Path-integral–expanded-ensemble Monte Carlo method in treatment of the sign problem for fermions

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(Received 14 August 2009; published 3 December 2009)

Expanded-ensemble Monte Carlo method with Wang-Landau algorithm was used for calculations of the ratio of partition functions for classes of permutations in the problem of several interacting quantum particles (fermions) in an external field. Simulations for systems consisting of 2 up to 7 interacting particles in harmonic or Coulombic field were performed. The presented approach allows one to carry out calculations for low enough temperatures that makes it possible to extract data for the ground-state energy and low-temperature thermodynamics.

DOI: 10.1103/PhysRevE.80.066702 PACS number(s): 07.05.Tp, 05.30.−d, 87.55.kd

I. INTRODUCTION

Path integral Monte Carlo (PIMC) method was designed for simulation of systems of interacting quantum particles at finite temperatures [1–4]. A serious difficulty of the PIMC approach in application to fermionic systems is the so-called sign problem. The wave function, describing N fermions, must change its sign (be antisymmetric) upon transposition of any pair of particles. Hence the density matrix should be also antisymmetric upon particles transpositions. It results in alternating signs in the coordinate representation of the density matrix which defines the weight function within the PIMC method. At low temperatures, contributions from positive and negative terms in the weight function are almost perfectly canceled leaving no hope to obtain reliable results of simulations [2].

In one-dimensional problems the PIMC approach can be formulated in a way that the sign problem disappears completely [5,6], but unfortunately for two and three dimensions it is not the case. Several approaches aiming to relax the sign problem for simulations of fermions using PIMC have been suggested in the literature: introduction of pseudopotential approximations to eliminate the Fermi-Dirac antisymmetry and the resulting negative sign, before Monte Carlo integration [7,8]; replacing the path through pure states with a path through idempotent density matrices based on rotational averaging around the two-particle center of mass [9]; restricted path integrals [10]; multilevel blocking approach [11,12] as well as some others.

In this paper a technique is introduced that is based on precise computation of ratios of opposite sign contributions in the fermionic partition function using the expanded-ensemble (EE) method [13], complemented with Wang-Landau (WL) algorithm [14] for tuning the EE parameters. First we test our approach for systems of noninteracting particles in harmonic field by gradual transformation of positive part of fermionic partition function into negative part and compare the obtained results with exact expressions. Some preliminary calculations of this kind for systems of two and three fermions were performed in [15]. For systems of interacting particles we suggest to compute the change in free energy (ratio of partition functions) due to transformation of the system with interaction to the system of noninteracting particles in the external harmonic field. The partition function of the latter system and their "positive" and "negative" contributions are known analytically, that enables us to reconstruct the partition function of the interacting system.

The paper is organized as follows: the methodology is described in Sec. II. Section III contains details of its application to specific systems as well as calculated results and their discussion. Concluding remarks are given in Sec. IV.

II. BACKGROUND OF THE METHOD

A. System of identical particles

Consider a system of N *identical* particles with a spin. Canonical partition function (PF) of such a system can be presented as a symmetrical (antisymmetrical) sum over all $N!$ permutations P in the density matrix in the canonical PF for a system of N *distinguishable* particles [16,17],

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

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

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

In the coordinate presentation $Z_c^{(D)}$ is written in the form:

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

where $\mathbf{r}=(r_1,\ldots,r_N)$ is dN-dimensional vector, d is dimensionality, $\rho^{(D)}(\mathbf{r},\mathbf{r}';\beta)=\langle\mathbf{r}|\exp(-\beta\hat{H})|\mathbf{r}'\rangle$ is the density matrix for a system of spinless distinguishable particles in the coordinate presentation, $\hat{H}$—Hamiltonian of the system.

The spin part in the Eq. (2) has the form [18,19]

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

where $\delta(\sigma_i,\sigma_j)$ is the Kronecker symbol. Sum in Eq. (4) is taken over all $2s+1$ values of the spin projection for each particle, and s is the value of their spin.

Following [16,18,19] we rewrite the partition function (1) as a sum over classes of permutations. Each class is designated by an ordered set of numbers $\{C_\nu\}$, $1\le\nu\le N$, each C_ν is the number of cycles of length ν in the given class. Then $\xi^{[P]}=\xi^{[G]}$, $K(P)=K(G)=(2s+1)^{\Sigma_\nu C_\nu(G)}$, so that $\Sigma_\nu C_\nu(G)$ is the total number of cycles in the class G $(1\le\Sigma_{\nu=1}^{N}C_\nu(G)\le N)$. Since the value of the integral over all coordinates depends only on the cycle structure of the permutation $Z^{(D)}(P)=Z^{(D)}(G)$. This way (1) yields

$$Z^{(A,S)}(\beta) = \frac{1}{N!}\sum_G \xi^{[G]}K(G)M(G)Z_c^{(D)}(\beta;G), \tag{5}$$

where $M(G)=N!/\prod_{\nu=1}^{N}(C_\nu!\,\nu^{C_\nu})$ is the number of permutations in the given class G [16]. The number of classes grows with N much slower than the total number of permutations $N!$, making summation (5) tractable in calculations even for large N.

Each term of the PF (5) is described by the standard bead approximation of the density matrix [16,20] with the boundary condition $\mathbf{r}_{n+1}=P(\mathbf{r}_1)$, where P is any permutation of the class G (here and below the reduced units are used in which m (mass), $\hbar$ (Planck constant), and e (electron charge) are equal to Eq. (1):

$$Z_c^{(D)}(\beta,G) = \left(\frac{n}{2\pi\beta}\right)^{ndN/2}\int d\mathbf{x}\,\exp(-h),$$

$$h = -\frac{n}{2\beta}\left[\sum_{j=1}^{n}(\mathbf{r}_j-\mathbf{r}_{j+1})^2\right]_{\mathbf{r}_{n+1}=P(\mathbf{r}_1)} - \frac{\beta}{n}\sum_{j=1}^{n}V(\mathbf{r}_j). \tag{6}$$

In the following we shall use notation $\mathbf{x}$ for the whole set of bead coordinates $\{\mathbf{r}_i\}$, $i=1,\ldots,n$.

The partition function (6) is equivalent to the classical configurational PF of $\Sigma_\nu C_\nu(G)$ ring polymers, each consisting of nC_ν beads. This approximation becomes exact in the limit $n\to\infty$.

B. Method of expanded ensembles for the path-integral partition function

In order to calculate the PF for a system of identical particles it is necessary to obtain either a ratio of PFs for two different classes $Z_c^{(D)}(\beta,G_1)/Z_c^{(D)}(\beta,G_2)$ or a ratio of PFs for a given class with and without interparticle interactions (see details in Sec. III). Here we describe, how such ratio of PFs can be computed using the expanded-ensemble approach previously developed for classical calculations of free-energy differences.

Consider two systems with the cofigurational part of Hamiltonian $h_A(\mathbf{x})$ and $h_B(\mathbf{x})$ treated within canonical ensemble (it is supposed that factor β is included into h, $h=-\beta H$, and $\mathbf{x}$ represents all configurational variables). Both $h_A(\mathbf{x})$ and $h_B(\mathbf{x})$ depend on the same set of coordinates $\mathbf{x}$. A set of intermediate Hamiltonians $h_0=h_A,h_1,\ldots h_M=h_B$ is introduced, e.g., within a linear dependence:

$$h_m = (1-\lambda_m)h_0 + \lambda_m h_M,$$

$$0=\lambda_0<\lambda_1<\ldots<\lambda_M=1. \tag{7}$$

For each m the canonical PF is defined, $Z_m=\int d\mathbf{x}\exp(h_m)$. For the whole set of Hamiltonians an *expanded-ensemble* is introduced with the PF

$$Z = \sum_{m=0}^{M} Z_m \exp(-\eta_m), \tag{8}$$

where η_m are balancing (weighting) factors, so that each of the ensembles with the index m becomes a subensemble of the expanded or *generalized* ensemble [13].

The MC random walks in the EE is being carried out according to a conventional Metropolis procedure with two kinds of steps: (1) configurational moves within a certain subensemble and (2) change in parameter λ_m to the neighboring one $m\to m\pm1$ at fixed configuration $\mathbf{x}$. In both cases the transition probability is determined as:

$$p_{i\to i'} = \min\{1,\exp[(-h_{m(i')}-\eta_{m(i')})-(-h_{m(i)}-\eta_{m(i)})]\}. \tag{9}$$

In the course of MC run the number of visits to the m-th subensemble, n_m, is determined and the related probability (the weight) is then estimated as $p_m=n_m/n_{MC}$, where n_{MC} is the total number of MC steps. On the other hand it is clear that $p_m=Z_m e^{-\eta_m}/Z$ and hence it follows:

$$\frac{n_m}{n_k} = \frac{Z_m}{Z_k}\exp(-\eta_m+\eta_k). \tag{10}$$

Thus the ratio of PFs for any pair of subensembles can be obtained. In the following, we shall use EE technique to compute ratio of PFs corresponding to different classes of permutations, as well as to PFs differing by interaction potential.

It is evident that for the EE method to be successful, the probabilities p_m should not be too small (in the perfect case they should be equal). This condition can be achieved by a proper choice of the balancing factors η_m. In the previous applications [13,21,22] the balancing factors were often optimized by an iterative procedure. Here we describe an adjusting procedure for η_m based on Wang-Landau algorithm which provides automatic optimization of the balancing factors.

C. Wang-Landau (WL) algorithm

The WL algorithm [14] was originally elaborated for precise calculating the density of states for lattice systems in the entropic sampling MC method [23]. The main idea of WL algorithm can be used for fine-tuning of balancing factors η_m in EE method as well. We construct a set of Hamiltonians using linear dependence (7). Then we present two sets of $M+1$ accumulators, i. e. for balancing factors η_m and for the number of visits n_m. All initial values of η_m and n_m are taken to be zero. At each step the transition probability is determined by Eq. (9). If the trial state (i') is accepted, the value of corresponding balancing factor $\eta_{i'}$ is augmented by $\Delta\eta$ and the value of the number of visits $n_{i'}$ by 1; in the opposite case, it is the values of η_i and n_i corresponding to the initial state (i) that should be increased. It means that the probability to visit the already visited subensembles is being decreased in further run.

A certain number of such elementary steps constitute a sweep. At the end of the current sweep the value of $\Delta\eta$ is being reduced: $\Delta\eta \to a\Delta\eta$, where $0<a<1$ is an increment. After several sweeps the η_m dependence is formed providing flat character of the histogram n_m. Now the main contribution to the calculated ratio of PFs in Eq. (10) is in $\eta_M - \eta_0$ and the second term yields a relatively small correction.

In our calculations initial value $\Delta\eta_0$ was chosen regarding two circumstances. It should be large enough to provide fast formation of η_m dependence and n_m histogram, but not too large to produce a systematic error due to non-Markovian character of the simulation. In most of our calculations $\Delta\eta_0$ was taken equal to 0.01, that is significantly smaller than ΔS in entropic sampling [14], and the value of the increment was much larger, i.e., in the range of 0.95–0.975 compared to 0.5 in Ref. [14]. The number of sweeps was in the range of 1200–2000. This way starting from the second half of a single calculation $\Delta\eta$ became less than 10^{-15}. It practically means that further run was performed at constant η_m.

III. NUMERICAL CALCULATIONS, RESULTS AND DISCUSSION

A. Noninteracting particles in harmonic field

For testing purposes we consider first a system of noninteracting particles in a three-dimensional (3D) harmonic external field $V(r)=r^2/2$. It was shown previously that contribution to the PF of N identical noninteracting particles in an external field coming from a permutation cycle of length ν is equal to the PF of a single particle in the same field at inverse temperature $\nu\beta$ [19,24]. For a harmonic external field this yields:

$$Z_\nu = \left(2\sinh\frac{\nu\beta}{2}\right)^{-1}. \tag{11}$$

So the exact expression for PF of any class of permutations G is:

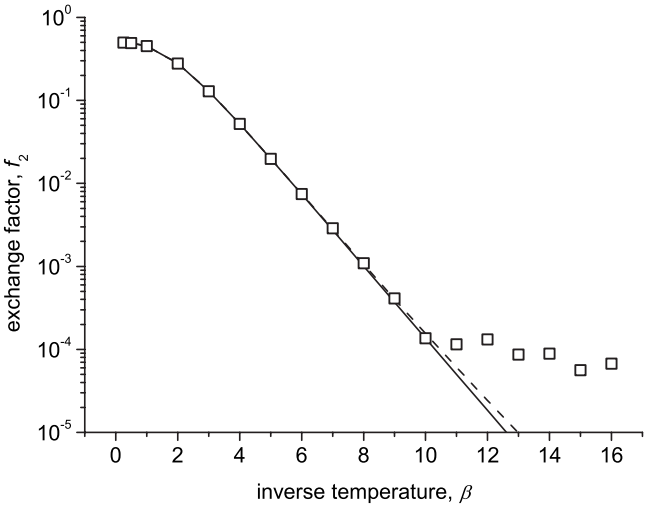

FIG. 1. β dependency of exchange factor f_2 for the system of two noninteracting spinless particles in 3D harmonic field. Solid line is exact dependency obtained from Eq. (16) according to Eqs. (11) and (12). Dashed line is that for the five-bead approximation [26] corrected by Takahashi-Imada term [25]. Simulation conditions: $n_{MC}=1200\times 2.5\cdot 10^6$, $\Delta\eta_0=0.01$, $a=0.95$, and $M=1$ (two subensembles)

$$Z_c^{(D)}(\beta,G) = \prod_{\nu=1}^{N} Z_\nu^{C_\nu}. \tag{12}$$

Finally the total PF of a system of identical noninteracting particles is determined according to Eq. (5).

We start with $N=2$ noninteracting spinless particles. The PF of the system is:

$$Z_2^{(A)}(\beta) = \frac{1}{2}[Z_{20}(\beta) - Z_{01}(\beta)]. \tag{13}$$

Here and below indices of PF represent numbers C_ν defining class of permutation G (see Sec. II A). Thus for two particles index {20} denotes two separate cycles (which is equivalent to two distinguishable particles) and {01} is a cycle of two particles corresponding to the exchange contribution. As a first step we applied EE MC to obtain the ratio Z_{01}/Z_{20} for a set of β values and compared our results with the exact expression.

In the framework of EE MC we constructed a set of Hamiltonians

$$h_m = -(1-\lambda_m)[H_K(\mathbf{x})]_{x_{k(n+1)}\equiv x_{k1}} - \lambda_m [H_K(\mathbf{x})]_{x_{2(n+1)}\equiv x_{11}}^{x_{1(n+1)}\equiv x_{21}} - H_P(\mathbf{x}), \tag{14}$$

where

$$H_K(\mathbf{x}) = \frac{n}{\beta}\sum_{k=1}^{2}\sum_{j=1}^{n}(\mathbf{x}_{kj} - \mathbf{x}_{k(j+1)})^2,$$

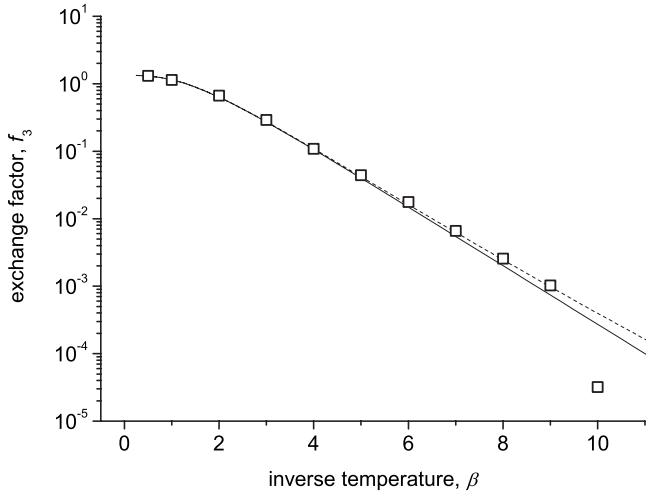

FIG. 2. β dependency of factor f_3 for the system of three noninteracting particles with spin $s=1/2$ in 3D harmonic field. Solid line is exact dependency. Dashed line is that in 10-bead approximation [26]. Simulation conditions: see Fig. 1.

$$H_P(\mathbf{x}) = \frac{\beta}{n}\sum_{k=1}^{2}\sum_{j=1}^{n}(\mathbf{x}_{kj})^2. \tag{15}$$

So with the increase in m two separate trajectories of the class {20} are transformed ("mutated") into the cycle {01}. We used five-bead approximation and in order to compensate small number of beads the Takahashi-Imada correction [25] was introduced. Due to simplicity of the system we composed expanded-ensemble in this case of only two subensembles. We performed 1200 sweeps of $2.5\cdot 10^6$ steps each, with $\Delta\eta_0=0.01$ and the increment $a=0.95$.

In order to illustrate the sign problem, we, following our study [15], introduced a factor $f_2(\beta)$ which reveals relationship between the total PF for two spinless fermionic particles $Z^{(A)}(\beta)$ and the PF for distinguishable particles Z_{20}:

$$Z_2^{(A)}(\beta) = Z_{20}(\beta)f_2, \quad f_2(\beta) = \frac{1}{2}\left[1 - \frac{Z_{01}(\beta)}{Z_{20}(\beta)}\right]. \tag{16}$$

The sign problem manifests itself in $Z_{01}/Z_{20}\to 1-0$ and hence in $f_2\to 0$ for $\beta\to\infty$. Thus, the precision of the obtained data can be checked by comparison of obtained f_2 with the exact curve. In Fig. 1 the computed EE data for f_2 are displayed together with the exact curve according to Eqs. (11) and (12) and the exact curve for five-bead approximation for the same system [26]. It is clearly seen that f_2 follows the exact curve very accurately up to $\beta=10$, reaching values of the order 10^{-4}. At greater values of β deviation of Z_{01}/Z_{20} from 1 becomes smaller than precision of calculations, that manifests the sign problem within the current approach.

We have also considered the case of $N=3$ fermions, for which expansion of the total PF in terms of contributions from classes of permutations reads:

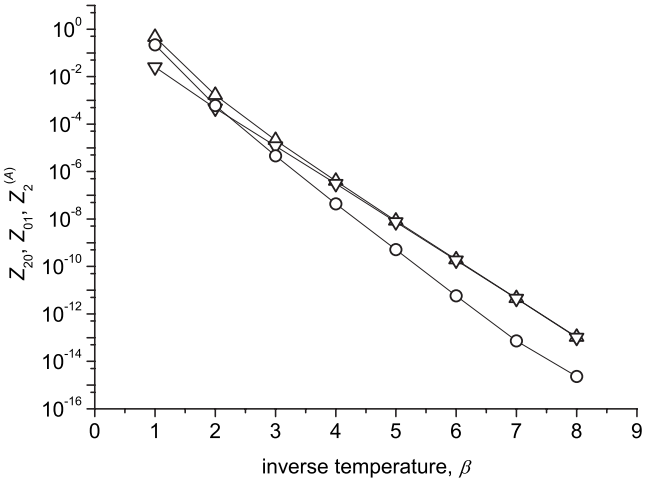

FIG. 3. β dependency of Z_{20} (triangles), Z_{01} (reverse triangles), and $Z^{(A)}=\frac{1}{2}(Z_{20}-Z_{01})$ (circles) for the system of two identical spinless particles with Coulomb repulsion in 3D harmonic field. Simulation conditions: $n_{MC}=2000\times 10^6$, $\Delta\eta_0=0.01$, $a=0.975$, and $M=9$ (ten subensembles)

$$Z_3^{(A)}(\beta) = \frac{1}{6}[K_{300}Z_{300}(\beta) - 3K_{110}Z_{110}(\beta) + 2K_{001}Z_{001}(\beta)]$$
$$= Z_{300}(\beta)f_3(\beta), \tag{17}$$

where

$$f_3(\beta) = \frac{1}{6}\left[K_{300} - 3K_{110}\frac{Z_{110}(\beta)}{Z_{300}(\beta)} + 2K_{001}\frac{Z_{001}(\beta)}{Z_{300}(\beta)}\right], \tag{18}$$

{300}, {110}, and {001} correspond to classes of three distinguishable particles, of one separate particle and a cycle of two particles and of cycle of three particles. For spin $s=0$ $K_{300}=K_{110}=K_{001}=1$, while for $s=1/2$ $K_{300}=8$, $K_{110}=4$, $K_{001}=2$.

We performed calculations for ratios Z_{110}/Z_{300} and Z_{001}/Z_{300}, using 10-bead approximation. Other simulation parameters were the same as for the case of two particles. The result for f_3 in the case $s=1/2$ (Fig. 2) demonstrates a good agreement with exact curves up to $\beta=9$.

Data presented in this section demonstrate that the EE-WL method accurately reproduces the ratio of PFs known analytically. Next we treat several systems with interaction using the noninteracting system as a reference.

B. Two identical particles in harmonic field with Coulomb repulsion

In this section two fermionic particles with Coulomb repulsion $V_{coul}(r)=1/|r|$ in a harmonic field are considered. We use the fact that the PF of noninteracting system is analytically known, and compute the ratio of PF (free-energy difference) due to switching on the interactions in the system for each class. This approach has a clear analogy with the so-called thermodynamical cycle frequently used in free-energy calculations of macromolecular systems [27]. Gradual change in the interaction potential within the same trajectory linkage structure (the same permutation class G)

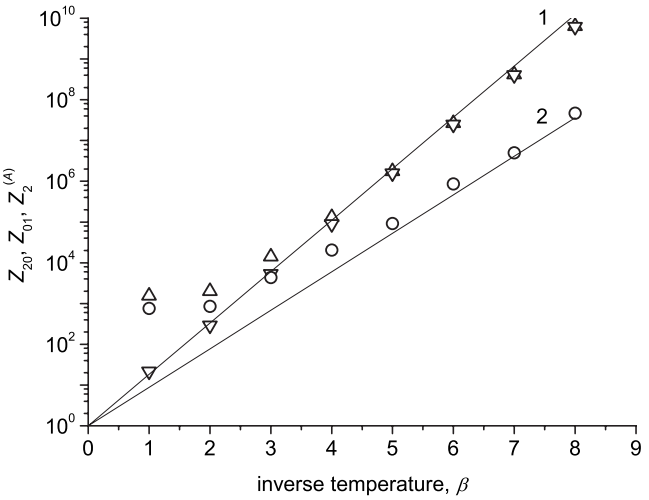

FIG. 4. β dependencies of Z_{20} (triangles), Z_{01} (reverse triangles), and $Z^{(A)}=\frac{1}{2}(Z_{20}-Z_{01})$ (circles, $s=0$) for the system of two fermions with Coulomb repulsion in the attractive Coulomb field of charge 2 (Helium atom). Data for the case $s=1/2$ nearly match to that for Z_{20} and are not shown. Straight lines are the asymptotes corresponding to ground (1) and triplet (2) states of He. Simulation conditions: $n_{MC}=2000\times 10^6$, $\Delta\eta_0=0.01$, $a=0.975$, and $M=21$.

makes transitions between subensembles much easier and allows us to reach higher precision compared to the case of direct transformation of one trajectory structure into another.

Now, we rewrite expression (13) in the following way:

$$Z_2^{(A)}=\frac{1}{2}\left[Z_{20}^0\frac{Z_{20}}{Z_{20}^0}-Z_{01}^0\frac{Z_{01}}{Z_{01}^0}\right], \tag{19}$$

where Z_{20}^0 and Z_{01}^0 denote corresponding PFs for the system without interaction which are known exactly. For each ratio, Z_{20}/Z_{20}^0 and Z_{01}/Z_{01}^0, we performed a separate EE MC computation. The set of Hamiltonians in EE MC method for the case Z_{20}/Z_{20}^0 is

$$h_m=-[H_K(\mathbf{x})]_{x_{k(n+1)}\equiv x_{k1}}-H_P(\mathbf{x})-\lambda_m I(\mathbf{x}),$$

$$I(\mathbf{x})=\frac{\beta}{n}\sum_{j=1}^{n}\frac{1}{|\mathbf{x}_{1j}-\mathbf{x}_{2j}|}, \tag{20}$$

so that $\lambda_0=0$ corresponds to the system of two particles without interaction and $\lambda_M=1$ corresponds to the system with Coulomb repulsion completely switched on. Expanded-ensemble was composed of 10 subensembles. The set of Hamiltonians in the case Z_{01}/Z_{01}^0 differs from Eq. (20) by cycle closure condition for $H_K(\mathbf{x})$, i.e., $x_{1(n+1)}\equiv x_{21}$, $x_{2(n+1)}\equiv x_{11}$. Using exact values for Z_{20}^0 and Z_{01}^0 in Eq. (19), we obtain $Z_2^{(A)}$ depending on β (Fig. 3).

For rather low-temperatures contributions from exited states become negligible compared to that of the ground state, so that for the PF we can write:

$$Z(\beta)\approx\exp(-\beta E_0), \tag{21}$$

and hence $-\ln[Z(\beta)]$ is proportional to βE_0. Discriminating high-temperature points and performing linear least-squares fit we get an estimation for the ground-state energy. For a system of two spinless fermions with Coulomb repulsion in 3D harmonic field we obtained $E_0=4.55\pm 0.05$, compared with $E_0=4$ for the system without interaction. We also studied one-dimensional (1D) case and found the ground-state energy $E_0=2.70\pm 0.02$, which is in a very good agreement with the value 2.71 obtained in [28]. ($E_0=2$ for noninteracting particles.) This result can also be compared to the ground-state energy, $E_0=2.65$, obtained by Kestner and Sinanoglu in [29] for the same model though their coefficient in the Coulomb repulsion term (0.94) is slightly different from that of ours (1.0). Later the result of [29] was approximately reproduced also by Newman and Kuki in their version of PIMC method [9].

C. Two interacting particles in the Coulomb field: Helium atom

Simulation of systems in an attractive Coulomb potential $V_{ex}=-q/r$ is a great challenge for MC methods. As long as the integrand for the finite bead approximation in Eq. (6) serves as a weight in the importance sampling procedure and the latter tends to maximize the integrand, it is clear that factor

$$\exp\left(+\frac{\beta}{n}\sum_{j=1}^{n}\mathbf{x}_j^{-1}\right), \tag{22}$$

will force trajectory to localize very close to the origin if the number of beads n is not large enough. To avoid this problem one should significantly increase the number of beads (at least to many thousands) and hence the number of MC steps. The problem of very large number of beads for attractive Coulomb potential can be substantially relaxed by using the method of Cole-De Raedt [30] based on application of Jensen's inequality to the propagator resulting in smearing out the singularity of the potential. The attractive Coulomb potential for k-th particle $1/\mathbf{x}_{k,j}$ is replaced by the following integral

$$W\left(d_{k,j},d_{k,(j+1)},\theta,\frac{\beta}{n}\right)=\int_0^{\pi/2}d\phi\frac{erf\left(\left(\frac{n}{\beta}\right)^{1/2}(d_{k,j}^2\tan^2\phi+2d_{k,j}d_{k,(j+1)}\cos\theta+d_{k,(j+1)}^2\cot^2\phi)^{1/2}\right)}{(d_{k,j}^2\tan^2\phi+2d_{k,j}d_{k,(j+1)}\cos\theta+d_{k,(j+1)}^2\cot^2\phi)^{1/2}}, \tag{23}$$

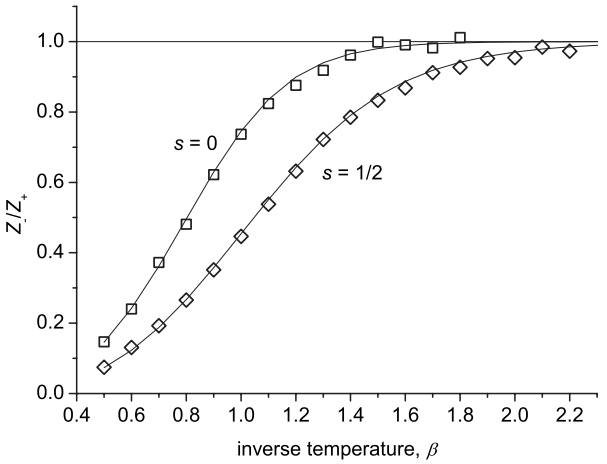

FIG. 5. β dependencies of ratios Z_-/Z_+ for the system of $N=5$ identical noninteracting particles in 3D harmonic field with spin $s=0$ (squares) and $s=1/2$ (diamonds). Solid lines are exact dependencies. Simulation conditions: $n_{MC}=1000\times10^7$, $\Delta\eta_0=0.01$, $a=0.95$, and $M=9$.

were $d_{k,j}=|\mathbf{x}_{k,j}|$ and θ is the angle between $\mathbf{x}_{k,j}$ and $\mathbf{x}_{k,(j+1)}$ ($\mathbf{x}_{k,(n+1)}\equiv\mathbf{x}_{k,1}$).

We simulated a system of two fermions with Coulomb repulsion in the attractive Coulomb field of charge $q=2$ (Helium atom) in 100-bead approximation. For the PF $Z_{He}=Z_2^{(A)}$ we used expression (19). As a reference we used the system of noninteracting particles in harmonic field. Within the EE procedure, we transform the external harmonic potential to the Coulombic one and simultaneously switch on the Coulombic repulsion between the particles (electrons). So the set of Hamiltonians in EE MC has the following form (written for Z_{20}/Z_{20}^0):

$$h_m = -[H_K(\mathbf{x})]_{x_{k(N+1)}\equiv x_{k1}} - (1-\lambda_m)H_P(\mathbf{x}) - \lambda_m\left[W\left(|\mathbf{x}_{1i}-\mathbf{x}_{2i}|,|\mathbf{x}_{1(i+1)}-\mathbf{x}_{2(i+1)}|,\theta,\frac{\beta}{n}\right) - 2\sum_{k=1}^{2} W\left(|\mathbf{x}_{ki}|,|\mathbf{x}_{k(i+1)}|,\theta,\frac{\beta}{n}\right)\right]_{x_{k(N+1)}\equiv x_{k1}}. \quad (24)$$

The number of subensembles was set to 22. As long as computation of three integrals in Eq. (23) for each bead at each MC step require a lot of CPU time, it was replaced by an interpolation in the set of precalculated tables.

The obtained β dependencies are shown in Fig. 4. Performing linear least-squares fit for dependencies at low temperatures we obtained $E_t=-2.03\pm0.07$ for $s=0$, and $E_0=-2.83\pm0.05$ for $s=0.5$. These results can be compared with the exact values for Helium triplet state $E_t=-2.175$ [31] and the ground (singlet) state $E_0=-2.904$ [31], contributions from these exact ground states $[\exp(-\beta E)]$ are also shown in Fig. 4 as straight lines. One can see that in the low-temperature limit the computed points are very close to these theoretically exact results.

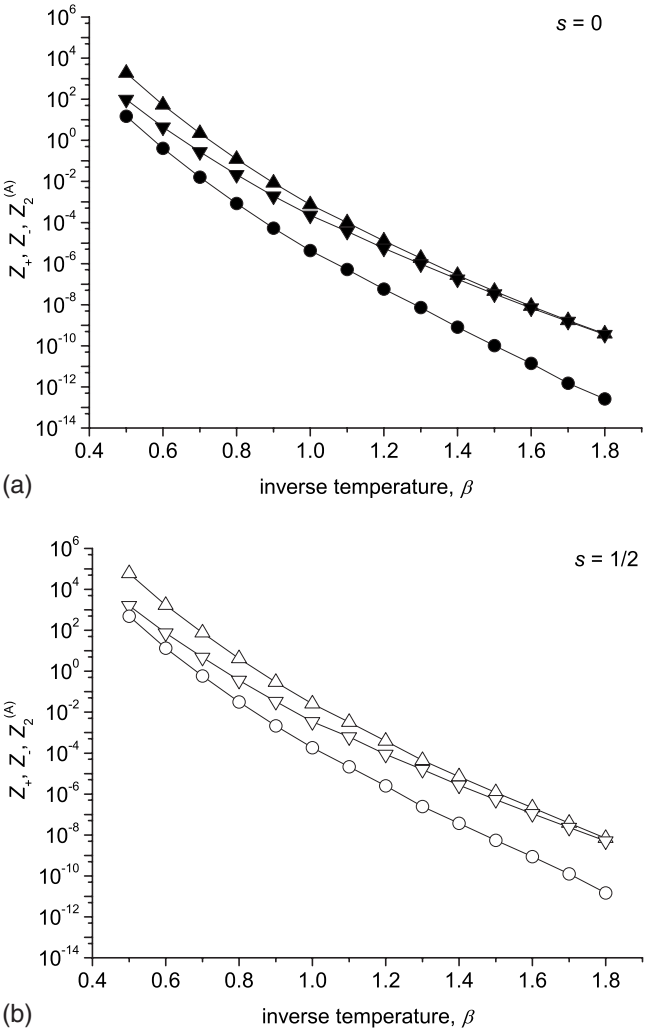

FIG. 6. β dependencies of Z_+ (triangles), Z_- (reverse triangles), and $Z^{(A)}=Z_+-Z_-$ (circles) for the system of $N=5$ fermions with Coulomb repulsion in 3d harmonic field with spin (a) $s=0$ and (b) $s=1/2$. Simulation conditions: see Fig. 5.

D. Several (5–7) fermionic particles in a harmonic field: Generalization of the method

To apply the proposed technique to a system of larger number of quantum particles one has to carry out separate computations for all classes of permutations. The number of classes increases with N considerably fast: for $N=5$ there are seven classes, 11 classes for $N=6$, 15 classes for $N=7$, 22 classes for $N=8$, etc. The idea is to separate contributions in Eq. (5) into two groups—positive and negative:

$$Z^{(A)} = Z_+ - Z_-, \quad (25)$$

and to perform computations in the similar way as it was done for the case $N=2$. Analogously to Eq. (16) we presented $Z^{(A)}$ as

$$Z^{(A)} = Z_+\left[1-\frac{Z_-}{Z_+}\right], \quad (26)$$

$$Z_{\pm}(\beta) = \frac{1}{N!}\sum_{G_{\pm}} K(G_{\pm})M(G_{\pm})Z_c^{(D)}(\beta;G_{\pm}), \tag{27}$$

where summation is taken over either positive or negative classes of permutations. Expressions for Z_+ and Z_- contain spin contributions which now are included into the weight function [see Eq. (32)], so it is necessary to make separate calculations for each value of spin (0 or 1/2).

Let us consider a system of $N=5$ particles with 7 classes of permutations. In Table I we gathered data on coefficients $M(G)$, $K(G)$ and sign for each class of permutations.

Expressions for Z_+ and Z_-, $N=5$, are

$$Z^{+} = \frac{1}{5!}[K_{50000}Z_{50000} + 20K_{20100}Z_{20100} + 24K_{00001}Z_{00001} + 15K_{12000}Z_{12000}], \tag{28}$$

$$Z^{-} = \frac{1}{5!}[10K_{31000}Z_{31000} + 30K_{10010}Z_{10010} + 20K_{01100}Z_{01100}]. \tag{29}$$

As in the case of two particles, we started with the system in a harmonic field without interactions and compared our results for Z_-/Z_+ with exact dependencies:

$$Z_{+} = \frac{1}{5!}\left\{K_{50000}\left[2\sinh\left(\frac{\beta}{2}\right)\right]^{-5d} + 20K_{20100}\left[2\sinh\left(\frac{\beta}{2}\right)\right]^{-2d}\left[2\sinh\left(\frac{3\beta}{2}\right)\right]^{-d} + 24K_{00001}\left[2\sinh\left(\frac{5\beta}{2}\right)\right]^{-d} + 15K_{12000}\left[2\sinh\left(\frac{\beta}{2}\right)\right]^{-d}[2\sinh(\beta)]^{-2d}\right\}, \tag{30}$$

$$Z_{-} = \frac{1}{5!}\left\{10K_{31000}\left[2\sinh\left(\frac{\beta}{2}\right)\right]^{-3d}[2\sinh(\beta)]^{-d} + 30K_{10010}\left[2\sinh\left(\frac{\beta}{2}\right)\right]^{-d}[2\sinh(2\beta)]^{-d} + 20K_{01100}[2\sinh(\beta)]^{-d}\left[2\sinh\left(\frac{3\beta}{2}\right)\right]^{-d}\right\}. \tag{31}$$

The set of Hamiltonians used in EE MC has the following form

$$h_m = -P(\mathbf{x}) + (1-\lambda_m)\ln\{K_{50000}\exp(-[H_K(\mathbf{x})]_{50000}) + 20K_{20100}\exp(-[H_K(\mathbf{x})]_{20100}) + 24K_{00001}\exp(-[H_K(\mathbf{x})]_{00001}) + 15K_{12000}\exp(-[H_K(\mathbf{x})]_{12000})\} + \lambda_m\ln\{10K_{31000}\exp(-[H_K(\mathbf{x})]_{31000}) + 30K_{10010}\exp(-[H_K(\mathbf{x})]_{10010}) + 20K_{01100}\exp(-[H_K(\mathbf{x})]_{01100})\}. \tag{32}$$

In order to smooth transition from h_0 to h_M we choose the number of subensembles equal to 9. In Fig. 5 ratios Z_-/Z_+ for the cases $s=0$ and $s=1/2$ are shown. Each point is a result of a single run, with EE balancing factors fitted automatically by the Wang-Landau algorithm. Our data follow exact curves accurately, up to the values of β at which ratios of PFs reaches the limiting value 1. Deviations occurring at high values of β are related to insufficient number of MC steps.

TABLE I. Classes of permutations for $N=5$ fermions. Each class is designated by an ordered set of numbers $\{C_\nu\}$, sign is that of $(-1)^{[G]}$ in expression (5), $M(G)$ is the number of elements in class G. Spin part (4), for $s=0$, $K(G)=1$ for each G; for $s=1/2$, $K(\{C_\nu\})=2^{\Sigma C_\nu}$.

#	$\{C_\nu\}$	Sign	M (G)	$K(G)$, $s=1/2$
1	50000	+	1	32
2	31000	−	10	16
3	20100	+	20	8
4	10010	−	30	4
5	00001	+	24	2
6	12000	+	15	8
7	01100	−	20	4

Now as a second stage we performed calculations for a system of $N=5$ particles with Coulomb repulsion in a harmonic field. The PF for the system of identical particles is presented in the way similar to Eq. (19), i.e.,

$$Z^{(A)} = Z_+^0\frac{Z_+}{Z_+^0} - Z_-^0\frac{Z_-}{Z_-^0}, \tag{33}$$

where Z_+^0 and Z_-^0 are positive and negative parts of the PF for a system without interaction which is considered as a reference system. We performed calculations of ratios Z_+/Z_+^0 and Z_-/Z_-^0 in the range $0.5\leq\beta\leq1.8$ and using exact values for Z_+^0 and Z_-^0 Eqs. (30) and (31) we obtained $Z_5^{(A)}$ (Fig. 6).

In this range of temperatures the simple approximation (21) for obtaining the ground-state energy is not valid. Taking into account the shape of the curve we tried the following function to fit our simulation points:

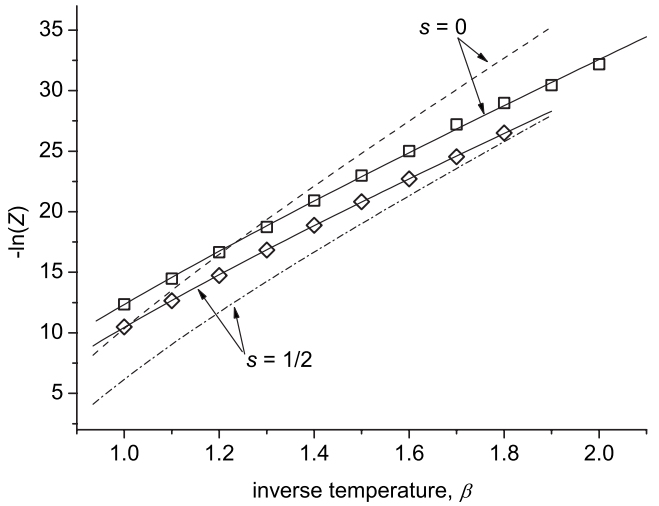

FIG. 7. Nonlinear least square fits for β dependencies of $-\ln(Z^{(A)})$, $N=5$ fermions with Coulomb repulsion in 3D harmonic field with spin $s=0$ (squares) and $s=1/2$ (diamonds). Dashed and dash-dotted lines are exact curves for the system without interaction, spin $s=0$ and $s=1/2$ correspondingly. Simulation conditions: see Fig. 5.

$$-\ln Z = \beta E_0 + C/\beta. \tag{34}$$

Using nonlinear least-squares method in $\beta \geq 1$ range, we get the following estimations of the ground-state energy: $E_0 = 17.5 \pm 0.2$, $(C = -5.1 \pm 0.4)$ for $s=0$ and, $E_0 = 16.60 \pm 0.03$ $(C = -6.14 \pm 0.06)$ for $s=0.5$ These fits are shown in Fig. 7. In order to test our fitting procedure, we also constructed sets of points for the noninteracting reference system using exact expressions (30) and (31) and fit them according to Eq. (34) (shown in Fig. 7 as dot-dashed lines). In this test we got an estimation for the ground-state energies of ideal systems 12.5 and 10.5 (for $s=0$ and $s=1/2$ respectively) with an error less than 0.1%.

Multiplying $-\ln(Z)$ by dimensionless temperature $\tau = 1/\beta$, we obtained temperature dependence of the free energy (Fig. 8). Taking into account that for $\tau=0$ the derivative of the free energy F must be equal to zero, we used the following simple parabolic approximation in τ scale

$$F = E_0 + A\tau^2. \tag{35}$$

By a nonlinear least squared fit we got temperature dependence of the free energy and estimations of the ground-state energies: $E_0 = 17.64 \pm 0.09$ $(A = -5.3 \pm 0.2)$ for $s=0$ and $E_0 = 16.59 \pm 0.03$ $(A = -6.13 \pm 0.05)$ for $s=1/2$, which are in a good agreement with the fitting procedure based on expression (34).

As soon as we have an explicit expression for the free energy in the form (35), we can get low-temperature thermodynamics for the system: entropy $S = -\frac{dF}{d\tau}$, internal energy $U = F + \tau S$, heat capacity $C = \frac{dU}{d\tau}$. These curves are shown in Fig. 9.

We performed similar calculations for systems of $N=6$ and $N=7$ fermions with Coulomb repulsion in 3D harmonic field, $s=1/2$. We constructed tables of coefficients for $M(G)$ and $K(G)$ analogous to Table I for all classes of permutations

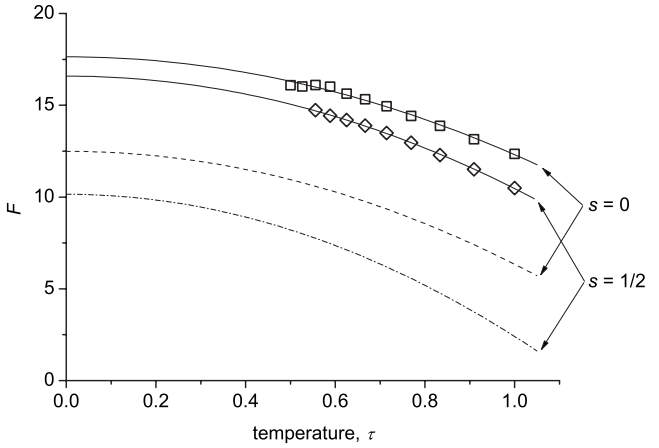

FIG. 8. Temperature dependence of free energy for the system of $N=5$ fermions with Coulomb repulsion in 3D harmonic field with spin $s=0$ (squares) and $s=1/2$ (diamonds). Lines show nonlinear least-squares fits using Eq. (35). Dashed and dash-dotted lines are exact curves for the system without interaction, spin $s=0$ and $s=1/2$ correspondingly. Simulation conditions: see Fig. 5.

for 6 and 7 particles (not shown) and built a set of Hamiltonians in the form (32). Using fits based on Eq. (34) in β-scale (not shown) and Eq. (35) (Fig. 10) in τ scale we obtained the following estimations of the ground-state energies: for $N=6$ $E_0 = 21.3 \pm 0.1$ and for $N=7 - E_0 = 26.1 \pm 0.4$ (for noninteracting particles $E_0 = 13$ and $E_0 = 15.5$ correspondingly).

IV. CONCLUSIONS

We have presented a combined path integral—expanded-ensemble Monte Carlo method with Wang-Landau algorithm for simulating system of many fermions. It was shown that the proposed approach provides reasonably accurate results with comparatively small computational effort. Typical cal-

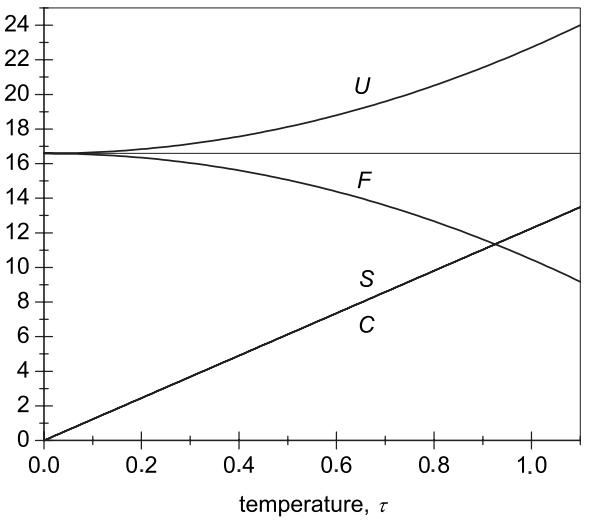

FIG. 9. Low-temperature thermodynamics for the system of $N=5$ fermions with Coulomb repulsion in 3D harmonic field, $s=1/2$.

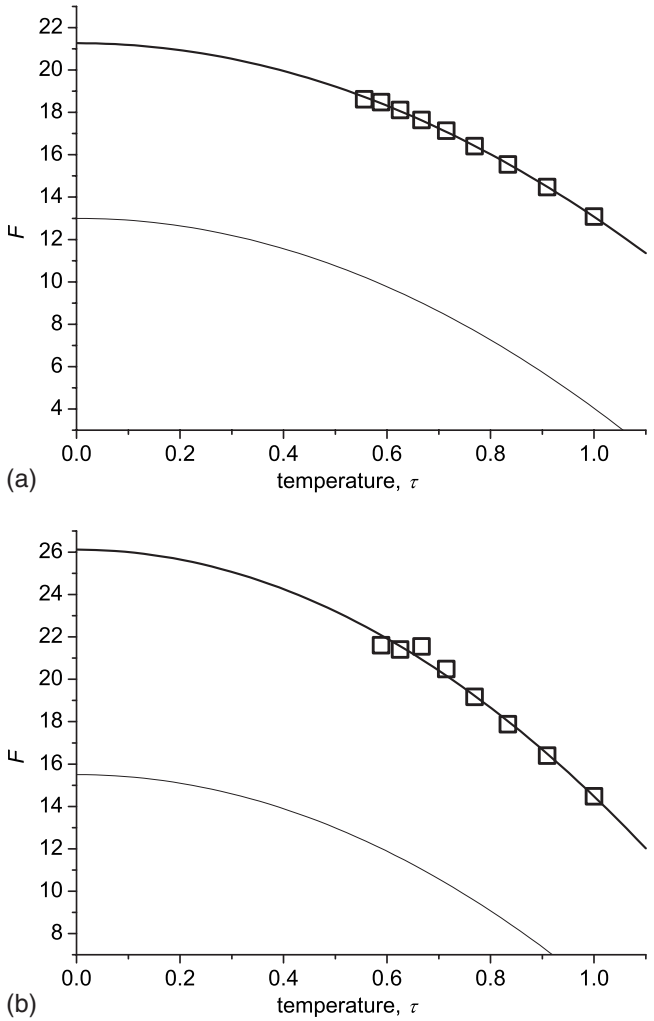

FIG. 10. Temperature dependence of free energy for the system of (a) $N=6$ and (b) $N=7$ fermions with Coulomb repulsion in 3D harmonic field, $s=1/2$. Lines show nonlinear least-squares fits using Eq. (35). Thin lines are exact data for corresponding systems without interaction.

culation time per one point ranged from 1 h for a system of two particles without interaction up to 40 h for helium atom on a single Pentium 4 node. Method can be combined with other approaches, for example the one using idempotent density matrices [9] or bead-Fourier path integrals [19]. It is also worth to point out here that in most of our calculations we used the simplest form of high-temperature approximation for the density matrix known as the "bead" form (see Eq. (6)). Meanwhile in a series of recent works [32–34] there were constructed other forms of discrete action which seemingly could benefit to PIMC simulations including those performed in the present paper. These improvements could appear to be helpful in our further work though a special comparative study here is apparently required. Also method can be straightforwardly parallelized, that is very important for simulation of many particles systems.

Though the presented approach does not bring a complete solution of the sign problem, it has two important advantages. First, the EE-WL technique provides very accurate, close to the optimal, estimation of the thin balance between positive and negative contributions to the fermionic PF at low temperatures. Advantages of the expanded-ensemble technique for precise estimation of free-energy differences have been discussed elsewhere [21,22], and, being applied to computations of the ratio of path integral partition functions, it allows to descend to lower temperatures compared to standard sampling techniques. Second, the EE method gives direct access to the free energy and hence thermodynamic of the system. Examples of simulation of model systems with 5–7 interacting fermions show that with the presented approach it is possible to extract information about the ground-state energy as well as on low-temperature thermodynamics.

Finally it should be pointed out that we tried to check the reliability of the proposed approach wherever it was possible. Thus, in Sec. III A we compared our simulation results with the exact data for $N=2$ and $N=3$ noninteracting fermions in 3d harmonic field, Figs. 2 and 3. Similar comparison was made in Sec. III D for $N=5$, Fig. 5. Results obtained for He atom we compared with experimental values of the ground-state energies for singlet and triplet states of Helium, Sec. III C. Our data for two particles with Coulomb repulsion in 1D harmonic field was compared with appropriate results of other authors in Sec. III B. Unfortunately we could not find appropriate literature results for $N=5-7$ to check our simulation data.

ACKNOWLEDGMENTS

The work has been supported by the Russian Foundation for Basic Research (RFBR), (Grant No. 08-02-00041a) and by the Swedish Royal Academy of Sciences.

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