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BOSE–EINSTEIN CONDENSATION OF NONINTERACTING FREE OR TRAPPED PARTICLES: A COMMON TREATMENT OF THE BOTH THEORIES*

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The Bose–Einstein condensation of noninteracting identical particles is investigated, both in the case of free gas in a box, and the trapped particles confined in a harmonic potential. The importance of the low temperature behavior of the exact single-particle canonical partition function is pointed out. The elementary proof of the phase-transition in the thermodynamical limit is presented.

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The developments on Bose–Einstein condensation (BEC) in trapped atoms [1] allow us to reconsider the general idea of BEC phenomenon, in order to discuss some distinction with the former theory of free particles in a box [2, 3], which is reflected by a different meaning of thermodynamical limit in both cases. The behavior of finite system of particles in a confining harmonic potential looks qualitatively similar to that of the free gas in a box, in a sense that the rapid increase of the ground state occupation is experimentally [4] observed, in agreement with theoretical predictions [5–7], when the temperature becomes sufficiently low. This is accompanied by other pre-transition effects, *e.g.*, by an appearance of a maximum in the specific heat (*versus* temperature), which may be used to identify the temperature at which BEC occurs for finite system [7]. The standard continuous version of both theories predicts (under certain conditions) the true phase-transition [3, 5], however the corresponding thermodynamical limits are different (it is not still the average density constant, in the case of trapped particles [1, 5, 6]).

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In fact the source of any distinction between theories of the same set of identical noninteracting particles in equilibrium is the single-particle canonical partition function. Within grand canonical ensemble approach (for its general use and application to the fermions system see Ref. [8] of this issue) it is visualized by the structure of most important relations [3]

$$N\ [\log \Xi]\ = \sum_{j=1}^{\infty} (\pm)^{j+1} z^j Z_1(\beta j)\ \left[\times j^{-1}\right]\,, \tag{1}$$

where Ξ and Z_1 are appropriate partition functions and the fugacity z is determined by the (average) number of particles N ($\pm$ is for bosons or fermions, respectively). Because of a separation (with respect to the dimension coordinates) of both canonical partition functions of interest [2,3,6,7] it is sufficient to consider the one-dimensional case only. The partition functions are

$$Z_1 = \sum_{n=-\infty}^{+\infty} e^{-\pi \frac{\lambda^2}{L^2} n^2} \equiv \vartheta\left(\lambda^2/L^2\right)\,, \tag{2}$$

— where L is a size of a one dimensional box (length), $\lambda = \sqrt{\beta h^2/2\pi m}$ is a thermal wavelength, and where the ϑ, defined by Eq. (2), is the Jacobi theta-function (see, *e.g.*, [2,9]) of a heat conductance (and also elliptic functions) theory — and

$$Z_1 = \sum_{n=0}^{+\infty} e^{-\beta h f n} = \frac{1}{1-e^{-\beta h f}} \equiv \chi(\beta h f)\,, \tag{3}$$

where f is a frequency related to the harmonic trap [1, 5–7]; respectively. Both $\vartheta(x^2)$ and $\chi(x)$ considered as functions of variable x diverges (like x^{-1}) if $x \to 0$, both monotonically decrease with x, rapidly approaching unity for $1 < x \to \infty$. Both, what seems important in the present context, exhibit a typical for the transition phenomena different *scaling* behavior from both sides of the "critical" value $x = 1$. The last is evident for χ and in the case of Jacobi function is reflected by functional equation [2]

$$\vartheta(\omega) = \omega^{-1/2}\vartheta\left(\omega^{-1}\right)\,. \tag{4}$$

The physical meaning of the transition (at unity) is evident in the case of free quantum particle (in d-dimensional box), allowing the analysis of some details of the standard thermodynamical limit procedure [3]

$$\sum_{\vec{p}} \longrightarrow h^{-d}\int d^d x d^d p = h^{-d} V \int_{-\infty}^{+\infty} d^d p\,. \tag{5}$$

In fact, writing the partition function

$$Z_1(V,T) = \vartheta^d(\lambda^2/L^2) = \frac{(2\pi mkT)^{d/2}V}{h^d}\vartheta^d\left(\bar{L}^2\right) , \tag{6}$$

where the volume $V = L^d$ and $\bar{L} = L/\lambda$ is a dimensionless length in the thermal wavelength units, we immediately see that (5) is equivalent to the assumption that $\vartheta(\bar{L}^2) \approx 1$. Because of the extraordinary fast (Gaussian-type) convergence of Jacobi series the last condition means practically $\bar{L} \geq 1$, or *length* $\geq$ *thermal wavelength*, which is the ordinary limitation of continuous theory approximation. The corresponding canonical density distribution is of course $\rho(\vec{x},\vec{p}) = e^{-\beta\vec{p}^2/2m}$. However, in the opposite case, $\bar{L} \leq 1$, the density distribution becomes (on the same very fast manner) $\rho(\vec{x},\vec{p}) = \delta^d(\vec{p})$, representing the condensed (BEC) phase.

Because $\vartheta(x^2)$ and $\chi(x)$ do not look differ much, maybe except for some vicinity of unity, where the relative difference does not exceed 50% [the maximum is for $x \approx 0.95$, where $[\chi(x) - \vartheta(x^2)]/\vartheta(x^2) \approx 0.46$], one could expect that for the appropriate choice of parameters both theories lead to comparable results. However, equating the proper quantities in (2) and (3), $\lambda/L = \beta hf$, we obtain $L = f^{-1}\sqrt{kT/2\pi m}$, so the physical size of a box (of the old theory) becomes dependent on temperature. Thus thermodynamical limit is no longer possible, unless $f = f(T) \propto T^{1/2}$. And the latter was not a case of both experimental [4] and theoretical study (the frequency of a trap was constant). On the other hand by forcing the temperature independent relation $L^2 = \hbar/(mf)$ or, equivalently, $\bar{L}^2 = (\beta hf)^{-1}$ we get canonical partition function (2) $\vartheta(\beta hf) = (\beta hf)^{-1/2}\vartheta(\bar{L}^2) \propto (\beta hf)^{-1/2}$ having the different asymptotic than $\chi(\beta hf) \propto (\beta hf)^{-1}$. Thus the similar predictions of both theories cannot be any way expected. The reasoning above gives therefore simple explanation why the thermodynamical limit properties of one theory cannot be deduced from the corresponding properties of other theory.

Let us finally present an *elementary* proof of BEC for free noninteracting N particles in d-dimensional box of a length L. Using Eq. (1) and denoting $z = e^{-\nu}$ the equation for particles balance is

$$1 = \frac{1}{N}\sum_{j=1}^{\infty} e^{-\nu j}\vartheta^d\left(j/\bar{L}^2\right) . \tag{7}$$

The point is that, irrespectively on how high the temperature is, formally *almost all* terms in (7) represent the contribution from condensed phase (the argument of each ϑ with $j > \bar{L}^2$ exceeds the unity). In order to perform the thermodynamical limit rigorously we must divide the sum (7) into two parts, say, from $j = 1$ to $M - 1$, and for $j \geq M$, where $M = M(\bar{L})$, and $M \to \infty$ slower than $\bar{L}^2$. It appears further that it is convenient to choose the asymptotic of the form

$$M\left(\bar{L}\right) \sim \bar{L}^2/\epsilon(\bar{L})\,, \tag{8}$$

where $\epsilon(L)$ is a very slowly divergent in infinity, *e.g.*, like

$$\epsilon(\bar{L}) \sim \log\left(\log \ldots \log(\bar{L}) \ldots\right)\,.$$

Then, we can apply the thermodynamical limit [3]

$$N/\bar{L}^d \equiv \lambda^d N/V = \rho\lambda^d \equiv \xi\,, \qquad L \to \infty \tag{9}$$

to the first sum and write the Eq. (7) as

$$\xi = \sum_{j=1}^{\infty} \frac{e^{-\nu j}}{j^{d/2}} + \lim_{\bar{L}\to\infty} \frac{e^{-\nu(\bar{L})M}}{\bar{L}^d} \sum_{j=0}^{\infty} e^{-\nu(\bar{L})j} \vartheta^d\left([M+j]/\bar{L}^2\right)\,. \tag{10}$$

It is clear that if $\nu = \lim_{\bar{L}\to\infty} \nu(\bar{L}) > 0$, then the limit in Eq. (10) is zero, especially because of the exponential damping ($e^{-\nu M(\bar{L})}$), and thus the standard equation for the fugacity — $\rho\lambda^d = g_{d/2}(z)$ — is obtained. For dimensions $d \leq 2$ the $g_{d/2}(z)$ diverges when $z \to 1$, so the BEC may occur only for $d > 2$. Moreover, the following analysis will show that for $d \leq 2$ it is not possible to get a finite positive contribution from the second part if (anyway) $\nu(\bar{L}) \to 0$. To complete our consideration we should prove that there exists a limit — independent on $M(\bar{L})$ — leading to nonvanishing contribution from the second part of (10), in the case of $\nu(\bar{L}) \to 0$ and $d > 2$. The asymptotic behavior of the form $\nu(\bar{L}) \sim c\bar{L}^{-\gamma}$, where $\gamma \geq 2$, is *a priori* necessary to prevents the exponential decay of the quantity of interest. Then $e^{-\nu(\bar{L})M(\bar{L})} \to 1$, so we consider the expression

$$\lim_{\bar{L}\to\infty} \frac{1}{\bar{L}^d} \sum_{j=0}^{\infty} e^{-c\bar{L}^{-\gamma}j} \vartheta^d\left([M(\bar{L})+j]/\bar{L}^2\right)\,. \tag{11}$$

We divide again the sum into two parts, for $j \in [0, \bar{L}^2\bar{\epsilon}(\bar{L}))$, and for $j \geq \bar{L}^2\bar{\epsilon}(\bar{L})$, where $\bar{\epsilon}$ is similar to ϵ. Then in the second part we may replace all ϑ by $\vartheta(+\infty) = 1$, obtaining

$$\lim_{\bar{L}\to\infty} \frac{1}{\bar{L}^d} \frac{e^{-c\bar{L}^{2-\gamma}\bar{\epsilon}(\bar{L})}}{1 - e^{-c\bar{L}^{-\gamma}}} = \frac{1}{c} \qquad \text{if and only if} \qquad 2 < \gamma = d\,. \tag{12}$$

The first sum contains $\bar{L}^2\bar{\epsilon}(\bar{L})$ summands, each of them is less than the first one $\vartheta^d(M(\bar{L})/\bar{L}^2) \sim \epsilon^{d/2}(\bar{L})$ (see Eqs. (4) and (8)), so the whole expression is evaluated by

$$\bar{L}^{2-d}\epsilon^{d/2}(\bar{L})\bar{\epsilon}(\bar{L}) \to 0 \qquad \text{if} \qquad d > 2\,. \tag{13}$$

This finishes the proof.

Identical consideration with $\bar{L} = (\beta hf)^{-1}$, $\xi = N(\beta hf)^{-d}$, $M(\bar{L}) = \bar{L}/\epsilon(\bar{L})$, and with ϑ replaced by χ leads to

$$\xi = g_d(z) + \lim_{\bar{L}\to\infty} \frac{e^{-\nu(\bar{L})M(\bar{L})}}{\bar{L}^d(1 - e^{-\nu(\bar{L})})}\,, \tag{14}$$

requiring $\nu(\bar{L}) \to c\bar{L}^{-d}$ and $d > 1$ for the occurrence of true phase transition in a trapped gas model. Under such condition the limit in (14) returns $1/c$, as in the previous case. The dimension $d = 2$ or $d = 1$ is critical for BEC phenomenon in infinite system of free or trapped particles, respectively. However the pre-transition effects in finite systems will also be observed in such a case.

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