Diffusion Monte Carlo for fermions with replica reduction

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We propose an improved framework of diffusion Monte Carlo method for quantum many-fermion systems. This approach enables us to find the ground state of the system without any *a priori* information on the nodal structure of the wave function. The main idea in this approach is to use sign-carrying replicas which are the basis vectors in a restricted Hilbert space. For efficiency, we propose to reduce the number of replicas in a proper manner. We test our method on a spinless fermion system, and compare the results with the exact values. We also discuss this method in relation to exact diagonalization.

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For many-fermion systems, it is difficult, in general, to diagonalize the Hamiltonian and find the exact ground-state energy, because the dimension of the Fock space increases exponentially with the system size. In order to circumvent this difficulty, one can use the Lanczös method,[1] or the density matrix renormalization group.[2] The Lanczös method, however, can be applied only to systems with limited size. On the other hand, the density matrix renormalization group method cannot handle long-range interactions. The so-called fermion Monte Carlo formalism was invented to treat many-fermion systems in continuum space.[3] A detailed study showed that there are still uncontrolled approximations in the fermion Monte Carlo methods.[4] Furthermore, it is known that usual quantum Monte Carlo formalisms in continuum space suffer from severe sign problems.[5]

Recently, a new fermion Monte Carlo has been proposed to simulate correlated many-fermion systems in Slater determinant space.[6–8] The key achievement of this method is to ensure convergence to the solution of full configuration without any *a priori* information regarding the nodal structure of the wave function. Using a Monte Carlo method, even excited states can be calculated by eliminating the components of the lower states from the imaginary-time propagator.[9]

In this paper, following the procedure of diffusion Monte Carlo,[10–13] we propose an improved scheme for the new fermion Monte Carlo by using a replica reduction. Furthermore, we argue that, when there are symmetries in systems, it is necessary to restrict the replicas to walk only in the reduced Hilbert space. By introducing the concept of guiding state,[14] we determine the ground state without any guessing. For spinless fermion systems, we compare the exact values with those obtained by our method. In this approach, we show that we do not encounter the sign problem.

For a given Hamiltonian H, introducing an energy shift E and the inverse of energy τ, we consider a formal solution of the imaginary-time Schrödinger equation

$$|\Psi(\tau)\rangle = \pm \exp\{-(H - E)\tau\}|\Psi(0)\rangle. \tag{1}$$

As τ goes to infinity, with the properly chosen E, the state $|\Psi(\tau)\rangle$ becomes the ground state. This is the basic idea of the diffusion Monte Carlo method. We will discuss more on the $\pm$ sign included in Eq. (1) when we introduce replicas, which are the basis vectors performing random walks in this diffusion Monte Carlo.

For a M-fermion system, the simplest basis $\{|i\rangle\}$, which we call *easy basis*, is represented by a set of Slater determinants as

$$|i\rangle = c_{i_1}^\dagger c_{i_2}^\dagger \cdots c_{i_M}^\dagger |0\rangle \quad (i_1 < i_2 < \cdots < i_M). \tag{2}$$

Here, note that several subindices can be combined into the index i_n in the creation operator $c_{i_n}^\dagger$. For instance, a momentum and a spin are represented by a single index.

If there is no symmetry at all in H, this easy basis $\{|i\rangle\}$ should be used straightforwardly. However, when symmetries are involved, we should block diagonalize the matrix of H. In this case, any states in a decomposed space should not cross into other decomposed spaces in the diffusion Monte Carlo process. Since we should restrict the Hilbert space, we should find a proper basis. There are many methods to decompose the Hilbert space for systems with translation, rotation, reflection symmetries,[15,16] as well as spin symmetries.[17] Unless we make symmetry breaking explicitly in the Hamiltonian, we should restrict the Hilbert space until no further reduction through block diagonalization can be done. In the Lanczös method, we do this reduction only for saving of memory space but which is not mandatory. However, in the diffusion Monte Carlo method, the restriction of the Hilbert space is essential if the size of energy fluctuation is larger than energy differences between ground-state energies in different sectors.

For systems having symmetries, the process of restricting the Hilbert space is essentially equivalent to finding the symmetrized basis $\{|b_i\rangle\}$ in terms of the easy basis. It is well known in group representation theory[18] that, in order to find $\{|b_i\rangle\}$, we should use projection operators $p_{\alpha\beta}$ written as

$$p_{\alpha\beta} = \frac{n}{g} \sum_{t \in G} r_{\beta\alpha}(t^{-1}) \rho_t, \tag{3}$$

where n is the dimension of representation, g is the order of symmetry group G with group elements t, $r_{\beta\alpha}$ is the irreducible representation matrix elements, and ρ_t is the operator acting on the Hilbert space. Using $p_{\alpha\beta}$, we decompose the Hilbert space $\mathcal{H}$ as

$$\mathcal{H} = \bigoplus_{i=1}^{h} V_i^{\oplus m_i} = \bigoplus_{i=1}^{h} \left(\bigoplus_{\alpha=1}^{n_i} V_{i,\alpha}^{\oplus m_i} \right), \tag{4}$$

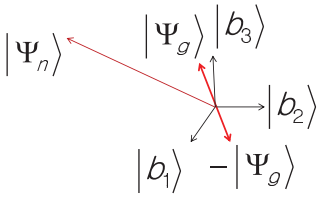

FIG. 1. (Color online) The normalized ground state $|\Psi_g\rangle$ is represented in terms of the basis $|b_i\rangle$, where the sign of the ground state is arbitrary. The state $|\Psi_n\rangle$, which is not normalized, is used in order to approximate the ground state.

where h is the number of irreducible representations, m_i is the multiplicity, and n_i is the dimension of the corresponding irreducible representation. Note that the vector space V_i is unique, while $V_{i,\alpha}$ depends on our choice of basis $\{|b_i\rangle\}$. Within the m_i-dimensional restricted space $V_{i,\alpha}^{\oplus m_i}$, we represent the Hamiltonian H in a $m_i \times m_i$ matrix C as

$$H|b_i\rangle = \sum_j C_{ji}|b_j\rangle, \tag{5}$$

where the matrix elements C_{ji} of C are given by complex numbers in general.

Once we find C in the symmetrized basis, we can divide C into two parts: diagonal A and off-diagonal B as

$$C = A + B. \tag{6}$$

With a small step $\Delta\tau = \tau/T$, we introduce the Suzuki-Trotter decomposition as

$$\begin{aligned} &\pm\exp\{-(H-E)\tau\} \to \pm\exp\{(E-C)\tau\} \\ &\quad = [\pm\exp\{(E-C)\Delta\tau\}]\cdots[\pm\exp\{(E-C)\Delta\tau\}] \\ &\quad \approx [\pm\exp\{(E-A)\Delta\tau\}\exp(-B\Delta\tau)] \\ &\qquad \cdots[\pm\exp\{(E-A)\Delta\tau\}\exp(-B\Delta\tau)]. \end{aligned} \tag{7}$$

We note that in most cases of physical interests, the matrix $D \equiv \exp(-B\Delta\tau)$ has negative elements. This is the origin of the sign problem.[19–21]

In a typical diffusion Monte Carlo, we approximate the ground state $|\Psi_g\rangle$ by $|\Psi_n\rangle$. We let $|\Psi_n\rangle$ perform random walks generating $|\Psi_{n+1}\rangle$, $|\Psi_{n+2}\rangle$, and so on. Finally we sum the states to find the ground state. However, as shown in Fig. 1, the state $|\Psi_n\rangle$ will wander around $|\Psi_g\rangle$ and sometimes may move close to $-|\Psi_g\rangle$ if negative elements are included in D. Then $|\Psi_n\rangle$ will wander around $-|\Psi_g\rangle$ also for some period of time. In this case, we may obtain a zero wave function for an averaged state. Thus, it is necessary to make a restriction on random walks. This restriction is incorporated in the process of *Flip*, which will be explained later.

In order to handle negative values in D and $|\Psi_n\rangle$, we extract the minus part of $D^{(-)}$ from D and rewrite D as $D = D^{(+)} - D^{(-)}$. Simultaneously we consider the minus part of $|\Psi^{(-)}\rangle$ from $|\Psi\rangle$ and rewrite it as $|\Psi\rangle = |\Psi^{(+)}\rangle - |\Psi^{(-)}\rangle$. Then, we can find the wave-function evolution as

$$\begin{aligned} D|\Psi_n\rangle &= (D^{(+)} - D^{(-)})(|\Psi_n^{(+)}\rangle - |\Psi_n^{(-)}\rangle) \\ &\to \begin{pmatrix} D^{(+)} & D^{(-)} \\ D^{(-)} & D^{(+)} \end{pmatrix}\begin{pmatrix} |\Psi_n^{(+)}\rangle \\ |\Psi_n^{(-)}\rangle \end{pmatrix} = \begin{pmatrix} |\Psi_{n+1}^{(+)}\rangle \\ |\Psi_{n+1}^{(-)}\rangle \end{pmatrix} \\ &\to |\Psi_{n+1}^{(+)}\rangle - |\Psi_{n+1}^{(-)}\rangle = |\Psi_{n+1}\rangle. \end{aligned} \tag{8}$$

We employ the spinorlike notation in the above in order to identify the effect of the sign. For an explicit numerical example for $D|\Psi_n\rangle$, we note

$$\begin{aligned} &\begin{pmatrix} 1 & -5 & 3 \\ -5 & 6 & 1 \\ 3 & 1 & -4 \end{pmatrix}\begin{pmatrix} 1 \\ -3 \\ 2 \end{pmatrix} \\ &\to \begin{pmatrix} 1\,0\,3\,0\,5\,0 \\ 0\,6\,1\,5\,0\,0 \\ 3\,1\,0\,0\,0\,4 \\ 0\,5\,0\,1\,0\,3 \\ 5\,0\,0\,0\,6\,1 \\ 0\,0\,4\,3\,1\,0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 2 \\ 0 \\ 3 \\ 0 \end{pmatrix} = \begin{pmatrix} 22 \\ 2 \\ 3 \\ 0 \\ 23 \\ 11 \end{pmatrix} \\ &\to \begin{pmatrix} 22 \\ 2 \\ 3 \end{pmatrix} - \begin{pmatrix} 0 \\ 23 \\ 11 \end{pmatrix} = \begin{pmatrix} 22 \\ -21 \\ -8 \end{pmatrix}. \end{aligned} \tag{9}$$

Here the key observation is that all numbers in the middle of the above equation are positive or zero. Thus, as far as we use the doubly enlarged space, it is conceptually possible to interpret the numbers as probabilities for random walks.

In order to find the ground state with as small memory as possible, we employ a Monte Carlo method.[22,23] We first represent $|\Psi_n\rangle$ in terms of integer multiples of basis as

$$|\Psi_n\rangle = \sum_i N_{ni}|b_i\rangle, \tag{10}$$

where N_{ni} can be negative integers. However, in the doubly enlarged space, the walkers are $|b_i\rangle$ or $-|b_i\rangle$ and the total number of walkers N_n is equal to $\sum_i |N_{ni}|$. The wave-function evolution from $|\Psi_n\rangle$ to $|\Psi_{n+1}\rangle$ is described by our algorithm of four steps which we explain below: *Walk, Branch, Cancel*, and *Flip*.

Walk. We now focus on the random walk of the symmetrized basis $|b_i\rangle$. For example, in Eq. (9), there are $6 = 1 + |-3| + 2$ walkers, which are one $|b_1\rangle$, three $-|b_2\rangle$'s, and two $|b_3\rangle$'s. A walker of $-|b_2\rangle$ will go to $|b_1\rangle$ with probability $\frac{5}{12}$, $-|b_2\rangle$ with probability $\frac{6}{12}$, and $-|b_3\rangle$ with probability $\frac{1}{12}$.

In fact, we find that, with known matrix elements D_{ji} of D, the replica $|R\rangle$ walks in the doubly enlarged space as

$$|R\rangle = \text{sign}(N_{ni})|b_i\rangle \to |R'\rangle = \text{sign}(D_{ji}) \times \text{sign}(N_{ni})|b_j\rangle,$$

where $\text{sign}(x)$ is -1, 0, 1 when $x < 0$, $x = 0$, $x > 0$, respectively. The corresponding transition probability is given by

$$\frac{D_{ji}^{(+)} + D_{ji}^{(-)}}{\sum_k (D_{ki}^{(+)} + D_{ki}^{(-)})} = \frac{|D_{ji}|}{\sum_k |D_{ki}|}. \tag{11}$$

We emphasize again that the values of $D_{ji}^{(+)}$ and $D_{ji}^{(-)}$ cannot be nonzero simultaneously.

Since D is a huge matrix in general, we need to truncate D. We propose an approximation as follows. For a small $\Delta\tau$, we find $D \approx 1 - B\Delta\tau$ in the first order of $\Delta\tau$. Hence, when a replica state walks from $|b_i\rangle$ to $|b_j\rangle$, nonzero values of B determine the next states $|b_j\rangle$ up to $O(\Delta\tau)$. Thus we consider

a small space whose basis vectors are connected from $|b_i\rangle$ such as

$$|b_i\rangle \cup \{|b_j\rangle | C_{ji} \neq 0\} = \{|b_i\rangle \equiv |j_0\rangle, |j_1\rangle, |j_2\rangle, \ldots, |j_m\rangle\}.$$

With this truncated space, we approximate D and find a manageable number of D_{ki} as

$$D|b_i\rangle = D|j_0\rangle \approx \sum_{k=0}^{m} D_{ki}|j_k\rangle. \tag{12}$$

The procedure to find D_{ki} is simple. We first write the matrix elements of B connected to $|b_i\rangle$ such as

$$B \approx \begin{pmatrix} 0 & C^*_{j_1 j_0} & \cdots & C^*_{j_m j_0} \\ C_{j_1 j_0} & 0 & & C^*_{j_m j_1} \\ \vdots & & \ddots & \\ C_{j_m j_0} & C_{j_m j_1} & & 0 \end{pmatrix}.$$

Then, we diagonalize the above matrix, and find that

$$B \approx \sum_a |\lambda_a\rangle \lambda_a \langle \lambda_a| \quad \text{and} \quad |\lambda_a\rangle = \sum_l U_{la}|b_l\rangle,$$

where $|\lambda_n\rangle$ are eigenvectors with the corresponding unitary matrix U. In consequence, we find a manageable number of matrix elements,

$$D_{ki} = \sum_{a=0}^{m} U_{ka} \exp(-\lambda_a \Delta\tau) U^{\dagger}_{a0}. \tag{13}$$

This approximation would be improved if we include more connected states produced by B^2.

Branch. As we see in Eq. (7), we have to handle the proportional factor $\exp\{(E - A)\Delta\tau\}$. After the random walk from $|b_i\rangle$ to $|b_j\rangle$ up to sign, the branching process is taken into account by using the factor F,

$$F = \exp\{(E - \langle b_j|H|b_j\rangle)\Delta\tau\} \sum_k |D_{ki}|, \tag{14}$$

where $\sum_k |D_{ki}|$ is due to the probability normalization in Eq. (11). Adopting the usual rule of birth-death process, we replicate the replica as many as $\text{int}(F + u)$, where u is a random number uniformly distributed in the interval $[0, 1]$.

Cancel. It is crucial to take the procedure of cancellation as shown in $|\Psi^{(+)}_{n+1}\rangle - |\Psi^{(-)}_{n+1}\rangle$ in Eq. (8). In fact, after all replicas perform random walks and branching, we have to find the difference between the number of $|b_j\rangle$ walkers and the number of $-|b_j\rangle$ walkers. As a result, we find the next-step replica numbers N_{n+1i}, which are positive or negative, for each symmetrized basis $|b_i\rangle$.

Flip. As shown in Eq. (1), the sign of the ground state $|\Psi_g\rangle$ is not determined. It is necessary to choose the sign in front of $|\Psi^{(+)}_{n+1}\rangle - |\Psi^{(-)}_{n+1}\rangle$ in order for $|\Psi_{n+1}\rangle$ to wander around only one among $|\Psi_g\rangle$ and $-|\Psi_g\rangle$. Using the guiding state $|\psi_g\rangle$ which is the sum of all previous replicas,

$$|\psi_g\rangle = \sum_{c=0}^{n} |\Psi_c\rangle, \tag{15}$$

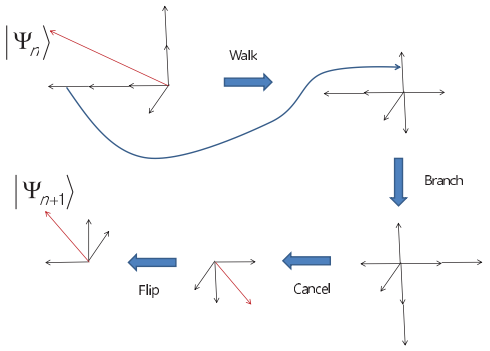

FIG. 2. (Color online) The state $|\Psi_n\rangle = |b_1\rangle - 3|b_2\rangle + 2|b_3\rangle$ walks into $|\Psi_{n+1}\rangle = -|b_1\rangle - |b_2\rangle + |b_3\rangle$ through the steps of Walk, Branch, Cancel, and Flip. In the process of Walk, a typical transition from $-|b_2\rangle$ to $|b_3\rangle$ is represented by using the curved arrow. In the process of Branch, the numbers of $\pm|b_i\rangle$ are changed. In the process of Cancel, the differences between the numbers of $|b_i\rangle$ and $-|b_i\rangle$ are calculated. After the process of Flip, we finally find the state $|\Psi_{n+1}\rangle$, which undergoes the four processes again.

we determine the sign in Eq. (7) with the following rule. For the case where the state $|\Psi_n\rangle$ walks into $|\Psi^{(+)}_{n+1}\rangle - |\Psi^{(-)}_{n+1}\rangle$, we calculate the overlap I as

$$I = \langle\psi_g|(|\Psi^{(+)}_{n+1}\rangle - |\Psi^{(-)}_{n+1}\rangle). \tag{16}$$

We choose the sign as plus if $I \geqslant 0$ or minus otherwise. Choosing the minus sign means flipping all replicas,

$$N_{n+1i} \to -N_{n+1i}. \tag{17}$$

Up to Flip, a cartoonlike numerical example is shown in Fig. 2.

Count. After the flip process, we have obtained another approximation $|\Psi_{n+1}\rangle$ to the ground state. This approximation is used to update the guiding state. Eventually the guiding state $|\psi_g\rangle$ becomes the ground state $|\Psi_g\rangle$ in the restricted Hilbert space. We also update the energy shift E using the energy expectation value with the guiding state:

$$E = \frac{\langle\psi_g|H|\psi_g\rangle}{\langle\psi_g|\psi_g\rangle}. \tag{18}$$

Since the true ground-state energy is always lower than any E, one may guess that the number of replicas will increase gradually. However, we find that there is some peak in the number of replicas during the simulation. And then all replicas eventually die out in the long run. In diffusion Monte Carlo, the extinction of replicas happens when the shift energy is lower than the ground-state energy. This controversy has originated from the truncation of D, since the approximated branching factor F is less than the exact value F_{exact} at the extinction of replicas:

$$\frac{F}{F_{\text{exact}}} = \exp\{(E - E_{\text{true}})\Delta\tau\} \frac{\sum_k |D_{ki}|}{\sum_k |D_{ki}|_{\text{full}}} < 1. \tag{19}$$

As far as the difference $\sum_k |D_{ki}|_{\text{full}} - \sum_k |D_{ki}|$ is in the order of $(\Delta\tau)^2$, we conclude that the expectation value E approaches the true ground-state energy E_{true} up to the order of $\Delta\tau$. The Suzuki-Trotter decomposition whose error is of the order of $(\Delta\tau)^2$ is not the main approximation in the procedure.[24]

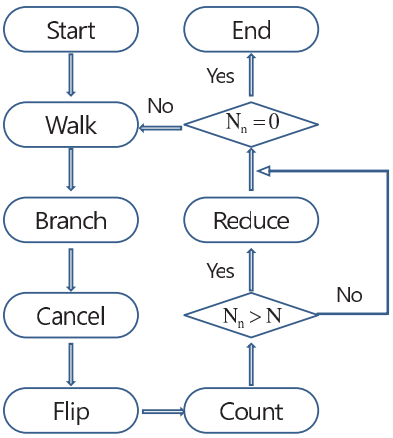

FIG. 3. (Color online) Flowchart for the algorithm in diffusion Monte Carlo for fermions with replica reduction.

Reduce. One may notice a drawback in this process. It is true that, when we handle a large fermion system, the number of replicas grows quickly and exceeds the limit of our resources: memory space and CPU time. In order to overcome this drawback, we propose the replica reduction. Whenever the number of replicas becomes bigger than some upper bound limit N, we reduce the replica numbers N_{n+1i} as

$$N_{n+1i} \to \text{sign}(N_{n+1i})\text{int}(f|N_{n+1i}| + u), \tag{20}$$

where the reduction factor f is sufficiently smaller than 1, and the random number u is distributed uniformly in $[0,1]$. Whenever the replica reduction takes place, the survivors become more important. This should be taken into account when we update the guiding state. We save Z when we do the Zth reduction so far. The power Z is used to update the guiding state as

$$|\psi_g\rangle \to |\psi_g\rangle + \frac{1}{f^Z}\sum |R\rangle. \tag{21}$$

We note that, as simulation goes on, the remaining replicas make the bigger contribution to the ground state.

The algorithm cycle for our method is described in Fig. 3. As we will see, if the number of replicas N_n in Fig. 3 does not become zero, the simulation runs in the loop of the cycle.

Now we present some results obtained by our method for the ground-state energy and wave function in a spinless fermion system.[25] The corresponding Hamiltonian is written as

$$H = t\sum_{i=1}^{L-1}(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + V\sum_{i=1}^{L-1} n_i n_{i+1}, \tag{22}$$

where $n_i = c_i^\dagger c_i$ and the single-particle states are characterized by the index i running from 1 to L. Since the Hamiltonian does not contain $c_L^\dagger c_1$, $c_1^\dagger c_L$, and $n_L n_1$, the translational symmetry is broken. The only symmetry is the reflection R, which acts on the Fock space such as

$$Rc_i^\dagger = c_{L+1-i}^\dagger R, \quad R|0\rangle = |0\rangle. \tag{23}$$

The symmetry group is $\{1,R\}$, and the one-dimensional irreducible representations Γ_1 and Γ_2 are given by

$$\Gamma_1: \quad r_{11}(1) = 1, \quad r_{11}(R) = 1,$$
$$\Gamma_2: \quad r_{11}(1) = 1, \quad r_{11}(R) = -1.$$

Thus, the Hilbert space is divided into two subspaces, which we call the Γ_1 sector and the Γ_2 sector. For the M-fermion case, the typical symmetrized bases before normalization are given by

$$(1+R)c_{i_1}^\dagger \cdots c_{i_M}^\dagger|0\rangle \quad \text{for } \Gamma_1 \text{ sector},$$
$$(1-R)c_{i_1}^\dagger \cdots c_{i_M}^\dagger|0\rangle \quad \text{for } \Gamma_2 \text{ sector}.$$

When we consider normalization, we should pay attention to some special bases which are eigenstates of R such as $Rc_{i_1}^\dagger \cdots c_{i_M}^\dagger|0\rangle = \pm c_{i_1}^\dagger \cdots c_{i_M}^\dagger|0\rangle$. With these symmetrized bases, we find the ground-state energy and wave function.

For the case of $L = 13$ and $M = 6$, we find the 848 dimensional Γ_1 sector and the 868 dimensional Γ_2 sector. Our method provides us with the ground-state energy in each sector, where the ground state in the Γ_1 sector is the first excited state in the system. The numerical results are summarized in Table I for the model of $t = 1$ and $V = 1$, where we compare them with the exact ground-state energy.

In order to see the effect of the upper bound number N, we also simulate with small numbers. The number of replicas and the ground-state energy of each cycle are presented in Fig. 4, where the upper bound replica number N is given by 200, 300, 400, 500, and 1000. We observe that a very small upper bound number makes no convergence toward the ground state. With a small number of replicas, the step of cancellation is not sufficient. It seems that there is a critical

TABLE I. Numerical results on the ground-state energy of Γ_1 and Γ_2 sectors in spinless fermion system of $t = 1$ and $V = 1$ for a small system of $L = 13$ and $M = 6$ with $f = \frac{1}{2}$. With the smaller time step $\Delta\tau$ and the bigger upper bound number N, the longer simulation time is needed to approach closer to the exact values of $-6.266\,05$ and $-6.813\,12$. The fluctuation of the energy values is roughly of the order of $\Delta\tau$. We find that the norm of wave-function difference $\|\Psi_{\text{MC}} - \Psi_{\text{exact}}\|$ is given by 0.016 503 for the Γ_2 sector and 0.020 135 for the Γ_1 sector in the case of $\Delta\tau = 0.001$ and $N = 200\,000$.

$\Delta\tau \setminus N$	2000	20 000	200 000
0.01	−6.22300, −6.76496	−6.24783, −6.79147	−6.25211, −6.79304
0.005	−6.24803, −6.77069	−6.25876, −6.80500	−6.26221, −6.80807
0.002	−6.25109, −6.79992	−6.26178, −6.81094	−6.26524, −6.81214
0.001	−6.25344, −6.81046	−6.26527, −6.81215	−6.26581, −6.81283

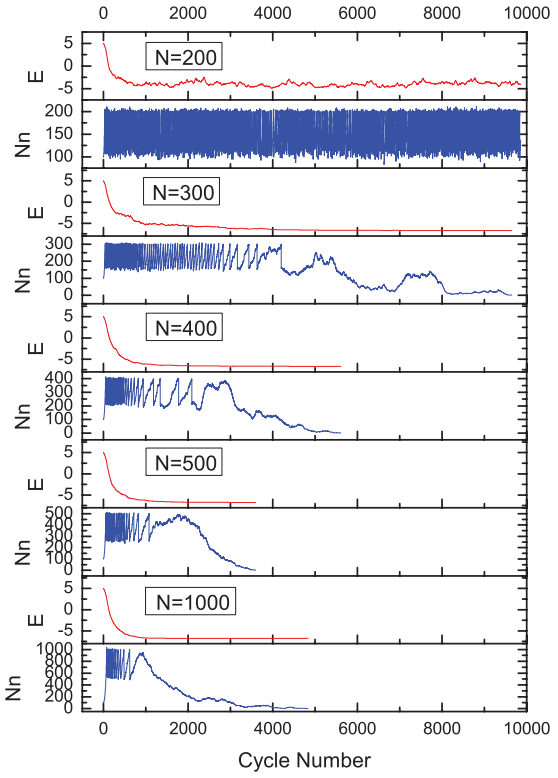

FIG. 4. (Color online) For each upper bound number $N = 200$, $N = 300$, $N = 400$, $N = 500$, and $N = 1000$, the ground-state energy E and the number of replicas N_n are shown in the condition of Table I with $\Delta\tau = 0.01$. The final ground-state energy is given by $-6.705\,16$ for $N = 300$, $-6.688\,63$ for $N = 400$, -6.7446 for $N = 500$, and $-6.761\,57$ for $N = 1000$. The number of the last cycle is given by 9645 for $N = 300$, 5606 for $N = 400$, 3592 for $N = 500$, and 4837 for $N = 1000$, while the simulation with $N = 200$ never ends.

value for the upper bound replica number in simulations. If the upper bound replica number N is less than a certain value N_c, which is between 200 and 300 in this example, we guess that the random walkers itinerate forever.

In order to test stability of the method, we calculate the ground-state energy up to ten fermions at the filling factor $\frac{1}{2}$, as shown in Table II. We observe the replica number diminishing to zero in all cases.

In order to compare this Monte Carlo method with exact diagonalization, let us consider the memory space. Since exact diagonalization by iteration needs at least two states, which are the initial state $|\psi_0\rangle$ and the resulting state $H|\psi_0\rangle$,

TABLE II. Monte Carlo (MC) results on ground-state energy of Γ_1 and Γ_2 sectors in a spinless fermion system of $t = 1$ and $V = 1$. We compare them with exact diagonalization (ED) results. The number of fermions increases from $M = 6$ to $M = 10$, while the filling factor is fixed as $L = 2M$. We fix the parameters as $\Delta\tau = 0.01$ and $f = \frac{1}{2}$. The upper bound number N should be increased as many fermions are involved. The exact ground-state energies are integers because of the specific value of $t = 1$ and $V = 1$ at half filling. We find the trend of less accuracy as many fermions are involved.

M	L	N	MC in Γ_1	ED in Γ_1	MC in Γ_2	ED in Γ_2
6	12	900	−5.32(3)	−5.40414	−5.96(2)	−6
7	14	3400	−6.92(3)	−7	−6.39(4)	−6.47936
8	16	12000	−7.92(4)	−8	−7.44(4)	−7.53782
9	18	48000	−8.48(5)	−8.58455	−8.87(8)	−9
10	20	180000	−9.46(9)	−9.62274	−9.82(11)	−10

the minimal memory space in exact diagonalization would be $m_i + m_i$ when we repeatedly calculate the Hamiltonian elements, where m_i is the restricted Hilbert space dimension. On the other hand, our Monte Carlo method needs roughly $m_i + 0.5m_i$ for the guiding state and replicas. We find that slightly less memory space is required in the Monte Carlo method, in principle. However, we need a longer simulation time but achieve a relatively lower accuracy.

Another useful application of this diffusion Monte Carlo method would be the case where a given Hamiltonian includes random parameters,[26,27] for instance, the Anderson localization model. Exact diagonalization is not adequate as far as the Hamiltonian contains random parameters. However, our method makes it possible to simulate systems without fixing parameters.

In summary, we have presented an improved diffusion Monte Carlo method to obtain the ground-state energy and wave function in a system where fermions are involved. Real physical applications will be possible if we find an efficient parallel computing scheme.

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