is

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

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

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

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

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

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

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

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

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

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

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

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

Of course, the $\mathbf{r} = 0$, $\mathbf{p} = 0$ state is not allowed quantum-mechanically, and the derivation leading to Eqs. (6), (7) needs a change. 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

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

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 $T = 0$ ($\mu_0 = 3/2\ \hbar\Omega$).

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 practically zero value below that temperature. The value of T_c^* is very near to T_{c0} at large number of particles, $N >> 1$.

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

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

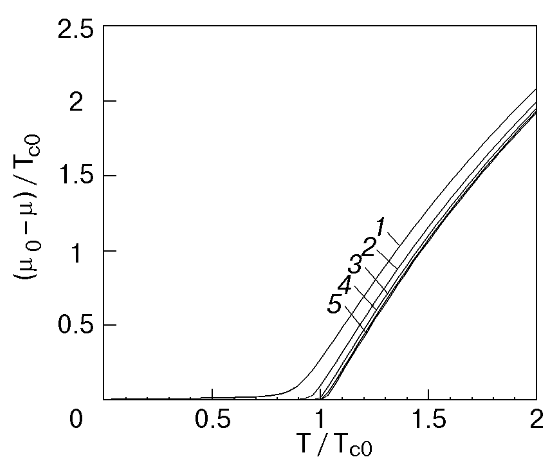

Fig. 1. Chemical potential vs temperature for various values of N: 10^2 (*1*), 10^3 (*2*), 10^4 (*3*), 10^5 (*4*), 10^6 (*5*).

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

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

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 its amplitude as temperature decreases, the real-space condensate. Formation of such condensate is even more explicit in the evolution of the z-projected density distribution, Fig. 3, as temperature reduces 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]) is attaining a value

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

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

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

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

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

$$\bar{n} \sim N/\bar{r}^3 , \text{ where } \bar{r} = \left(\frac{T}{m\Omega}\right)^{1/2} \sim r_0 N^{1/6} (T/T_0)^{1/2} . \quad (15)$$

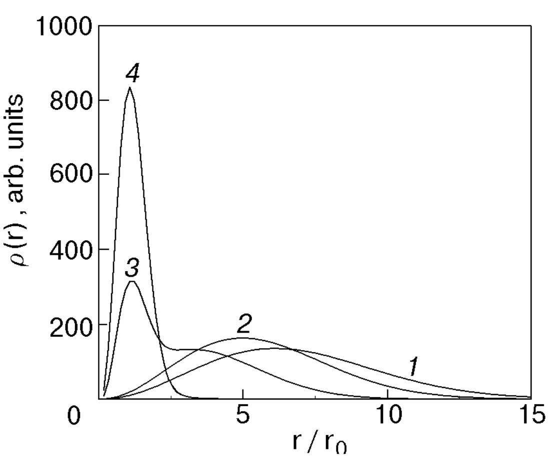

Fig. 2. Radial density distribution $\rho(r) = 4\pi r^2 n(r)$ for $N = 1000$ and various temperatures: $T/T_{co} = 0.2$ (*1*), 0.8 (*2*), 1.4 (*3*), 2.0 (*4*).

$\bar{r}$ is a confinement radius (mean radius of gaseous cloud). It relates to the minimal quantum radius r_0 according to $\bar{r} \sim r_0 N^{1/6} (T/T_c)^{1/2}$. By putting $T \sim T_c^*$ as defined above we receive T of the order of the BE condensation temperature (14). Therefore, the phenomenon we discussing is just the BE condensation mechanism [1]. Except that, in a trap the condensation occurs both in the momentum and in the coordinate spaces or, if we choose to explore the behavior of the dilute low-temperature Bose gas in a real space, it will condense there making a high-density globular fraction coexisting with the spatially dispersed «excitations» in the region of size comparable to the thermal confinement radius $\bar{r}$.

In the grand canonical ensemble which we sofar have been considering, the number of particle 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 receive $\mu \simeq \simeq \varepsilon_0 - T/N_0$ and $\langle \delta n_0^2 \rangle^{1/2} \simeq N_0$. This means huge fluctuation of particle number $\delta N \sim N$ at $T << T_0$, an unrealistic property of the model [17].

In a canonical ensemble, which better fits to experiments with dilute gases in traps, average value of 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 $\{n_\alpha\}'$ means collection of all state numbers except n_0, $\beta = 1/T$. The average over such states

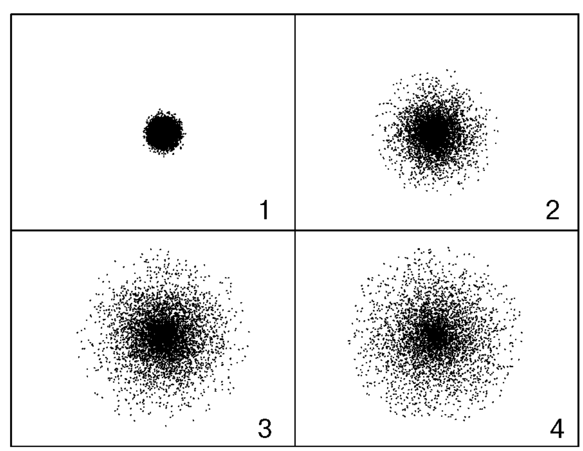

Fig. 3. Side view of particle distribution: *1* — $T = 0.2\,T_{c0}$, *2* — $T = 0.8\,T_{c0}$, *3* — $T = 1.4\,T_{c0}$, *4* — $T = 2.0\,T_{c0}$.

does not strongly fluctuates and therefore can be substituted with its grand canonical value corresponding to an appropriate choice of chemical potential $\mu = \mu_{N-n_0}$. Therefore we receive

$$\langle n_0 \rangle \cong \frac{\sum\limits_{n_0=0}^{N} n_0 Z_{N-n_0}}{\sum\limits_{n_0=0}^{N} Z_{N-n_0}} , \qquad (17)$$

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

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

$$\langle n_0 \rangle \cong \frac{\sum\limits_{n_0=N_0}^{N} n_0 \, e^{-\beta\Omega_{N-n_0}}}{\sum\limits_{n_0=N_0}^{N} e^{-\beta\Omega_{N-n_0}}} . \qquad (18)$$

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 $N << N_0$ (corresponding to $T >> T_0$), we receive for the thermodynamic potential Ω_N a value $\Omega_N \simeq -N T$ and $Z_N \simeq e^N$. This agrees with a conclusion reached in a different way in Ref. 12 that the thermodynamic properties of 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 same in the canonical and in the grand canonical ensembles [2].

In conclusion, I hope I reached the purpose of elucidating in a direct way the properties of 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.

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.* **A58**, 2359 (1998).
11. W. Ketterle and N. J. van Druten, *Phys. Rev.* **A54**, 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.* **E55**, 6795 (1997).
14. Y. Castin, J. Dalibard, and C. Cohen-Tannoudji, *Laser Cooling and Trapping of Neutral Atoms*, in: Atoms in Electromagnetic Fields, C. Cohen-Tannoudji (ed.), World Scientific, Singapore (1994).
15. I. S. Gradsteyn and I. M. Ryzhik, *Tables of Integrals, Sums and Products*, A. Jeffrey (ed.), Acad. Press, New York (1994).
16. E. P. Wigner, *Phys. Rev.* **40**, 749 (1932).
17. M. Fierz, *Helv. Phys. Acta* **29**, 47 (1995).