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The distribution function and fluctuations of the number of particles in an ideal Bose gas confined by a trap

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***Abstract*. The distribution function $w_0(n_0)$ of the number n_0 of particles in the condensate of an ideal Bose gas confined by a trap is found. It is shown that at the temperature above the critical one ($T > T_c$) this function has the usual form $w_0(n_0) = (1 - e^{\mu})e^{\mu n_0}$, where μ is the chemical potential in the temperature units. For $T < T_c$, this distribution changes almost in a jump to a Gaussian distribution, which depends on the trap potential only parametrically. The centre of this function shifts to larger values of n_0 with decreasing temperature and its width tends to zero, which corresponds to the suppression of fluctuations.**

Keywords: *Bose – Einstein condensate, distribution function.*

The concept of statistical independence of ensembles of particles occupying different quantum states [1] results in the factorisation of the distribution $W(n_0, n_1, ...)$ of the number n_k of particles in the states with energies $E_0 < E_1 \leqslant E_2 ...$:

$$W(n_0, n_1, ...) = \prod_k w_k(n_k), \quad w_k(n_k) = Q_k e^{(\mu - \varepsilon_k)n_k}, \qquad (1)$$

where $\varepsilon_k = E_k/T$; T is the temperature expressed in energy units; μ is the chemical potential expressed in temperature units; Q_k is the normalising factor [in the notation in formula (37.4) of [1], $Q_k = \exp(\Omega_k/T)$, where Ω_k is the thermodynamic potential]. In the case of the Bose – Einstein statistics, the probability of different values of n_k should be normalised by the condition

$$\sum_{n_k=0}^{N} w_k(n_k) = 1,$$

where N is the total number of gas particles. For $N \to \infty$, this gives

$$w_k(n_k) = (1 - e^{\mu - \varepsilon_k})e^{(\mu - \varepsilon_k)n_k}. \qquad (2)$$

Then, the chemical potential μ is determined by the requirement that a sum of average values

$$\langle n_k \rangle = \tilde{n}_k = \sum_{n_k=0}^{\infty} n_k w_k(n_k)$$

of n_k from (1) and (2) would be equal to the total number N of particles:

$$\sum_k \tilde{n}_k = N, \quad \tilde{n}_k = (e^{\varepsilon_k - \mu} - 1)^{-1}. \qquad (3)$$

The energy E_k can be measured from the ground-state energy. In this case, $\varepsilon_0 = 0$, and we obtain from (2) and (3)

$$w_0(n_0) = (1 - e^{\mu})e^{\mu n_0}, \quad \tilde{n}_0 = (e^{-\mu} - 1)^{-1}. \qquad (4)$$

At low temperature, at least for a system with a discrete spectrum, the distribution (1), (2) becomes inherently contradictory. For $T \to 0$, we obtain $\varepsilon_{k\neq0} \to \infty$ and $\tilde{n}_{k\neq0} \to 0$. This means that for $T = 0$, all the particles should be definitely found in the ground state, i. e., the distribution of the number of particles in the ground state should have the form

$$w_0(n_0) = \delta_{n_0,N}, \quad T = 0. \qquad (5)$$

In this case, however, it follows from (3) and (4) that $\tilde{n}_0 = N$, $\mu = -\ln(1 + 1/N) \simeq -1/N$, and the distribution takes the form

$$w_0(n_0) = N^{-1}e^{-n_0/N}, \qquad (6)$$

which drastically differs from (5). This results in the fluctuation catastrophe, which has been discussed in paper [2] irrespectively of the contradiction between (5) and (6). From Eqns (1) and (2) follows the known expression for the root-mean-square fluctuation $\langle \Delta n_k^2 \rangle = \tilde{n}_k(\tilde{n}_k + 1)$ (see [1], § 113), which yields certainly the incorrect result $\langle \Delta n_0^2 \rangle = N(N + 1)$ for $T = 0$, when $\tilde{n}_0 = N$.

In this paper, it will be shown that Eqns (1) and (2) correctly describe the distribution of the number of particles only in excited states. The distribution (4) of the number of particles in the ground state is valid only at temperatures above the critical temperature T_c, when $\langle n_0 \rangle \ll N$. For $T < T_c$, this distribution changes, and for a system with a discrete spectrum (gas in a trap) it takes a Gaussian shape. In this case, the fluctuation catastrophe is eliminated. In fact, this change in the distribution is caused by the necessity of the fulfilment of the exact relation

$$\sum_k n_k = N, \qquad (7)$$

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rather than expression (3), which is valid only for average values. This circumstance becomes substantial at $T < T_c$ and results in the statistical dependence of ensembles of particles occupying different quantum states.

The distribution function $w_0(n_0)$ is obtained by summing the Gibbs distribution

$$w_0(n_0) = \sum_{n_1+n_2+...=N-n_0} W(n_0, n_1, ...)$$
$$= S^{-1} \sum_{n_1+n_2+...=N-n_0} e^{-\varepsilon_0 n_0 - \varepsilon_1 n_1 - ...}, \quad (8)$$

where S is a normalising factor. The summation in (8) is performed over all positive n_1, n_2, ... satisfying the condition (7). This condition can be satisfied automatically if the sum in (8) is written in the form

$$w_0(n_0) = S^{-1} e^{-\varepsilon_0 n_0} \sum_{n_1, n_2 ...} e^{-\varepsilon_1 n_1 - \varepsilon_2 n_2 - ...}$$
$$\times \frac{1}{2\pi i} \oint z^{(-N+n_0-1)+n_1+n_2+...} dz. \quad (9)$$

The integration contour in (9) is a circle with a centre at the point $z = 0$. Only when the condition (7) is satisfied, the integrand in (9) has a simple pole and the integral is equal to $2\pi i$. In other cases, the integral is zero, which allows one to perform summation over all positive n_1, n_2, ... in (9) without any restrictions; only the convergence of all the sums appearing should be provided. This will be satisfied if the radius of the circle, which can be conveniently written in the form $|z| = e^{\mu}$, is limited by the condition $e^{\mu-\varepsilon_0} < 1$. After that, we can set $\varepsilon_0 = 0$ and require the fulfilment of the condition $\mu < 0$.

The summation in (9) gives

$$w_0(n_0) = S^{-1} \frac{1}{2\pi i} \oint z^{-N+n_0-1} e^{G(z)} dz, \quad (10)$$

$$e^{G(z)} = \prod_{k \neq 0} (1 - z e^{-\varepsilon_k})^{-1}, \quad G(z) = -\sum_{k \neq 0} \ln(1 - z e^{-\varepsilon_k}).$$

The function $G(z)$ inside the circle $|z| = e^{\mu} < 1$ has no singularities, so that $w_0(n_0 = N) = S^{-1} e^{G(0)} = S^{-1}$. For $n_0 = N - 1$, we obtain that the probability

$$w_0(n_0 = N-1) = S^{-1} \left(\frac{d}{dz} e^{G(z)} \right)_{z=0} = S^{-1} \sum_{k \neq 0} e^{-\varepsilon_k}$$

at $T \to 0$ is exponentially small and decreases with further decreasing n_0. This means that at $T \to 0$, we may restrict ourselves to two quantities

$$w_0(n_0 = N) = 1 - \sum_{k \neq 0} e^{-\varepsilon_k}, \quad w_0(n_0 = N-1) = \sum_{k \neq 0} e^{-\varepsilon_k}. \quad (11)$$

For $T = 0$, we obtain expression (5) from (11). It is natural that the fluctuation corresponding to (5) is $\langle \Delta n_0^2 \rangle = 0$.

The quantities $\varepsilon_{k \neq 0}$ decrease with increasing temperature, and it becomes impossible to obtain the distribution by such a simple method. For this reason, we proceed as follows. Having made the change of variables $z = e^{\mu + ix}$ in (10), we obtain

$$w_0(n_0) = S^{-1} e^{\mu n_0} \int_{-\pi}^{\pi} e^{-i(N-n_0)x + F(x)} dx,$$

$$F(x) = -\sum_{k \neq 0} \ln(1 - e^{\mu + ix - \varepsilon_k}). \quad (12)$$

We omitted in (12) all the factors independent of n_0, which are included in the normalisation S determined by the relation (12) itself.

The three first terms of the expansion of the function $F(x)$ have the form

$$F(x) = F(0) + iAx - Dx^2, \quad (13)$$

where

$$F(0) = -\sum_{k \neq 0} \ln(1 - e^{\mu - \varepsilon_k}); \; A = \sum_{k \neq 0} \tilde{n}_k; \; D = \frac{1}{2} \sum_{k \neq 0} (\tilde{n}_k + \tilde{n}_k^2).$$

The first term of this expansion enters into the normalisation after the substitution into (12) and can be omitted.

Let us now choose a parameter μ by requiring the fulfilment of the condition

$$A = \sum_{k \neq 0} \tilde{n}_k = N - \tilde{n}_0, \quad (14)$$

which coincides with (3), and consider the temperature dependences of A and D.

For $T \to 0$, we obtain $\varepsilon_{k \neq 0} \to \infty$, from which it follows that $\tilde{n}_{k \neq 0} \to 0$, $\tilde{n}_0 \to N$, $\mu \to -1/N$, so that $A \to 0$ and $D \to 0$. As temperature increases, the values of $\varepsilon_{k \neq 0}$ decrease, whereas the values of $\tilde{n}_{k \neq 0}$ and, hence, A and D increase, and for $T > T_*$ (where T_* is a characteristic temperature, which depends on the number N of particles and the trap potential) these quantities become of the order of N, i. e., very large. It is important that, if the number N of particles is large, the values of A and D are already very large when $\tilde{n}_0 = N - A$ is still very close to N, while $\mu = -1/\tilde{n}_0$ is still very small, i. e., the temperature T_* is certainly far less than the critical temperature (for example, for $N = 1000$ and $A = 100$, $D \geqslant 50$, we obtain $\tilde{n}_0 = 900$).

As temperature further increases, the values of $\varepsilon_{k \neq 0}$ continue to decrease, and the condition (14) can be fulfilled only at sufficiently large values of $|\mu|$. In this case, the value of $\tilde{n}_0$ becomes small, i. e., the condensate fraction disappears and A and D reach their maximum values $A = N$ and $D \geqslant N/2$.

Therefore, beginning from temperatures $T > T_*$, which are still much lower than the critical temperature, the real part of $F(x)$ becomes large already at $|x| \ll 1$. This allows one to substitute the expansion (13) into (12) and to tend the limits of integration to infinity. Taking into account (14), we obtain

$$w_0(n_0) = S^{-1} e^{\mu n_0} e^{-(n_0 - \tilde{n}_0)^2 / 4D}, \quad \mu = -\ln(1 + 1/\tilde{n}_0). \quad (15)$$

The distribution (15) has a universal form because it depends on the trap potential and the number N of particles only via the parameters $\tilde{n}_0$ and D appearing in it. This distribution has qualitatively different form for large and small $\tilde{n}_0$, i. e., at temperatures above and below the critical temperature.

In a broad temperature range below the critical temperature, when the conditions

$$\tilde{n}_0^2 \gg D, \quad N - \tilde{n}_0 \gg 1, \quad (16)$$

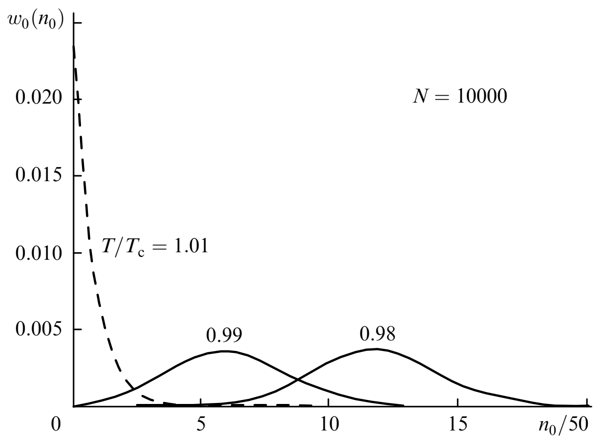

Figure 1. Distribution function (15) of the number of particles in a Bose-gas condensate confined by a trap at different temperatures and $N = 10000$. The quantities $\tilde{n}_0$ and D are calculated from formula (17).

are satisfied, the distribution function (15) is exponentially small at two extreme points $n_0 = N$ and $n_0 = 0$ [the second inequality is equivalent to the condition $D \gg 1$ and simultaneously provides the validity of (15)], i.e., it has in fact a Gaussian shape. As temperature decreases, $\tilde{n}_0$ increases, D decreases, the distribution (15) narrows down, and its centre shifts to larger values of n_0. In the calculation of the statistical sum S, we can pass from summation to integration with infinite limits, which gives $S = 2\sqrt{\pi D}\exp(\mu n_0 + \mu^2 D)$, $\mu = -1/\tilde{n}_0$. The calculation of the average values is reduced to the differentiation of S with respect to μ, and we find the average number of particles in the condensate $\langle n_0 \rangle = \tilde{n}_0(1 - 2D/\tilde{n}_0^2)$, which weakly differs from $\tilde{n}_0$ (but does not coincide with it), and the root-mean-square fluctuation $\langle \Delta n_0^2 \rangle = 2D$, which decreases along with D with decreasing temperature.

As temperature increases, $\tilde{n}_0$ also decreases, the first of the conditions (16) is no longer satisfied, and the distribution (15) presses itself increasingly to its left boundary $n_0 = 0$. Finally, for $n_0 \ll D$ (however, the condition $\tilde{n}_0 \gg 1$ can be still valid), the factor $e^{\mu n_0}$ becomes dominant in the distribution (15), and this distribution takes the form (4).

Similarly to (10), the joint distribution

$$w_{0,i\neq 0}(n_0, n_i) =$$
$$S^{-1} e^{-\varepsilon_i n_i} \frac{1}{2\pi i} \oint z^{-N-1+n_0+n_i} e^{G(x)} (1 - z e^{-\varepsilon_i}) dz.$$

can be written. Having performed the same transformations as in deriving (15), we find that the distribution function

$$w_{i\neq 0} = \sum_{n_0=0}^{N} w_{0,i\neq 0}(n_0, n_i)$$

of the excited particles coincides with (1), (2) at all temperatures.

In the case of a parabolic trap at the temperature $T_* < T < T_c + \Delta T$, where $T_* = T_c N^{-1/3}$ and $\Delta T \ll T_c$, the quantities $\tilde{n}_0$ and D can be calculated exactly [3]:

$$\tilde{n}_0 = \frac{1}{2} N \Big\{ 1 - t^3 + [(1 - t^3)^2 + 4\gamma t^3/N]^{1/2} \Big\},$$

$$D = \gamma t^3 N/2, \quad t = T/T_c, \quad \gamma \simeq 1.37. \tag{17}$$

One can see from (17) that in this case, the distribution (15) changes its Gaussian shape to the form (4) in a narrow vicinity of the critical temperature $|T - T_c| \leqslant 1/\sqrt{N}$, i.e., for large N, virtually in a jump. It is shown [4] that this transition is accompanied by a jump in the heat capacity by $\Delta(dE/dT) \simeq -6.75N$. Fig. 1 shows a qualitative change in the shape of the distribution function (15) in the vicinity of the critical temperature.

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