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

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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 environment (walls, blackbody radiation at temperature \( T_1 \)) and second one the optical molasses at temperature \( T_2 \ll T_1 \). The equilibrium distribution of particles \( f(p, \mathbf{r}, t) \) can be obtained by solving the Boltzmann kinetic equation

\[
\frac{df}{dt} = \mathcal{I}_1 \{ f \} + \mathcal{I}_2 \{ f \},
\]

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

\[
\mathcal{I}_i = -\frac{f_i - \bar{f}_i}{\tau_i},
\]

then the solution for the equilibrium state will be
The relaxation rate $\tau_2^{-1}$ is proportional to the laser intensity $P$. At large intensity, assuming $\tau_2^{-1} \gg \tau_1^{-1}$, Eq. (3) gives $f = f_2^0$.

In a semiclassical approximation, particle energy is

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

(4)

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

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

(5)

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

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

(6)

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

$$
N = \frac{(4\pi)^2}{(2\pi \hbar)^3} (2mT)^{3/2} \left(\frac{2T}{m\Omega^2}\right)^{3/2} \times
$$

$$
\times \int_0^\infty x^2 \, dx \int_0^\infty y^2 \, dy \, \frac{1}{e^{x^2 + y^2} - 1},
$$

(7)

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

At low temperature, no nonzero value of $\zeta$ can satisfy Eq. (7). It therefore vanishes at temperature $T = T_{c_0}$ determined from the condition $\zeta = 0$ thus giving

$$
T_{c_0} = \hbar \Omega (N/\zeta(3))^{1/3} = 0.94 \hbar \Omega N^{1/3},
$$

(8)

where $\zeta(z)$ is the Riemann zeta function. Below $T_{c_0}$, $\zeta$ remains equal to zero with the total number of particles $N_0$ having both $r = 0$ and $p = 0$ values, determined from

$$
N_0 = \left(1 - \frac{T^3}{T_{c_0}^3}\right) N.
$$

(9)

Of course, the $r = 0$, $p = 0$ 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

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

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

$$
N = \sum_{n=0}^\infty \frac{S_n}{\eta^{n/2} - 1}
$$

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

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 $T_{c_0}$ 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

$$
\sum_{n_1 + n_2 + \ldots + n_m = n} r^{n_1 + n_2 + \ldots + n_m} = \prod_{k=1}^m \frac{H_{n_k}^2(x_k)}{2^{n_k} n_k!} =
$$

$$
= \sum_{m=0}^n \frac{1}{2^m m!} H_m^2 \left(\sum_{k=1}^r x_k^2 \right)^{m/2}
$$

(11)

![Fig. 1. Chemical potential vs temperature for various values of $N$: $10^6$ (1), $10^7$ (2), $10^8$ (3), $10^9$ (4), $10^{10}$ (5).](image)
where \( r_m = 1 \) at \( m \) even and \( r_m = 0 \) at \( m \) odd, we receive by putting \( r = 3 \)

\[
n(r) = e^{-r^2} \sum_{m=0}^{\infty} \frac{H_m^2(r)}{2^m m!} \sum_{k=0}^{\infty} \frac{1}{\eta e^{(m+2k)x} - 1}.
\]

(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 \( T_c^* \).

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

\[
W(p, r) = \frac{N_0}{\pi r_0^2} e^{-p^2 r_0^2} e^{-r^2 / r_0^2},
\]

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]

\[
T_0 = \frac{\hbar^2}{m n^2 / 3}.
\]

(14)

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

\[
\bar{n} \sim N / \bar{r}^3,
\]

where \( \bar{r} = \left( \frac{T}{m \Omega} \right)^{1/2} \sim r_0 N^{1/6} \left( T / T_0 \right)^{1/2} \).

(15)

\[
\bar{r}
\]

is a confinement radius (mean radius of gaseous cloud). It relates to the minimal quantum radius \( r_0 \) according to \( \bar{r} \sim r_0 N^{1/6} (T / T_0)^{1/2} \). By putting \( T \sim T^* \) 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 \( \alpha \) is \( \langle \delta n_{\alpha}^2 \rangle = n_{\alpha} (n_{\alpha} + 1) \). In a condensate, by putting \( \langle n_{\alpha, q} \rangle = N_0 \) we receive \( \mu = z \varepsilon_0 - T / N_0 \) and \( \langle \delta n_{\alpha}^2 \rangle^{1/2} = N_0 \). This means 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, average value of condensate population is given by

\[
\sum_{n=0}^{N} \sum_{n_{\alpha} = 0}^{N} e^{-\beta \sum_{\alpha} (\varepsilon_{\alpha} - \varepsilon_0) n_{\alpha}} \delta \sum_{\alpha} n_{\alpha}, N - n_{\alpha}
\]

\[
\langle n_{\alpha} \rangle = \sum_{n_{\alpha} = 0}^{N} \sum_{n_{\alpha} = 0}^{N} e^{-\beta \sum_{\alpha} (\varepsilon_{\alpha} - \varepsilon_0) n_{\alpha}} \delta \sum_{\alpha} n_{\alpha}, N - n_{\alpha}
\]

where \( n_{\alpha} \) is collection of all state numbers except \( n_{\alpha} \), \( \beta = 1 / T \). The average over such states
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

$$\langle n'_0 \rangle \equiv \frac{\sum_{n_0=0}^{N} n_0 Z_{N-n_0}}{\sum_{n_0=0}^{N} Z_{N-n_0}} ,$$

(17)

where $Z_n = e^{-\beta \Omega_n}$, $\Omega_n$ 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

$$\langle n'_0 \rangle \equiv \frac{\sum_{n_0=N_0}^{N} n_0 e^{-\beta \Omega_{N-n_0}}}{\sum_{n_0=N_0}^{N} e^{-\beta \Omega_{N-n_0}}} .$$

(18)

The quantity $\Omega_n$ is strongly peaked at $n = N_0$ thus giving $\langle n'_0 \rangle = N_0$ 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 receive for the thermodynamic potential $\Omega_N$ a value $\Omega_N = -N T$ and $Z_N = e^{N}$.

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.