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METHODOLOGICAL NOTES

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On the Bose – Einstein condensate partition function for an ideal gas

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Contents

Abstract. Recursive approaches determining the canonical ideal Bose gas partition function are reviewed that enable the Bose – Einstein condensate occupation probability to be calculated for a finite number of particles ensemble, where the thermodynamic limit approximation fails. In addition to the earlier known method recursive with respect to the number of particles, an iteration procedure with respect to the number of quantum states is proposed. The efficiency of both methods is demonstrated for an ideal Bose gas in a three-dimensional isotropic harmonic trap.

1. Introduction

As is well known, the formation of the Bose–Einstein condensate (BEC) of an ideal gas as its temperature decreases (or the density increases) was predicted in Albert Einstein's second paper devoted to the quantum theory of a monoatomic ideal gas [1]. This inference was based on the calculation of the average number of particles with a continuous energy distribution. For a temperature below a certain critical (density-dependent) value, it turned out to be less than the given number of particles, and hence Einstein proposed that "...a certain number of molecules make a transition to the first quantum state with zero kinetic energy" [1]. This was actually a brilliant conjecture rather than the result of a systematic proof.

Einstein used a continuous atomic energy distribution, wherein the zero-energy state was not separated from the continuous spectrum. A more rigorous treatment of this issue was given in [2 – 4] for the model of a large canonical ensemble employing the Darwin–Fowler method. Interest in the investigation of condensate properties was rekindled only recently, after it was experimentally obtained in a dilute gas confined in magnetic traps [5, 6]. In these cases, the number of trapped atoms was of the order of $10^3 - 10^6$, which is below the value required for a legitimate treatment of the problem in the thermodynamic limit approximation with the use of the density of states. The thermodynamic functions of these systems are not singular in temperature and the critical temperature is no longer a strictly defined quantity. In this case, we are dealing merely with a temperature interval in which a phase transition occurs.

A substantial improvement in the BEC model with a moderate number of atoms was achieved with taking the discreteness of the energy spectrum of quantum states into account. In addition to the generalization of the Darwin–Fowler method, which applies to the grand canonical ensemble [7–11], the method of the kinetic equation for both microcanonical and canonical ensembles was used [12–17], as was the method of quasiparticles for the canonical ensemble. The latter enabled obtaining approximate analytic expressions for all momenta of the particle number distribution function in the condensate for both an ideal gas and a gas with a weak interparticle interaction [18, 19]. A comprehensive analysis of different methods for studying statistical properties of the Bose–Einstein condensate can be found in [20] and in review [21].

In this paper, which is inherently methodological, we enlarge only on recursive approaches to the calculation of the partition function for the canonical ensemble of an ideal Bose gas; the results of their application are frequently treated as references for more complex models. Along with

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the Landsberg method [22, 23], in which an iterative procedure is used with respect to the number of particles, we propose a method of iterations with respect to the number of states. We simultaneously propose an improvement of Landsberg's method to facilitate its application to ensembles consisting of a larger number of particles and its use in a wider temperature range than was done before. We demonstrate the efficiency of recursion techniques in the example of a Bose gas in a three-dimensional isotropic trap and compare our results with those obtained in the framework of the traditional semiclassical approach for the grand canonical ensemble. The results of precision calculations outlined below allow quantitatively estimating the variation of statistical BEC characteristics with respect to the number of particles in the ensemble. In particular, attention is drawn to the radical change in the variance of the number of BEC particles at near-critical temperatures in comparison with the semiclassical result.

2. Thermodynamic limit for the grand canonical ensemble

The conventional method of investigating the statistical properties of the Bose–Einstein condensate for the grand canonical ensemble relies on the Darwin–Fowler theory. It involves a semiclassical approximation in the thermodynamic limit, which is understood as the possibility of neglecting the discrete energy structure of the system and introducing the density-of-state distribution function.

The probability to find n particles in the same quantum state with an energy E at a temperature T is

$$P_n = \left[1 - \exp\left(-\frac{E-\mu}{k_{\rm B}T}\right)\right] \exp\left[-\frac{(E-\mu)\,n}{k_{\rm B}T}\right], \qquad (1)$$

where $k_{\rm B}$ is the Boltzmann constant and μ is the chemical potential, which is determined from the condition that the total average number of particles in the gas is equal to a given value N. It follows from (1) that the average number of particles in the state under consideration is

$$\bar{n} = \frac{1}{\exp\left[(E-\mu)/k_{\rm B}T\right] - 1}\,. \qquad (2)$$

The average number of particles in the energy interval $(E,\, E + \mathrm{d}E)$ is

$$\mathrm{d}\bar{n} = \frac{F(E)\,\mathrm{d}E}{\exp\left[(E-\mu)/k_{\rm B}T\right] - 1}\,, \qquad (3)$$

where $F(E)$ is the density of states. The chemical potential is determined from the integral relation

$$N = \int_0^\infty \frac{F(E)\,\mathrm{d}E}{\exp\left[(E-\mu)/k_{\rm B}T\right] - 1}\,. \qquad (4)$$

2.1 BEC in a three-dimensional trap

For an isotropic harmonic trap with an eigenfrequency ω, we have $F(E) = (1/2)\,E^2/(\hbar\omega)^3$. We express the energy in units of $\hbar\omega$ and accordingly the temperature in units of $\hbar\omega/k_{\rm B}$ to obtain

$$\mathrm{d}\bar{n} = \frac{1}{2}\,\frac{E^2\,\mathrm{d}E}{\exp\left[(E-\mu)/T\right] - 1}\,. \qquad (5)$$

The equation for the critical temperature $T_{\rm c}$, which follows from the condition $\mu = 0$, takes the form

$$N = \int_0^\infty \frac{1}{2}\,\frac{E^2\,\mathrm{d}E}{\exp(E/T_{\rm c}) - 1} = \frac{T_{\rm c}^3}{2}\int_0^\infty \frac{x^2\,\mathrm{d}x}{\exp(x) - 1} = T_{\rm c}^3\zeta(3)\,, \qquad (6)$$

where $\zeta(3) \approx 1.202$ is the value of the Riemann ζ function at 3. Hence, it follows that

$$T_{\rm c} = \left(\frac{N}{\zeta(3)}\right)^{1/3}. \qquad (7)$$

For $T \leqslant T_{\rm c}$, the average number of particles with a positive energy, i.e., residing outside the condensate, is defined by a formula similar to (6),

$$N_{\rm p} = \int_0^\infty \frac{1}{2}\,\frac{E^2\,\mathrm{d}E}{\exp(E/T) - 1} = T^3\zeta(3)\,. \qquad (8)$$

If the average number of BEC particles is denoted by N_0, it follows from (6) and (8) that

$$\frac{N_0}{N} = \frac{N - N_{\rm p}}{N} = 1 - \frac{T^3}{T_{\rm c}^3}\,. \qquad (9)$$

As is well known, the variance of the number of Bose particles in one state with an energy E is $D(E) = \bar{n}(\bar{n}+1)$.

If it is assumed for an estimate that the variance D_0 of the number of BEC particles is equal to the variance of the number of particles outside the condensate, as should be the case for the canonical ensemble, then this variance can be represented as

$$D_0 = \int_0^\infty \frac{1}{\exp(E/T) - 1}\left(\frac{1}{\exp(E/T) - 1} + 1\right)\frac{1}{2}\,E^2\,\mathrm{d}E$$
$$= \frac{T^3}{2}\int_0^\infty \left(\frac{1}{\exp(x) - 1} + 1\right)\frac{x^2\,\mathrm{d}x}{\exp(x) - 1} \approx 1.645\,T^3. \qquad (10)$$

From (9), we obtain

$$D_0 = 1.369 N\,\frac{T^3}{T_{\rm c}^3} = 1.369(N - N_0)\,. \qquad (11)$$

Hence, it follows that the variance of the number of noncondensed particles is close to the average number of noncondensed particles, and therefore the corresponding particle number probability distribution must be close to the Poisson distribution

$$P_{N-n} = \exp\left[-(N - N_0)\right]\frac{(N - N_0)^{N-n}}{(N-n)!} \qquad (12)$$

or, more precisely, to the Gaussian distribution

$$G_{N-n} = \frac{1}{\sqrt{2\pi D_0}}\exp\left[-\frac{(n - N_0)^2}{2D_0}\right]. \qquad (13)$$

Here, n is the number of particles in the condensate. These distributions simultaneously define the probability of n particles residing in the BEC.

With the aid of formulas (7) and (8), it is possible to estimate the maximal energy value that would yield the accuracy necessary for determining the mean and the variance of the particle number in the BEC. By replacing the infinite upper integration limit with a finite value $E_{\max}$, we obtain

$$N_{\mathrm{p}} = \int_0^{E_{\max}} \frac{1}{2}\,\frac{E^2\,\mathrm{d}E}{\exp(E/T) - 1} = \frac{T^3}{2}\int_0^{E_{\max}/T} \frac{x^2\,\mathrm{d}x}{\exp(x) - 1}\,. \quad (14)$$

In view of formula (8), we can say that the relative error of the value of N_{p} is given by the integral

$$\delta = \frac{1}{2\zeta(3)}\int_{E_{\max}/T}^{\infty} \frac{x^2\,\mathrm{d}x}{\exp(x) - 1}\,. \quad (15)$$

Setting, e.g., $E_{\max}/T = 10$, we obtain $\delta \approx 3\times 10^{-3}$. About the same uncertainty is also obtained for the variance in this case.

2.2 Bose gas at above-critical temperatures

At temperatures exceeding the critical one, the chemical potential is nonzero and is determined, as stated above, from condition (4). Introducing the new function $\eta(T) = -\mu/k_{\mathrm{B}}T$, we obtain

$$N = \int \frac{F(E)\,\mathrm{d}E}{\exp(E/k_{\mathrm{B}}T + \eta) - 1} \quad (16)$$

instead of Eqn (4). In particular, for an isotropic harmonic trap, we obtain

$$N = \int_0^{\infty} \frac{1}{2}\,\frac{E^2\,\mathrm{d}E}{\exp(E/T + \eta) - 1}\,. \quad (17)$$

Relation (17) permits expressing the temperature as a function of η:

$$T(\eta) = (2N)^{1/3}\left[\int_0^{\infty} \frac{x^2\,\mathrm{d}x}{\exp(x + \eta) - 1}\right]^{-1/3}. \quad (18)$$

Formula (5), rewritten in the new notation as

$$\mathrm{d}\bar{n} = \frac{1}{2}\,\frac{E^2\,\mathrm{d}E}{\exp\left[E/T(\eta) + \eta\right] - 1}\,, \quad (19)$$

defines the particle energy distribution function at a temperature $T(\eta)$. The parameter η ranges from zero, which corresponds to the critical temperature, to infinity. Before the classical distribution sets in, it is practically sufficient to restrict ourselves to the interval $[0 \ldots 3]$ for η.

We describe the temperature dependence of the heat capacity for a Bose gas confined in a harmonic trap. The internal energy of the gas is represented as

$$U = \int_0^{\infty} \frac{1}{2}\,\frac{E^3\,\mathrm{d}E}{\exp(E/T + \eta) - 1} = \frac{1}{2}\,T^4\int_0^{\infty} \frac{x^3\,\mathrm{d}x}{\exp(x + \eta) - 1}\,. \quad (20)$$

Accordingly, the heat capacity at temperatures $T(\eta) \geqslant T_{\mathrm{c}}$ can be calculated in accordance with the formula

$$C = \frac{\mathrm{d}U}{\mathrm{d}T} = \frac{2T(\eta)^3}{N}\int_0^{\infty} \frac{x^3\,\mathrm{d}x}{\exp(x + \eta) - 1} - \frac{T(\eta)^4}{2N}\left(\frac{\mathrm{d}T}{\mathrm{d}\eta}\right)^{-1}\int_0^{\infty} \frac{x^3\exp(x + \eta)\,\mathrm{d}x}{\left[\exp(x + \eta) - 1\right]^2}\,. \quad (21)$$

At temperatures below the critical one, the expression for the heat capacity corresponds to $\eta = 0$ and takes a simpler form:

$$C = \frac{\mathrm{d}U}{\mathrm{d}T} = 2T^3\int_0^{\infty} \frac{x^3\,\mathrm{d}x}{\exp(x) - 1}\,, \quad (T \leqslant T_{\mathrm{c}})\,. \quad (22)$$

In both expression (21) or (22), the heat capacity is expressed in units of Nk_{B}.

2.3 Incorporating the discreteness of energy levels

Because it has been possible to experimentally obtain the Bose–Einstein condensate of an ideal gas at ultralow temperatures ($T < 10^{-6}$ K), the authors of several papers proposed an improvement in the theory, which reduces to the inclusion of energy level discreteness and to the replacement of the integration over energy by summation over these discrete levels [5, 6, 8, 9, 13, 14]. Then the chemical potential is to be found from the condition

$$N = \sum_{m=0}^{\infty} \frac{g_m}{\exp\left[-(E_m - \mu)/k_{\mathrm{B}}T\right] - 1}\,, \quad (23)$$

which replaces Eqn (4). Here, g_m is the degeneracy of the mth level.

Specifically, it has been possible to effect this improvement for an isotropic harmonic trap. In this case,

$$E_m = \hbar\omega\left(m + \frac{3}{2}\right), \quad (24)$$

$$g_m = \frac{1}{2}\,(m + 1)(m + 2)\,. \quad (25)$$

The probability that n particles are found in one state of the mth level is given by

$$P_n^{(m)} = \frac{\exp\left[-(E_m - \mu)\,n/k_{\mathrm{B}}T\right]}{\sum_{n'=0}^{N}\exp\left[-(E_m - \mu)\,n'/k_{\mathrm{B}}T\right]}\,. \quad (26)$$

Assuming N to be sufficiently large and taking into account that $\mu - E_m < 0$, we can write

$$P_n^{(m)} = \exp\left[\frac{(\mu - E_m)\,n}{T}\right]\left[1 - \exp\left(\frac{\mu - E_m}{T}\right)\right], \quad (27)$$

and for the ground state, in particular,

$$P_n^{(0)} = \exp\left[\frac{(\mu - E_0)\,n}{T}\right]\left[1 - \exp\left(\frac{\mu - E_0}{T}\right)\right]. \quad (28)$$

It follows that the ground-state particle number distribution for the grand canonical ensemble is described by an exponential law. In what follows, we show that this result is significantly different from the corresponding distribution for the canonical ensemble.

3. Recursion techniques for calculating the Bose gas canonical partition function

We now turn to the exact formulation of the problem for the canonical ensemble of an ideal Bose gas consisting of N particles. Each gas particle may reside in one of the single-particle stationary states with discrete energy eigenvalues E_i. For the ideal Bose gas, the total energy $E_{\{n_i\}}$ is the sum of single-particle energies,

$$E_{\{n_i\}} = \sum_i n_i E_i \,, \tag{29}$$

where n_i are the occupation numbers of the single-particle states. The probability that the N-particle system is in the state described by a collection of occupation numbers $\{n_i\}$ is given by

$$P_{\{n_i\}} = \frac{1}{Z_N} \exp\left(-\frac{E_{\{n_i\}}}{k_B T} \right), \tag{30}$$

where Z_N is the partition function of the N-particle system:

$$Z_N = \sum_{\{n_i\}} \exp\left(-\frac{E_{\{n_i\}}}{k_B T} \right), \tag{31}$$

with the summation performed over all combinations of the occupation numbers that satisfy the condition

$$\sum_i n_i = N \,. \tag{32}$$

If our interest is only with the kth single-particle state, the probability of finding n_k particles in it is written as

$$P^{(k)}_{n_k} = \frac{Z^{(k)}_{N-n_k}}{Z_N} \exp\left(-\frac{n_k E_k}{k_B T} \right), \tag{33}$$

where $Z^{(k)}_{N-n_k}$ is the partition function for $N - n_k$ particles, with the kth single-particle state excluded from the sum.

3.1 Iterative procedure with respect to the number of particles

It has been a relatively long time since Landsberg proposed a recursion method for calculating the partition function of a canonical ensemble using iterations with respect to the number of particles [22]. He proposed that the partition function be calculated by a simple algorithm:

$$Z_n = \frac{1}{n} \sum_{p=1}^{n} S_p Z_{n-p} \,, \quad Z_0 = 1 \,, \quad n = 1, 2, \ldots, N \,, \tag{34}$$

where

$$S_p = \sum_j \exp\left(-\frac{pE_j}{k_B T} \right). \tag{35}$$

We note that summation in expression (35) is performed over all single-particle states, and therefore this method is advantageous when the summation can be performed analytically. For instance, for a three-dimensional isotropic harmonic trap,

$$S_p = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \sum_{m_3=0}^{\infty} \exp\left(-p \frac{m_1 + m_2 + m_3}{T} \right) = \frac{1}{\left[1 - \exp(-p/T) \right]^3} \,. \tag{36}$$

Here, we omitted the 'zero' oscillator energy and expressed the temperature in units of $\hbar\omega / k_B$.

To find the particle number distribution in the BEC, it is useful to temporarily exclude the ground state from consideration. We let $\widetilde{Z}_n$ denote the new partition function for n particles. Then

$$P^{(0)}_n = \frac{\widetilde{Z}_{N-n}}{\sum_{p=0}^{N} \widetilde{Z}_{N-p}} = \frac{\widetilde{Z}_{N-n}}{Z_N} \,. \tag{37}$$

Elimination of the ground state is effected by subtracting the first term from S_k. Therefore, $\widetilde{S}_k = S_k - 1$. Then the recurrent relation for $\widetilde{Z}_n$ can be written as

$$\widetilde{Z}_n = \frac{1}{n} \sum_{k=1}^{n} \widetilde{S}_k \widetilde{Z}_{n-k} \,, \quad \widetilde{Z}_0 = 1 \,. \tag{38}$$

We note that $\widetilde{Z}_{N-n} = Z_{N-n} - Z_{N-n-1}$. Hence, $P^{(0)}_n$ can also be represented in the form

$$P^{(0)}_n = \frac{Z_{N-n} - Z_{N-n-1}}{Z_N} \,, \tag{39}$$

as was done in [13].

Landsberg's method was used to calculate the partition function of a Bose gas for systems consisting of a moderate number of particles ($N \leqslant 1000$) at sufficiently low temperatures ($T \leqslant T_c$) [8, 9, 13]. This is because increasing the temperature and the number of particles leads to a rapid loss of accuracy and to an excess over "the largest computer real number." To obviate these computational difficulties, we propose an improvement in the use of the method by performing the normalization of partition functions at each iteration step:

$$Z^{\{0\}}_0 = 1 \,,$$

$$Z^{\{n-1\}}_n = \sum_{p=0}^{n-1} \frac{S_{n-p} \, Z^{\{n-1\}}_p}{n} \,, \quad n = 1, \ldots, N, \tag{40}$$

$$Z^{\{n\}}_k = \frac{Z^{\{n-1\}}_k}{\sum_{p=0}^{n} Z^{\{n-1\}}_p} \,, \quad k = 0, \ldots, n \,.$$

The probability to find n particles in the BEC, which we are concerned with, can be represented in the form

$$P^{(0)}_n = Z^{\{N\}}_{N-n} \,. \tag{41}$$

The partition function of the Bose gas is written as

$$Z_N = Z^{\{N\}}_N \prod_{n=1}^{N} \sum_{p=0}^{n} Z^{\{n-1\}}_p \,.$$

3.2 Iterative procedure with respect to the number of states

Only low-energy states are efficiently populated at low temperatures. We can therefore expect sufficiently exact information about the particle number distribution to be obtainable in this case if we restrict ourselves to a finite number of states. The accuracy of this approximation can be estimated using relation (15).

Let $Z_{m,n}$ denote the partition function with the inclusion of the first $m + 1$ states for a system of n particles. We then have the evident relation

$$Z_{m,n} = \sum_{p=0}^{n} \exp\left(-\frac{E_m p}{k_B T} \right) Z_{m-1,n-p} \,, \quad m \geqslant 1 \,, \tag{42}$$

with

$$Z_{0,n} = \exp\left(-\frac{E_0 n}{k_B T}\right). \tag{43}$$

The ground-state energy E_0 may be set equal to zero. Then $Z_{0,n} = 1$.

To express the probability $P_n^{(k)}$ of finding n particles in the kth state, we must first exclude this state from consideration and calculate the corresponding partition functions $Z_{M,p}^{(k)}$, $p = 0, \ldots, N$, with the aid of recurrent relation (42). Here, M is the greatest number of states included. Then

$$P_{M,n}^{(k)} = \frac{Z_{M,N-n}^{(k)} \exp(-E_k n/k_B T)}{\sum_{p=0}^{N} Z_{M,N-p}^{(k)} \exp(-E_k p/k_B T)}. \tag{44}$$

We return to the Bose gas confined in an isotropic harmonic trap and restrict ourselves to the investigation of ground-state ($k = 0$) statistics. For simplicity of notation, we omit the superscript (0) of the partition function. Formula (42) can be somewhat modified by passing from summation over states to summation over energy levels. The subscript m then labels not states but energy levels. Taking the degeneracy of the energy levels into account, we obtain

$$Z_{m,n} = \sum_{p=0}^{n} C_{p+g_m-1}^{g_m-1} \exp\left(-\frac{mp}{T}\right) Z_{m-1,n-p}, \qquad Z_{0,p} = \delta_{0,p}, \tag{45}$$

where $C_{p+g_m-1}^{g_m-1}$ is the binomial coefficient, equal to the number of partitions of p particles into g_m states of the mth level. As previously, we express the temperature in $\hbar\omega/k_B$ units and omit the 'zero' oscillator energy value, which cancels in the final result.

The probability that the ground state contains n particles at a temperature T can be represented as

$$P_{M,n}(T) = \frac{Z_{M,N-n}}{\sum_{p=0}^{N} Z_{M,N-p}}, \tag{46}$$

where M is the number of the highest level included. Accordingly, the mean number of particles $\bar{n}$ in the ground state and the variance of this quantity are found from the formulas

$$\bar{n} = \sum_{n=0}^{N} n P_n, \quad D = \sum_{n=0}^{N} n^2 P_n - \bar{n}^2. \tag{47}$$

In performing iterations, it is useful to resort to the recurrent formula for the probabilities $P_{m,p}$ implied by Eqns (44) and (45):

$$P_{m,n} = \frac{\sum_{p=0}^{n} C_{p+g_m-1}^{g_m-1} \exp(-mp/T) P_{m-1,p}}{\sum_{n'=0}^{N} \sum_{p=0}^{n'} C_{p+g_m-1}^{g_m-1} \exp(-mp/T) P_{m-1,p}}, \tag{48}$$

where $m = 1, \ldots, M$, $n = 0, \ldots, N$, and $P_{0,n} = \delta_{0,n}$.

We introduce the notation

$$W_{m,n} = \sum_{p=0}^{n} C_{p+g_m-1}^{g_m-1} \exp\left(-\frac{mp}{T}\right) P_{m-1,p}, \tag{49}$$

to finally obtain

$$P_{M,n} = \frac{W_{M,n}}{\sum_{n'=0}^{N} W_{M,n'}}, \tag{50}$$

$$Z_{M,N} = W_{M,N} \prod_{m=1}^{M-1} \sum_{n=0}^{N} W_{m,n}. \tag{51}$$

4. Application of the recursive methods to the BEC in a three-dimensional harmonic trap

Here, we illustrate the application of the recursive methods described above with the example of the canonical ensemble of a Bose gas confined to a three-dimensional isotropic harmonic trap. The results yielded by both methods are indistinguishable in accuracy; we compare them with the corresponding results obtained in the thermodynamic limit (see Section 2) for the grand canonical ensemble. The calculations were performed for ensembles with the number of particles ranging from 10^2 to 10^5.

Figure 1 shows the temperature evolution of the particle number distribution function in the BEC for an ensemble of 1000 atoms with the inclusion of the first 100 energy levels. We recall that the temperature is expressed in units of $\hbar\omega/k_B$, where ω is the eigenfrequency of the harmonic trap. According to the standard theory, it follows from (7) that the critical temperature T_c for such an ensemble is approximately equal to 9.4. It can be seen from Fig. 1 that at temperatures close to the critical one, the distribution decays exponentially with n and centers about zero. As the temperature decreases, the distribution broadens to acquire a bell shape and shifts toward larger particle numbers. As the temperature decreases further, the distribution becomes narrower, to turn into a peak concentrated at the maximum number of particles in the zero-temperature limit.

Figure 2 shows the temperature dependence of the mean number of BEC particles for the same ensemble obtained via two methods: the standard method [with the use of formula (9)] and the recursive one. The difference is more pronounced at temperatures close to the critical one. A

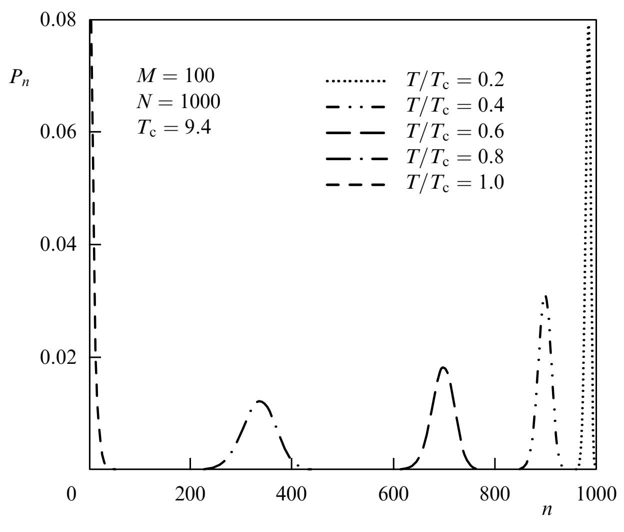

Figure 1. Temperature evolution of the particle number distribution function in the BEC for an ensemble of 1000 Bose particles confined to an isotropic harmonic trap.

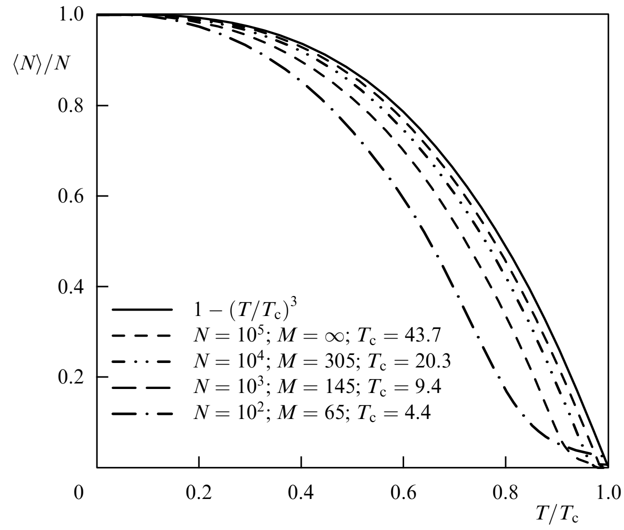

Figure 2. Temperature dependence of the mean number of particles in the BEC for ensembles of 100, 1000, 10,000, and 100,000 particles confined to a three-dimensional isotropic harmonic trap.

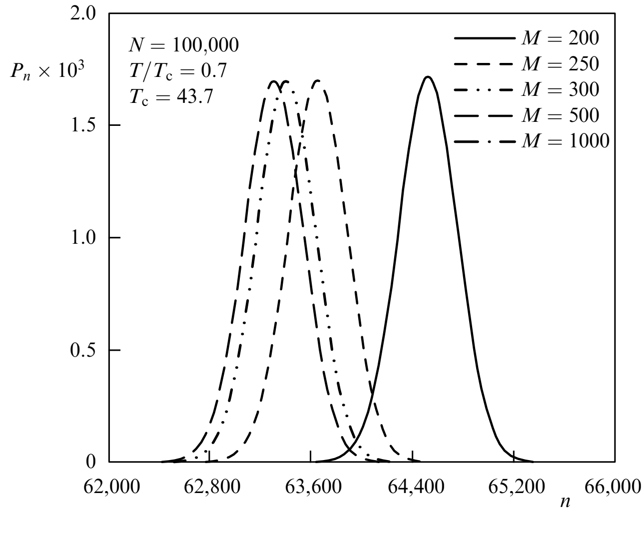

Figure 4. BEC particle-number distribution function for an ensemble of 100,000 particles with the inclusion of different numbers of states.

difference of this kind was previously obtained for a discrete model in Refs [2–4].

The departure of the standard theory from the recursive method is seen much more clearly in the determination of the particle number variance in the vicinity of the critical temperature, as is exemplified by Fig. 3. According to the standard theory, the variance has a maximum at $T \approx T_c$, whereas in reality it is minimal.

To represent the temperature evolution of the particle number distribution in one picture, we selected an ensemble of a moderate number of particles. For a larger number of particles, these distributions would look like very narrow peaks. Separately in Fig. 4 we give the BEC particle number distribution for an ensemble of 10^5 bosons at the temperature $T = 30$. For this number of bosons, $T_c \approx 43.7$. In this picture, we simultaneously demonstrate the accuracy of the recursive method, which depends on the number of states included or on the number of energy levels. We calculated the BEC particle number distributions with the inclusion of 200, 250, 300, 500, and 1000 levels. The last two curves completely merge, and hence the inclusion of 500 levels affords sufficiently high accuracy. According to our estimate (14), $m_{\max} \approx 350$.

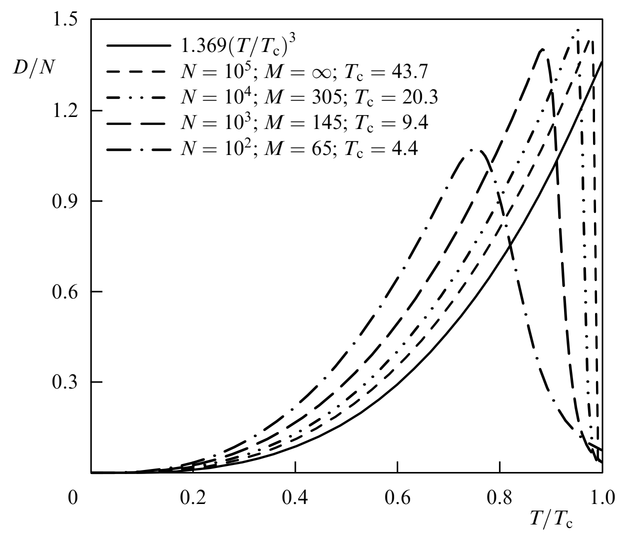

Figure 3. Temperature dependence of the variance of the number of BEC particles for ensembles of 100, 1000, 10,000, and 100,000 particles confined to a three-dimensional isotropic harmonic trap.

Figure 5 gives a comparison of the BEC particle number distribution function with the Poisson and Gauss distributions, Eqns (12) and (13), obtained in the semiclassical theory. As could be expected based on the resultant temperature dependence of the mean number of particles (Fig. 2) and the variance (Fig. 3), the difference between the distributions is most pronounced for temperatures close to the critical one. The semiclassical distributions are narrower and are shifted toward larger particle numbers.

We note that the use of the recursive method is not limited to the below-critical temperature range. The calculation of the partition function of a Bose gas permits calculating the temperature dependence of the thermodynamic system characteristics in a broader temperature domain. In particular, the standard procedure applied to the resultant partition function yields the heat capacity of the Bose gas (in units of $k_B N$)

$$C = \frac{1}{N}\frac{\mathrm{d}}{\mathrm{d}T}\left[T^2\,\frac{\mathrm{d}\ln(Z)}{\mathrm{d}T}\right]. \qquad (52)$$

Figure 6 shows the temperature dependence of the heat capacity of the canonical ensemble in a harmonic trap. We can see that the heat capacity is close to the semiclassical value at above-critical temperatures and approaches the classical limit $3Nk_B$ for temperatures $T \geqslant 1.5T_c$. Our calculations confirm the previously obtained results [7–17], which testify that the heat capacity of ensembles comprising a finite number of particles does not experience a discontinuity in the vicinity of the semiclassical critical temperature. The temperature variation of the heat capacity becomes smoother with a decrease in the number of ensemble particles. The heat capacity of a Bose gas confined to a box trap was considered in Ref. [24].

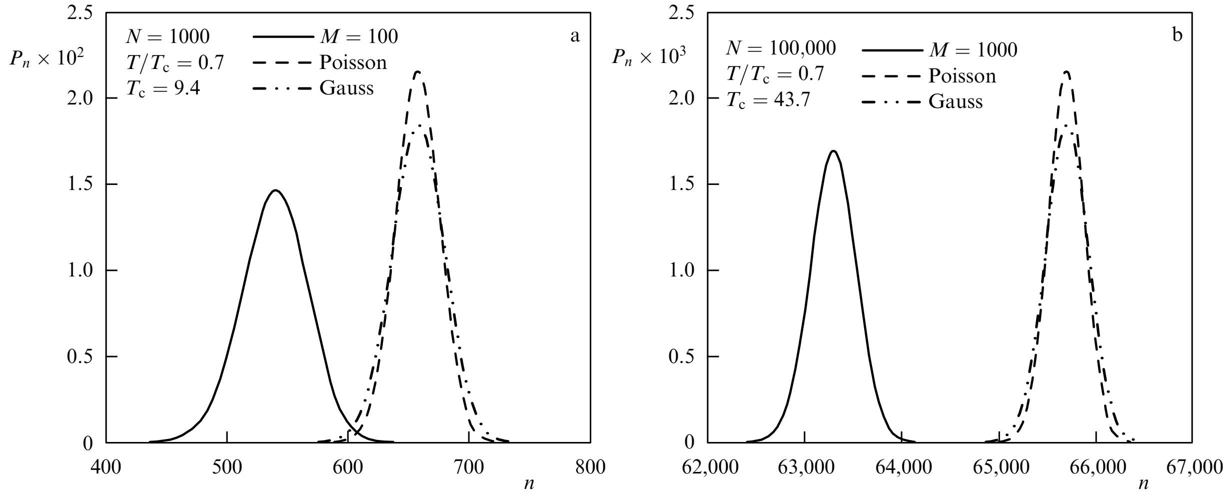

Figure 5. Comparison of the BEC particle number distribution functions for canonical ensembles of 1000 (a) and 100000 (b) particles with the Poisson and Gauss distributions derived for the grand canonical ensemble in the thermodynamic limit.

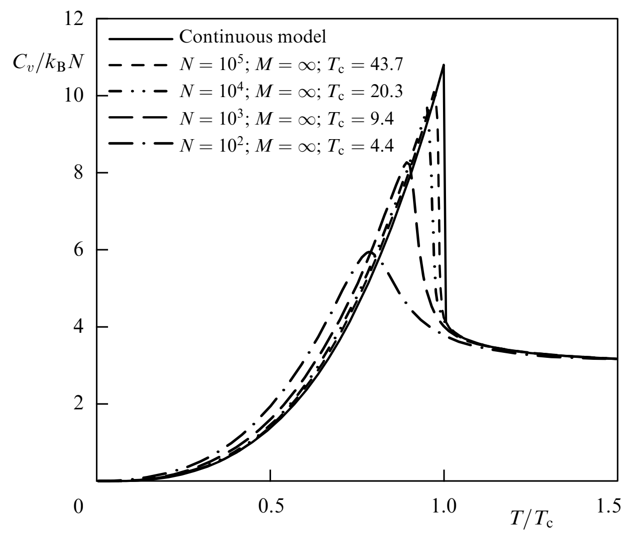

Figure 6. Temperature dependence of the heat capacity of a Bose gas confined to a three-dimensional isotropic harmonic trap for ensembles of 100, 1000, 10,000, and 100,000 particles. The heat capacity of a grand canonical ensemble calculated in the thermodynamic limit is plotted with a solid curve.

5. Conclusion

Our aim in this paper was to show how the statistics of the BEC of an ideal gas can be investigated using two recursive methods for calculating the partition function of the canonical ensemble of Bose particles. The calculation we performed using the two methods lead to virtually identical results. As noted above, the recursive (in the number of particles) Landsberg method offers computational advantages in the cases where an analytic expression for the single-particle partition function is known, in particular, in the example of a three-dimensional harmonic trap considered above. The second method (recursive with respect to the number of states), which is derived in this paper, would be appropriate for use in elucidating the effect of single-particle energy spectrum features on the thermodynamic properties of the system.

The use of recursive methods allows clarifying the statistical BEC properties determined previously in the so-called thermodynamic semiclassical limit. In the Bose gas model considered above, the discrete energy level structure and the finiteness of the number of particles are taken into account explicitly. The application of recursive methods does not involve a derivation of the chemical potential. Furthermore, recursive methods allow obtaining exhaustive information about statistical properties of the BEC of mesoscopic atomic systems (not only the mean and the variance but also the distribution function for the number of condensed particles). Yet another area of application of recursive methods may involve investigations of the statistics of one- and two-dimensional mesosystems, for which the thermodynamic limit pronounces a negative verdict as regards the possibility of BEC formation. We have shown that the utility of resorting to recursive methods is limited by a value of the order of 10^5 for the number of particles, which is typical for experiments involving the preparation of the BEC of dilute gases realized to date [5, 6]. For ensembles with a large number of particles, statistical characteristics derived by the semiclassical method depart from 'exact' values by only a small fraction of a percent.

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