Quantum gas in an external field: Exact grand canonical expressions and numerical treatment

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An exact Feynman-type presentation of the grand canonical partition function and averages as series over cycles for a system of noninteracting identical particles with a spin in an arbitrary external field is derived, and a numerical procedure for obtaining $\mu(\beta)$ and other dependencies at constant N is developed. It is shown that the same series can be obtained also from the conventional form of the grand potential Ω (i.e., a sum over single-particle energy states). Numerical calculations at constant N are carried out for quantum gas of bosons and fermions in three-dimensional harmonic field and in the Pöschl-Teller potential. [S1063-651X(99)03301-2]

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I. INTRODUCTION

Development of new computer simulation schemes always implies an appropriate means of their test. The most desirable in this aspect is to compare simulation data with analytical expressions which eventually exist or can be derived in certain particular cases.

In [1] we proposed a variant of path integral Monte Carlo (MC) method combining the previously existed ''bead'' and Fourier approximations, which are the extreme (and nonoptimal) cases of our approach. For a single particle in an external field we tested our method reproducing the ground-state energy and distribution function of an electron in the hydrogen atom and canonical averages of the harmonic oscillator.

The proposed method was extended in [1] also to systems of interacting identical particles (fermions and bosons) and appropriate MC procedures were created. To test them properly we arrived at an urgency to find cases described analytically. Exact expressions were obtained indeed for the canonical partition function and averages in the case of noninteracting quantum particles with a spin in d-dimensional harmonic field [1] (for $d=1$ and $s=0$ they reproduce preceding results of [2]). With their aid tests of MC data were performed in [1] for systems with the number of particles $N=2,3$. Unfortunately, canonical ensemble expressions become more and more cumbersome as N increases.

Meanwhile it is known that the grand canonical approach yields sometimes quite simple expressions since in this case the restriction on the constant number of particles is being removed. This was one of the motivating points of the present work. The most important for us in this aspect is the Feynman expression for the grand potential Ω in the form of a series over powers of activity for a system of free spinless bosons in a box [3]. Coefficients of this series include exactly determined canonical partition functions for cyclic permutations (cycles) of increasing number of quantum particles, hence the whole expression is often called ''a series over cycles.'' Recently a similar series for a system of noninteracting spinless quantum particles in a harmonic field was derived in [4].

In the present work a Feynman-type series over cycles for the grand potential Ω is constructed in a more general case, i.e., for a system of noninteracting identical particles (bosons and fermions) with a spin in an *arbitrary* external potential field (including [3] and [4] as specific cases).

The structure of the paper is as follows. Section II contains transformation of the canonical partition function, transition to the grand canonical ensemble, creation of the grand potential Ω, and averages. The obtained relations are then written down for specific cases of d-dimensional isotropic harmonic field and Pöschl-Teller potential [5,6]. It is shown as well that the canonical partition function for a cycle of ν noniteracting particles at temperature T is equal to that for a single particle at T, ν times less. We demonstrate also how the series over cycles for Ω can be derived from the conventional series over single particle energy states. The calculation scheme is described and numerical results for temperature dependencies of chemical potential, energy, heat capacity, and other averages at constant N for systems of noninteracting bosons and fermions both in harmonic and Pöschl-Teller fields are presented in Sec. III. Section IV contains concluding remarks.

II. SYSTEM OF IDENTICAL NONINTERACTING PARTICLES WITH A SPIN IN AN EXTERNAL FIELD

A. Canonical ensemble

We consider a system of N identical particles with a spin. Canonical partition function of such a system can be presented as a symmetrical (antisymmetrical) sum over all $N!$ permutations P in the density matrix of the canonical partition function for a system of N distinguishable particles $Z^{(D)}(\beta;P)$ [3]:

$$Z^{(S,A)}(\beta)=\frac{1}{N!}\sum_{\{P\}}\xi^{[P]}Z^{(D)}(\beta;P), \tag{1}$$

where $\xi=\pm 1$ for bosons and fermions correspondingly, $[P]$—parity of the permutation P, $\beta=T^{-1}$—inverse temperature. If the Hamiltonian of the system does not depend on spin, $Z^{(D)}(\beta;P)$ is being split into a product of the spin and the coordinate parts:

$$Z^{(D)}(\beta;P)=Z_{sp}^{(D)}(P)Z_c^{(D)}(\beta;P). \tag{2}$$

The coordinate part can be written in the form

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$$Z_c^{(D)}(\beta;P)=\int \rho(\mathbf{x},P\mathbf{x};\beta)d\mathbf{x}, \tag{3}$$

where $\mathbf{x}=(\vec{r}_1,\ldots,\vec{r}_N)$ is the dN-dimensional vector, d, dimensionality, $\rho(\mathbf{x},\mathbf{x}';\beta)=\langle\mathbf{x}|e^{-\beta\hat{H}}|\mathbf{x}'\rangle$, the density matrix for a system of spinless distinguishable particles in the coordinate presentation, $\hat{H}$, Hamiltonian of the system.

The spin part in Eq. (2) has the form

$$Z_{sp}^{(D)}(P)=\sum_{\{\sigma\}}\prod_{i=1}^{N}\delta(\sigma_i,P\sigma_i), \tag{4}$$

where $\delta(\sigma_i,\sigma_j)$ is the Kronecker symbol. Sum in Eq. (4) is over all $2s+1$ values of the spin projection for each particle, and s is the value of its spin. Note that for the identical permutation P_0 it yields: $Z_{sp}^{(D)}(P_0)=(2s+1)^N$ [e.g., for electrons $s=1/2$ and $Z_{sp}^{(D)}(P_0)=2^N$]. Consider that first ν particles in the P permutation are involved in a cycle. Then it is possible to make an independent summation over variables σ_i, included into this cycle:

$$\sum_{\sigma_1,\sigma_2,\ldots,\sigma_\nu}\delta(\sigma_1,\sigma_2)\,\delta(\sigma_2,\sigma_3)\ldots\delta(\sigma_{\nu-1},\sigma_\nu)\,\delta(\sigma_\nu,\sigma_1)=2s+1, \tag{5}$$

i.e., each cycle, regardless of its length, yields an equal contribution into Eq. (4) and the spin part is expressed as [7]

$$Z_{sp}^{(D)}(P)=\prod_{\nu=1}^{N}(2s+1)^{C_\nu(P)}=(2s+1)^{\Sigma_{\nu=1}^{N}C_\nu(P)}, \tag{6}$$

where $C_\nu(P)$ is the number of cycles involving ν particles in the P permutation. In the canonical ensemble $C_\nu(P)$ must satisfy the fixed number of particles' condition for each P:

$$\sum_{\nu=1}^{N}\nu C_\nu(P)=N. \tag{7}$$

The coordinate part $Z_c^{(D)}(\beta;P)$ can be also presented in the form of a product over cycles analogous to Eq. (6) for a system of *noninteracting* particles in an arbitrary external field. Indeed, as far as in this case $\hat{H}=\Sigma_{i=1}^{N}\hat{H}_1(i)$, where $\hat{H}_1(i)$ is a single-particle Hamiltonian of the ith particle,

$$\rho(\mathbf{x},\mathbf{x}';\beta)=\langle\mathbf{x}|e^{-\beta\hat{H}}|\mathbf{x}'\rangle=\prod_{i=1}^{N}\rho_1(\vec{r}_i,\vec{r}_i{}';\beta). \tag{8}$$

Here $\rho_1(\vec{r}_i,\vec{r}_i{}';\beta)=\langle\vec{r}_i|e^{-\beta\hat{H}_1(i)}|\vec{r}_i{}'\rangle$, a single-particle density matrix for the ith particle. Consider again that the coordinates of first ν particles in the P-permutation form a cycle. Then the following independent factor in $Z_c^{(D)}(\beta;P)$ emerges:

$$Z_\nu(\beta)=\int\rho_1(\vec{r}_1,\vec{r}_2;\beta)\rho_1(\vec{r}_2,\vec{r}_3;\beta)\ldots\times\rho_1(\vec{r}_\nu,\vec{r}_1;\beta)\prod_{i=1}^{\nu}d\vec{r}_i \tag{9}$$

The remaining part of $Z_c^{(D)}(\beta;P)$ splits into similar factors (partition functions of cycles), and the whole $Z_c^{(D)}(\beta;P)$ is now presented as a product:

$$Z_c^{(D)}(\beta;P)=\prod_{\nu=1}^{N}Z_\nu(\beta)^{C_\nu(P)}. \tag{10}$$

Finally as far as each ν cycle in the P permutation is a result of $\nu-1$ pair transpositions [3,8], the parity $[P]$ in Eq. (1) is determined as $[P]=\Sigma_\nu(\nu-1)C_\nu(P)$. Now, substituting $[P]$ in this form together with Eqs. (2), (6), and (10) into (1) we arrive at the following expression:

$$\begin{aligned}Z^{(S,A)}(\beta)&=\frac{1}{N!}\sum_{\{P\}}\xi^{\Sigma_{\nu=1}^{N}(\nu-1)C_\nu(P)}(2s+1)^{\Sigma_{\nu=1}^{N}C_\nu(P)}\times\prod_{\nu=1}^{N}Z_\nu(\beta)^{C_\nu(P)}\\&=\frac{1}{N!}\sum_{\{P\}}\prod_{\nu=1}^{N}[\xi^{(\nu-1)}(2s+1)Z_\nu(\beta)]^{C_\nu(P)}.\end{aligned} \tag{11}$$

According to the group theory the permutation group splits into classes, each of the latter having its specific cyclic structure [a set of indices $C_\nu(P)$]. Hence the sum over permutations, in Eq. (1) or in Eq. (11), can be reduced to the sum over classes (see [3,7]). For Eq. (11) it yields

$$Z^{(S,A)}(\beta)=\frac{1}{N!}\sum_{\{C_\nu\}}M(\{C_\nu\})\prod_{\nu=1}^{N}[\xi^{(\nu-1)}(2s+1)Z_\nu(\beta)]^{C_\nu}. \tag{12}$$

Summing over classes is presented in Eq. (12) as a sum over all sets $\{C_\nu\}$, provided the condition (7) is fulfilled. The number of elements in each class $M(\{C_\nu\})$, is determined as [3,7]

$$M(\{C_\nu\})=\frac{N!}{\prod_{\nu=1}^{N}(C_\nu!\,\nu^{C_\nu})}. \tag{13}$$

As a result we obtain the expression for the canonical partition function (11) in the form

$$Z^{(S,A)}(\beta)=\sum_{\{C_\nu\}}\prod_{\nu=1}^{N}\frac{a_\nu^{C_\nu}}{C_\nu!},\quad a_\nu=\frac{\xi^{(\nu-1)}(2s+1)Z_\nu(\beta)}{\nu}. \tag{14}$$

B. Grand canonical ensemble

Now we start with the general expression for the grand canonical partition function:

$$\Xi^{(S,A)}(\beta,\mu)=\sum_{N=0}^{\infty}\lambda^N Z_N^{(S,A)}(\beta). \tag{15}$$

Here $\lambda = e^{\beta\mu}$ is the activity, μ the chemical potential, and $Z_N^{(S,A)}(\beta)$ the canonical partition function for a system of N identical particles.

Substituting expression (14) into Eq. (15) and following Feynman [3], we arrive at a set of transformations:

$$\Xi^{(S,A)}(\beta,\mu) = \sum_{\{C_1,C_2,\ldots=0\}}^{\infty} \prod_{\nu=1}^{\infty} \frac{[\lambda^\nu a_\nu]^{C_\nu}}{C_\nu!} = \prod_{\nu=1}^{\infty} \sum_{C_\nu=0}^{\infty} \frac{[\lambda^\nu a_\nu]^{C_\nu}}{C_\nu!} = \prod_{\nu=1}^{\infty} e^{(\lambda^\nu a_\nu)}. \quad (16)$$

It is taken into account that summation over N [Eq. (15)] in the infinite limit removes the restriction (7) imposed on the number of cycles C_ν and hence the sum over each C_ν is performed independently from zero to infinity.

For the grand potential Ω we get

$$\beta\Omega^{(S,A)}(\beta,\mu) = -\ln[\Xi^{(S,A)}(\beta,\mu)] = -(2s+1)\sum_{\nu=1}^{\infty} \frac{\xi^{(\nu-1)} Z_\nu(\beta)}{\nu} \lambda^\nu. \quad (17)$$

The obtained series over powers of activity (17) is valid for a system of noninteracting identical particles in an *arbitrary* external field. Coefficients of the series contain canonical partition functions for cycles of ν particles $Z_\nu(\beta)$ ($1 \leqslant \nu < \infty$).

Note that for

$$Z_\nu(\beta) = h_\nu = V\left(\frac{m}{2\pi\hbar^2\beta\nu}\right)^{3/2} \quad (18)$$

with $\xi = 1, s = 0$ we get the Feynman expression for the free spinless boson gas in a box of volume V [3]. For isotropic d-dimensional oscillator field

$$Z_\nu(\beta) = \left(2\sinh\frac{\hbar\omega\beta\nu}{2}\right)^{-d} \quad (19)$$

(see e.g., [1,4]), and Eq. (17) determines the Ω potential in this case.

For noninteracting particles we can point to the following important fact:

$$Z_\nu(\beta) = Z_1(\nu\beta). \quad (20)$$

It means that the canonical partition function for a cycle of ν particles at the inverse temperature β is equal to that of a single particle at β times ν. Indeed, starting with the partition function for a single particle at $\nu\beta$:

$$Z_1(\nu\beta) = \int d\vec{r}_1 \rho_1(\vec{r}_1,\vec{r}_1;\nu\beta), \quad (21)$$

where $\rho_1(\vec{r},\vec{r}';\nu\beta) = \langle\vec{r}|e^{-\nu\beta\hat{H}_1}|\vec{r}'\rangle$, and using the identity $e^{-\nu\beta\hat{H}_1} = (e^{-\beta\hat{H}_1})^\nu$, we get

$$Z_1(\nu\beta) = \int \rho_1(\vec{r}_1,\vec{r}_2;\beta)\rho_1 \times(\vec{r}_2,\vec{r}_3;\beta)\ldots\rho_1(\vec{r}_\nu,\vec{r}_1;\beta) \times\prod_{i=1}^{\nu} d\vec{r}_i. \quad (22)$$

This expression exactly reproduces (9) for $Z_\nu(\beta)$. Note that for specific cases (18) and (19) the validity of Eq. (20) is observed directly.

As a consequence of Eq. (20) it follows that the grand potential Ω at β for our system is expressed only through a single-particle canonical partition function at a set of increasing inverse temperatures $\nu\beta$ (decreasing T). If the energy spectrum of a particle in the given field is known then $Z_1(\beta)$ can be calculated at any temperature and hence Ω can be determined. Note that for $\beta\to\infty$ $Z_1(\beta)$ approaches its ground state term, $e^{-\beta E_0}$ (1 if $E_0 = 0$).

Finally, it is instructive to demonstrate another way of obtaining the series (17) for Ω. We start with $\Xi^{(S,A)}(\beta,\mu)$ for the system of noninteracting identical particles in a standard form [9]:

$$\Xi^{(S,A)}(\beta,\mu) = \prod_{\vec{k}} \Xi_{\vec{k}}^{(S,A)}(\beta,\mu), \quad (23)$$

$$\Xi_{\vec{k}}^{(S,A)}(\beta,\mu) = [(1-\xi\lambda e^{-\beta E_{\vec{k}}})^{-\xi}]^{(2s+1)}.$$

Here $\Xi_{\vec{k}}$ is the grand canonical partition function for the $\vec{k}$th single-particle state ($\vec{k}$, d-dimensional vector with integer components), $E_{\vec{k}}$ is its energy, and β,μ,λ,ξ,s are the same as determined earlier [e.g., in Eqs. (14)–(17)]. For Ω we get

$$\beta\Omega(\beta,\mu) = -\ln\Xi(\beta,\mu) = \xi(2s+1)\sum_{\vec{k}} \ln(1-x_{\vec{k}}), \qquad x_{\vec{k}} = \xi\lambda e^{-\beta E_{\vec{k}}}. \quad (24)$$

Using series decomposition for the ln function,

$$\ln(1-x_{\vec{k}}) = -\sum_{\nu=1}^{\infty} \frac{x_{\vec{k}}^\nu}{\nu},$$

we transform the right-hand side of Eq. (24):

$$\beta\Omega(\beta,\mu) = -\xi(2s+1)\sum_{\vec{k}}\sum_{\nu=1}^{\infty} \frac{x_{\vec{k}}^\nu}{\nu} = -(2s+1)\sum_{\nu=1}^{\infty} \frac{\xi^{\nu+1}\lambda^\nu}{\nu}\sum_{\vec{k}} e^{-\nu\beta E_{\vec{k}}} = -(2s+1)\sum_{\nu=1}^{\infty} \frac{\xi^{\nu-1} Z_1(\nu\beta)}{\nu}\lambda^\nu. \quad (25)$$

The latter expression coincides with Eq. (17) if Eq. (20) is taken into account.

C. Thermodynamical quantities in the form of cycle series

Differentiating Eqs. (17) and (25) over μ, we obtain the following expression for the number of particles N:

$$N=-\left(\frac{\partial\Omega}{\partial\mu}\right)_{\beta}=(2s+1)\sum_{\nu=1}^{\infty}\xi^{\nu-1}Z_1(\nu\beta)\lambda^{\nu}. \tag{26}$$

For the energy we use the relation [3]

$$E=\frac{\partial}{\partial\beta}(\beta\Omega)_{\mu}+\mu N \tag{27}$$

and finally we get

$$E=-(2s+1)\sum_{\nu=1}^{\infty}\xi^{\nu-1}\lambda^{\nu}\frac{dZ_1(x)}{dx}, \tag{28}$$

where $x=\beta\nu$.

In particular, for the d-dimensional isotropic oscillator field:

$$N=(2s+1)\sum_{\nu=1}^{\infty}\xi^{\nu-1}\left(2\,\mathrm{sh}\frac{\hbar\omega\nu\beta}{2}\right)^{-d}\lambda^{\nu}, \tag{29}$$

$$E=\frac{d\hbar\omega}{2}(2s+1)\sum_{\nu=1}^{\infty}\xi^{\nu-1}\coth\frac{\hbar\omega\nu\beta}{2}\left(2\,\mathrm{sh}\frac{\hbar\omega\nu\beta}{2}\right)^{-d}\lambda^{\nu}. \tag{30}$$

It is useful also to have N and E in the form of series over single-particle states

$$N=\sum_{\vec{k}}N_{\vec{k}},\quad N_{\vec{k}}=\frac{(2s+1)}{e^{\beta(E_{\vec{k}}-\mu)}-\xi}, \tag{31}$$

$$E=\sum_{\vec{k}}N_{\vec{k}}E_{\vec{k}} \tag{32}$$

($E_{\vec{k}}$ is the energy of the $\vec{k}$th state).

For d-dimensional isotropic oscillator d-dimensional sums (31) and (32) can be reduced to one-dimensional sums with

$$N_k=\frac{f_k(d)(2s+1)}{e^{\beta(E_k-\mu)}-\xi}, \tag{33}$$

where $E_k=\hbar\omega[k+(d/2)]$, and $f_k(d)=C_{k+d-1}^{d-1}$ is the degeneracy factor.

It is convenient to count the chemical potential from the ground-state level while in the above relations it is counted from the bottom of the potential well. In the oscillator case it yields the following substitutions in Eqs. (29), (30), and (33):

$$\mu-\frac{d}{2}\hbar\omega\rightarrow\mu,\quad \sinh\frac{\hbar\omega\beta\nu}{2}\rightarrow 1-e^{-\hbar\omega\beta\nu}. \tag{34}$$

III. NUMERICAL CALCULATIONS

A. General approach

Relations (17), (26), (28)–(30), (24), and (31)–(33), explicitly determine thermodynamic averages as functions of the grand canonical ensemble variables T, μ. To get dependencies at constant number of particles N we start with relations (26) and (31), which are treated now as equations for obtaining curves $\mu(T)$ at constant N. Then for each fixed N we calculate energy E as a function of β or $T=\beta^{-1}$ (it can be also presented as a function of μ). In this way, based on grand canonical ensemble relations, we can get explicit dependencies of calculated quantities on N and β, i.e., we reproduce canonical averages.

The (μ,T) pairs were chosen so as to reproduce the given value of N within the fixed accuracy δ (δ was taken equal to 10^{-5} for N from 10 to 1000). Truncating series (26) and (31) we compared consecutive terms of each series with the same δ. The first term whose modulus did not exceed δ was taken as the last term in the truncated series. For each temperature the chemical potential was determined with the aid of the half-division method. It is evident that series over cycles (17), (26), and (29) converge better at high temperatures, while series (24),(31)–(33) over single particle states do so at low T. So in the range of $\mu>0$ for fermions we used the series (31) (in this region series over cycles absolutely diverge). In the region $\mu\leqslant 0$, both series (31) and (26) were used for fermions as well as for bosons.

The practice of calculations with the aid of series over cycles (26) showed that the number of terms taken into account for attaining the required accuracy increased indeed with the decrease of T due to the nature of this series. So it was used mainly at high temperatures.

Coefficients in Eq. (26) include canonical partition functions of a single particle in a one-dimensional field (to the power of d). If this partition function is determined analytically (as in the case of the harmonic field) the series (26) for $\mu<0$ can be calculated quite fast both for bosons and fermions. However in most cases, e.g., for the Pöschl-Teller potential, the canonical partition function $Z_1(\beta)$ has to be calculated numerically based on the known energy spectrum. Convergence of $Z_1(\beta)$ falls with the increase of T and, as far as this sum must be calculated with accuracy higher than that of Eq. (26), the total computational rate in this case falls noticeably, especially as T increases.

The series over single particle states (31) is more difficult for calculations since in the general case it is a d-dimensional one. The number of terms to be taken into account at fixed accuracy is much greater than that for the series over cycles and it grows further with the increase of T. Practically, calculations at temperature higher than a certain limiting value, dependent on parameters of the system, appear to be impossible. Meanwhile for low temperatures Eq. (31) provides quite fast calculations with the required accuracy both for bosons and fermions. Calculations on a Pentium PC took, usually, several minutes for each N.

As a rule there exists a rather large temperature interval in which efficiency ranges of both series overlap, i.e., both of them can be practically used for calculations. In the range of this overlap $\mu(T)$ dependencies for fixed N, obtained from Eqs. (26) and (31), always coincided within the required accuracy.

B. Oscillator field

To estimate the range of interest in the μ-T plane it is convenient to determine ''reference points'' at each N, i.e.,

the chemical potential at zero temperature and temperature at zero chemical potential for fermions.

At $T=0$ relations (31) and (32) for the case of the oscillator are reduced to

$$\frac{N}{2s+1}=\frac{1}{2}\sum_{k=0}^{K_\phi}(k+1)(k+2), \tag{35}$$

$$\frac{E}{2s+1}=\frac{1}{2}\sum_{k=0}^{K_\phi}(k+\tfrac{1}{2})(k+1)(k+2), \tag{36}$$

where K_ϕ corresponds to the Fermi energy $\mu_0=E_\phi=K_\phi$ (in units of $\hbar\omega$). If the energy is counted also from the ground state then $\frac{1}{2}$ in the first parentheses of Eq. (36) should be omitted. It is easy to show that summation in Eqs. (35) and (36) yields ultimately

$$\frac{N}{2s+1}=\frac{1}{6}(K_\phi+1)(K_\phi+2)(K_\phi+3), \tag{37}$$

$$\frac{E}{2s+1}=\frac{1}{8}K_\phi(K_\phi+1)(K_\phi+2)(K_\phi+3). \tag{38}$$

For high values of N, K_ϕ is close to $[6N/(2s+1)]^{1/3}$. For the specific energy we get

$$\frac{E}{N}=\frac{3}{4}K_\phi. \tag{39}$$

Note that for nonrelativistic quantum fermi gas in a box the specific energy at $T=0$ is equal to $\frac{3}{5}E_\phi$, while for the ultrarelativistic case it is equal to $\frac{3}{4}E_\phi$ [9]. The coincidence of our result (39) with the latter can be caused by similar energy dependence for the density of states (in both cases it is a square of energy).

Now we write down the expression (31) for fermions at $\mu=0$ taking into the account Eq. (34):

$$\frac{N}{2s+1}=\frac{1}{2}\left[\sum_k\frac{k^2}{e^{\beta k}+1}+3\sum_k\frac{k}{e^{\beta k}+1}+2\sum_k\frac{1}{e^{\beta k}+1}\right]. \tag{40}$$

These sums can be calculated analytically if we reduce them initially to appropriate integrals [9]. Finally, we get

$$\begin{aligned}\frac{N}{2s+1}&=\frac{1}{2}[T^3(1-\tfrac{1}{4})\Gamma(3)\zeta(3)\\&\quad+3T^2(1-\tfrac{1}{2})\Gamma(2)\zeta(2)+2T\ln 2]\\&=T^3\left(0.75\times1.202+0.75\frac{\pi^2}{6}\frac{1}{T}+\ln 2\frac{1}{T^2}\right).\end{aligned} \tag{41}$$

Here $\Gamma()$ and $\zeta()$ are γ and ζ functions, $\zeta(3)=1.202$; $\zeta(2)=\pi^2/6$. At great N (and T) the left-hand side of Eq. (41) is practically equal to the first term, $0.9015\ T^3$.

For bosons the chemical potential is negative and is strictly equal to zero only at $T=0$. So, at μ close to zero, it can be set equal to zero in the first two sums (31) with their following substitution by integrals. The last term of Eq. (31) should be presented as a sum in which its first item ($k=0$) keeps the value $\mu\neq0$.

As a result (on calculating integrals [9]), we arrive at the expression

$$\begin{aligned}\frac{N}{2s+1}&=T^3\frac{1}{2}\Gamma(3)\zeta(3)+T^2\frac{3}{2}\frac{\pi^2}{6}\\&\quad+\sum_{k=1}^{\infty}\frac{1}{e^{\beta k}-1}+\frac{1}{e^{-\beta\mu}-1}.\end{aligned} \tag{42}$$

For great N the bose condensation starts at high temperatures and for estimation of the condensation point T_c, only the first term in Eq. (42), containing T^3, should be saved and

$$T_c=\left(\frac{N}{(2s+1)}\frac{1}{1.202}\right)^{1/3}. \tag{43}$$

In the range $T<T_c$ with the decrease of T the last term yields the major contribution into Eq. (42) being the number of particles in the ground state.

In the limit of high temperatures ($\beta\hbar\omega\ll1,\mu<0$) the dependency $\mu(\beta)$ is determined from the series (29) by saving only its first term,

$$\frac{N}{2s+1}=\frac{e^{\beta\mu}}{(\beta\hbar\omega)^3},\quad \mu=T\ln\left(\frac{N}{2s+1}(\beta\hbar\omega)^3\right). \tag{44}$$

Comparing Eq. (44) with the expression for the chemical potential of the Boltzmann gas in a box of volume V,

$$\mu=T\ln\left(\frac{N}{V}\Lambda^3\right), \tag{45}$$

where $\Lambda=(2\pi\beta\hbar^2/m)^{1/2}$ is the thermal wavelength, one can express Eq. (44) in a similar form, introducing effective volume V_{ef}:

$$\mu=T\ln\left(\frac{N}{V_{ef}}\Lambda^3\right),\quad V_{ef}=(2s+1)\left(\frac{2\pi T}{m\omega^2}\right)^{3/2}. \tag{46}$$

C. Pöschl-Teller potential and limiting cases

This potential is determined as [5,6]

$$V(x)=\frac{V_0}{2}\left[\frac{\kappa(\kappa-1)}{\sin^2(\alpha x)}+\frac{\lambda(\lambda-1)}{\cos^2(\alpha x)}\right],\quad V_0=\frac{\hbar^2\alpha^2}{m} \tag{47}$$

with parameters $\kappa>1,\lambda>1$ and the range of x: $0\leqslant x\leqslant\pi/2\alpha$. It has a smooth bottom and approaches asymptotically vertical walls at limiting values of x. The Schrödinger problem for this potential has an exact solution with eigenvalues $E_n=(V_0/2)(\kappa+\lambda+2n)^2$, $n=0,1,\ldots$. We consider only the symmetrical case of Eq. (47), $\kappa=\lambda$, with

$$V(x)=2V_0\frac{\kappa(\kappa-1)}{\sin^2(2\alpha x)} \tag{48}$$

and energy spectrum $E_n=2V_0(\kappa+n)^2$. Introducing dimensionless eigenvalues counted from the ground state we can write

$$\tilde{E}_n=\frac{E_n-E_0}{4V_0\kappa}=\frac{1}{2\kappa}[(\kappa+n)^2-\kappa^2]=n\left(1+\frac{n}{2\kappa}\right). \quad (49)$$

This form of $\tilde{E}_n$ is helpful in obtaining two limiting cases of Pöschl-Teller potential. At $\kappa=1$ it formally yields a box with hard walls and flat bottom while for $\kappa\to\infty$ it approaches the harmonic potential.

Indeed, the energy levels for a box of width L are $E_k=(\hbar^2/2m)(\pi/L)^2k^2\equiv\varepsilon k^2$, $k=1,2,\ldots$. Substituting $k=n+1$, $n=0,1,\ldots$ and introducing again dimensionless energies counted from the ground state, we get

$$\tilde{E}_n=\frac{E_n-E_0}{2\varepsilon}=\frac{(n+1)^2-1}{2}=n\left(1+\frac{n}{2}\right), \quad n=0,1,\ldots . \quad (50)$$

This coincides with Eq. (49) for $\kappa=1$ as long as $2V_0=2\hbar^2\alpha^2/m=(2\hbar^2/m)(\pi/2L)^2=\varepsilon$ if we assume $L=\pi/2\alpha$.

The analogous procedure for harmonic field eigenvalues $E_n=\hbar\omega(n+\frac{1}{2})$, $n=0,1,\ldots$ yields

$$\tilde{E}_n=\frac{E_n-E_0}{\hbar\omega}=n. \quad (51)$$

It coincides with Eq. (49) for $\kappa\to\infty$ if we assume $\hbar\omega=4\kappa V_0$ or $\omega=4(\hbar/m)\kappa\alpha^2$.

As long as the product $\beta\mu(\beta)$ exhibits linear behavior in $\ln T$ scale at high temperatures both for gas in a harmonic field and in a box [see Eqs. (44) and (45)] we can use these asymptotes for checking our numerical results.

In units adopted above we get

$$\beta\mu(\beta)=\ln\left(\frac{N}{2s+1}\right)+\frac{3}{2}\ln\frac{2}{\pi}-\frac{3}{2}\ln T \quad (52)$$

for the box and

$$\beta\mu(\beta)=\ln\left(\frac{N}{2s+1}\right)-3\ln T \quad (53)$$

for the three-dimensional harmonic field.

D. Obtained data

Computational results for systems in a three-dimensional isotropic oscillator field are presented in Figs. 1–3. For the Pöschl-Teller potential results are shown in Figs. 4 and 5.

Figure 1 gives $\mu(T)$ dependencies for bosons and fermions in a T-interval range from zero up to temperatures where difference between two statistics almost vanishes. Both μ and T are presented in $\hbar\omega$ units. Each pair of curves corresponds to a fixed value of $N/(2s+1)$ from 10 to 10^4 (for bosons with $s=0$ it is the number of particles N, for fermions with $s=1/2$ it is $N/2$). Condensation for bosons becomes more and more abrupt with the increase of N, which is particularly well observed in the inset of Fig. 1, and is also revealed in Fig. 2.

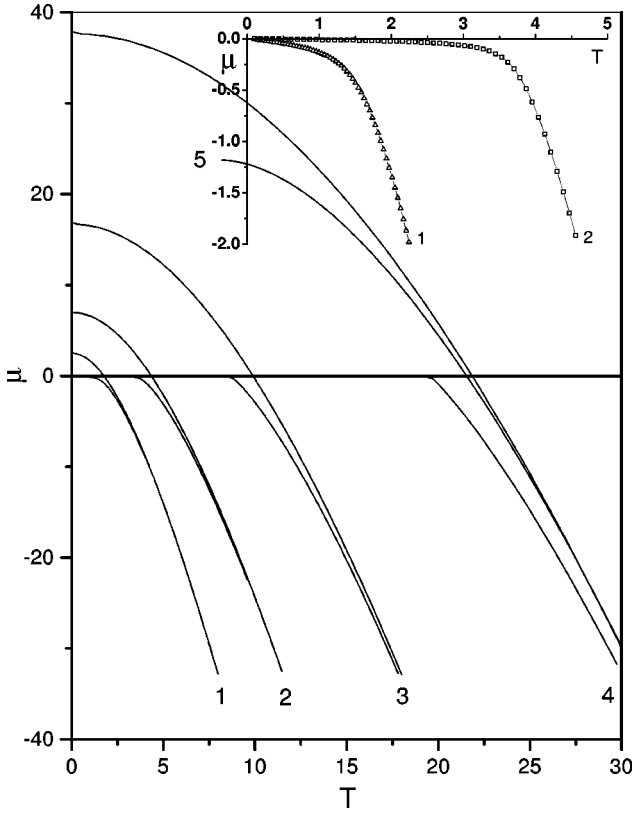

FIG. 1. μ vs T dependencies for boson and fermion gases in a 3D isotropic harmonic field at constant $N/(2s+1)$; curves 1–4 correspond to $N/(2s+1)=10,10^2,10^3,10^4$. The inset presents curves 1 and 2 for bosons in larger scale. Curve 5 is the Boltzmann gas in the case 4. μ and T are in $\hbar\omega$ units.

The T dependencies of averages (energy, heat capacity, population of levels) for the same values of N are presented in Fig. 2. T_c units for T are used to equalize scales for curves within the whole large N range, T_c being determined by Eq. (43). Data for bosons reproduce well canonical averages obtained in [4] with the aid of recurrent relations in the canonical ensemble. As far as very accurate comparison of both data requires recalculations according to relations from [4], we used another approach to check the difference between true canonical averages and results obtained within our procedure: we calculated the T dependency of energy for fermions, $s=1/2$, in oscillator field by the present method for the smallest number of particles, $N=2,3$ and compared them with exact canonical expressions from our previous paper [1]. The relative difference of these results as a function of T (in $\hbar\omega$ units), Fig. 3, testifies that even for $N=2$ maximum deviation (at $T=0.3$) does not exceed 7%. For $N=3$ it shifts to higher T and now is less than 3%. For limiting temperatures ($T\to0, T\to\infty$) the deviation vanishes. It is evident that for N about 10 we can completely neglect the difference between results of averaging in both ensembles. It justifies indeed application of the present approach: numerical calculation of averages at fixed N with the aid of grand canonical ensemble relations avoiding cumbersome formulas of the type [1] or recurrent relations [4].

It is worth mentioning here that while energy, Fig. 2(a), was calculated according to the suggested scheme, i.e., using series (30) and (32), the heat capacity, Fig. 3(b), was deter-

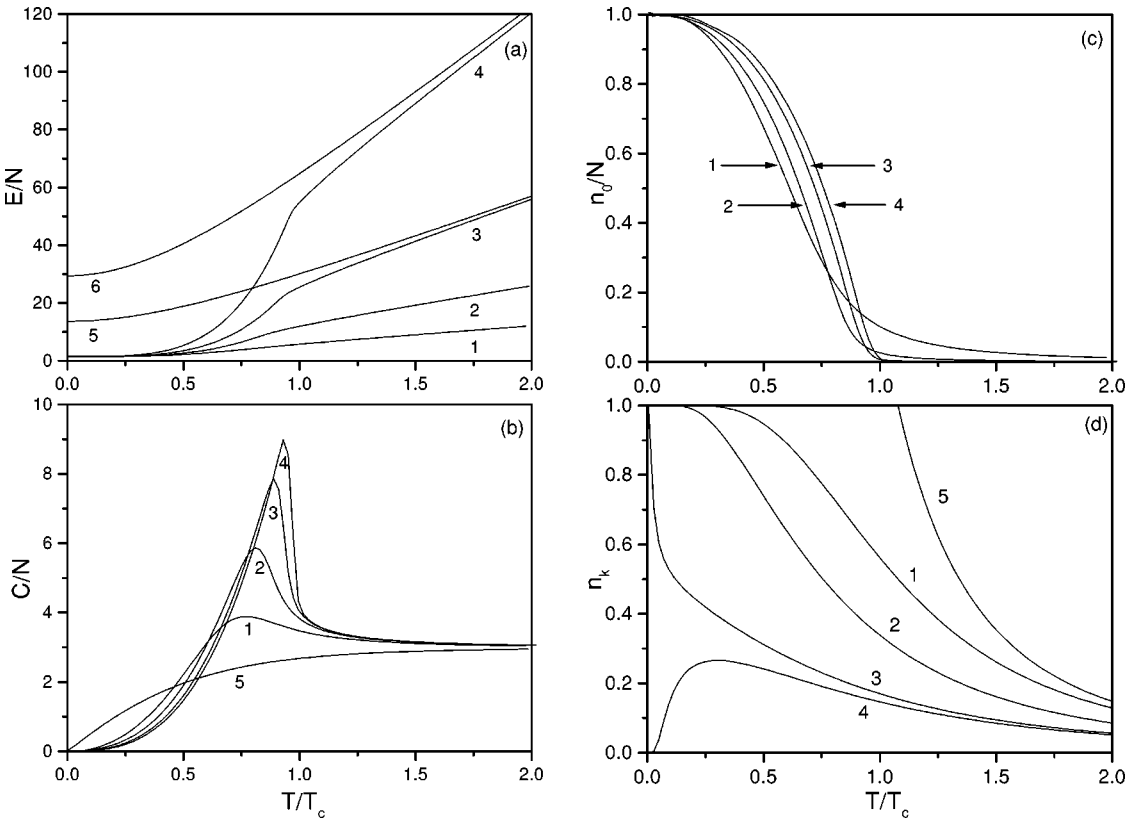

FIG. 2. Equilibrium properties vs T for boson and fermion gases in 3D harmonic field at constant $N/(2s+1)$: (a) specific energy, curves 1–4 correspond to $N/(2s+1)=10,10^2,10^3,10^4$ (bosons), 5 and 6 to 10^3 and 10^4 (fermions); (b) specific heat capacity: 1–4, for bosons as in case (a), 5, fermions, $N/2=10^4$; (c) specific population of the ground state for bosons, 1–4 as in cases (a) and (b); (d) population of levels for fermions, $N/2=10^4$: 1, ground state, 2, $0.5E_\phi$, 3, E_ϕ, 4, $1.1E_\phi$, 5, corresponds to the Boltzmann dependence for the ground-state level.

mined by numerical T differentiation of the above data for the energy. An attempt to get heat capacity by direct differentiation of series (30) and (32) yielded inadequate results especially for T above the condensation point for bosons.

The $\mu(T)$ dependencies for boson and fermion gases in the three-dimensional (3D) Pöschl-Teller potential for a set of κ is shown in Fig. 4. Limiting values $\kappa=1$ and $\kappa=\infty$ correspond to the cubic box and to harmonic field. In Fig. 5 we present corresponding $\beta\mu(\beta)$ versus $\ln T$ curves [T in Fig. 4 and 5 is in $4V_0\kappa$ units, see Eq. (49)]. It is clearly seen

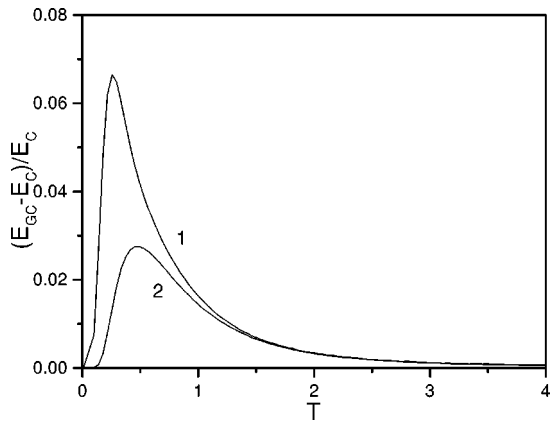

FIG. 3. Relative difference between canonical and grand canonical energies vs T ($\hbar\omega$ units) for fermions, $s=1/2$ in the 3D harmonic field. Curves 1 and 2 are for $N=2$ and 3.

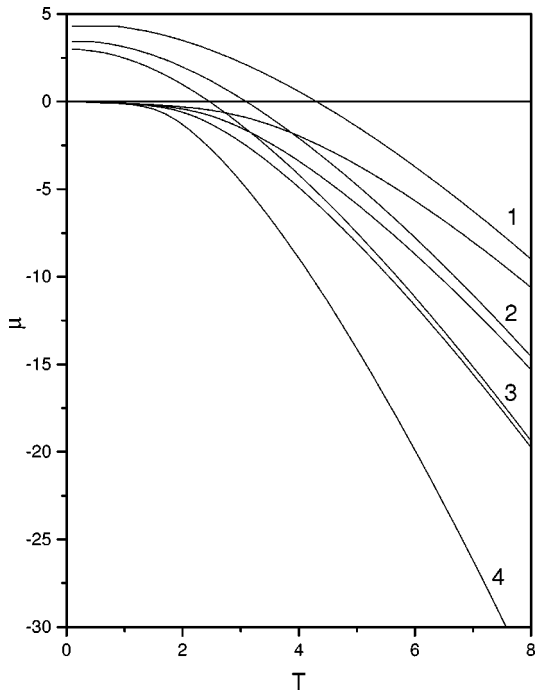

FIG. 4. μ vs T dependencies for boson and fermion gases in a 3D Pöschl-Teller field, $N/(2s+1)=10$. Curves 1–4 are for values of κ: 1 (cubic box), 2, 4, and oscillator field ($\kappa\to\infty$). μ and T are in $4V_0\kappa$ units, see Eq. (49).

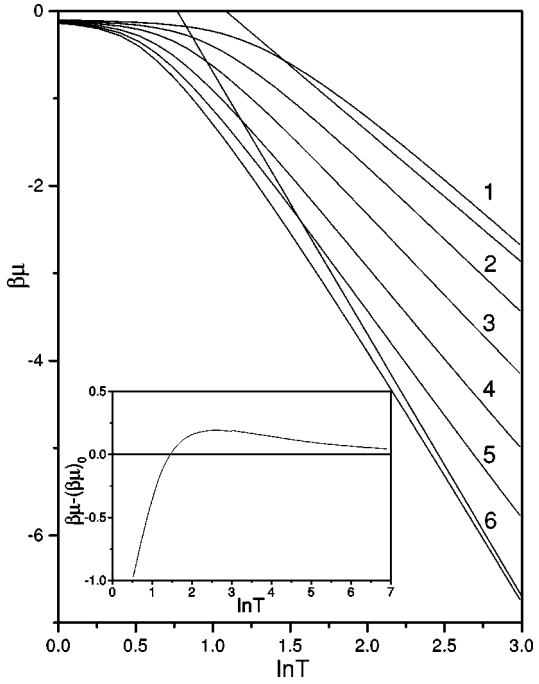

FIG. 5. $\beta\mu(\beta)$ dependencies in $\ln T$ scale for boson gas in 3D Pöschl-Teller field, in a range of T including high-temperature limiting behavior, $N/(2s+1)=10$. Curves 1–6 are for values of κ: 1 (cubic box), 2, 4, 10, 30, and harmonic field ($\kappa\to\infty$). Straight lines for 1 and 6, Boltzmann asymptotes for corresponding cases. The inset shows the difference of curve 1 and the Boltzman limit in a larger range of temperatures. T is in $4V_0\kappa$ units as in Fig. 4.

how these curves approach asymptotes with slopes increasing with the increase of κ, from -1.5 for the cubic box [curve 1, Eq. (52)] to -3 for the harmonic field [curve 6, Eq. (53)]. It is interesting to note that for the harmonic field the asymptote is monotonously attained from below while in the case of the cubic box it is attained nonmonotonously from above with crossing of both lines at a finite T. The asymptotic behavior of the curve 1 is presented in detail in the inset, Fig. 5. The maximum deviation of both lines is approximately 0.19. We made similar calculations for $N/(2s+1)=10^2,10^3$ and observed the same behavior with maximum deviation falling to 0.09 and 0.03, respectively. It means that the ''effect of intersection'' would completely vanish with further increase of N.

We can compare values of Fermi energies obtained in our calculations with the expression for macroscopic quantum fermion gas [9]:

$$E_\phi=\left(6\pi^2\frac{N}{(2s+1)V}\right)^{2/3}\frac{\hbar^2}{2m}, \tag{54}$$

or in adopted units,

$$E_\phi=\frac{1}{2}\left(\frac{6}{\pi}\frac{N}{2s+1}\right)^{2/3}. \tag{55}$$

This comparison is presented in Table I. It is seen how the relative difference tends to zero with the increase of N.

Finally it could be also noted that Feynman's expression for h_ν [Eq. (18)], strictly speaking, does not present the canonical partition function for a single particle in a box since it does not tend to 1 for $T\to 0$. We compare h_1 [Eq. (18)] with Z_1 for this case calculated numerically, Fig. 6. In adopted units their ratio as a function of T is

$$\frac{h_1}{Z_1}=\left(\frac{\sqrt{\frac{\pi}{2}T}}{\sum_{k=0}^{\infty}e^{-\frac{k(1+k/2)}{T}}}\right)^3. \tag{56}$$

It tends (though rather slowly) to 1 at large temperatures while at $T\to 0$ it falls to zero. It is interesting that these two kinds of behavior are separated by a pronounced peak.

TABLE I. Comparison of Fermi energy values for increasing number of particles N. $E_\phi^{(c)}$, our calculations; $E_\phi^{(a)}$, expression (55); Δ, relative difference.

$\frac{N}{2s+1}$	$E_\phi^{(c)}$	$E_\phi^{(a)}$	Δ
10	4.31	3.57	0.21
10^2	19.6	16.6	0.18
10^3	85.1	77.0	0.10
10^4	376.0	357.3	0.05

IV. CONCLUDING REMARKS

We have shown that Feynman presentation of the grand canonical potential Ω as a series over cycles can be treated in a more general sense than it was meant initially, i.e., it is valid for a system of noninteracting identical particles with a spin of both statistics in an arbitrary external field.

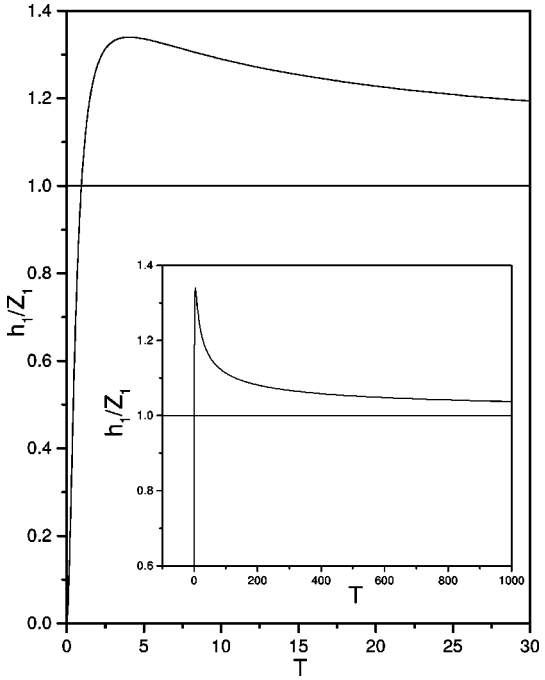

FIG. 6. Ratio of h_1 [Eq. (18)] to Z_1 for a cubic box vs T. In the inset it is shown at a much larger T scale. T is in 2ε units [see Eq. (50)].

A numerical procedure based on grand canonical expressions was developed enabling us to obtain very accurately the equilibrium data at constant N ranging from 10 to 10^4. In principle, there is no problem with increasing N by several orders. In the case of harmonic field when the canonical single-particle partition function exists in a closed form calculations run particularly fast. In cases when the single-particle energy spectrum is known but the partition function cannot be presented in a closed form our numerical procedure is still effective though it becomes noticeably slower. Such is the case for the Pöschl-Teller potential considered in this work.

It should, finally, be pointed out that for most potentials the single-particle Schrödinger problem has no exact solution and hence its spectrum is unknown. In this case we have to apply another procedure to estimate the single-particle canonical partition function that enters into series over cycles. An aproach that could be helpful here is the Monte Carlo method in the expanded esemble [10], which enables us to calculate the difference between the unknown partition function and that of the reference system (e.g., of the oscillator). Another question also exists: how to use (if possible) facilities developed here for systems of quantum noninteracting particles to the case when interaction is being switched on.

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