Density-matrix renormalization-group method in momentum space

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A momentum-space approach of the density-matrix renormalization-group (DMRG) method is developed. Ground-state energies of the Hubbard model are evaluated using this method and compared with exact diagonalization as well as quantum Monte Carlo results. It is shown that the momentum-space DMRG is a very useful numerical tool for studying the Hubbard model and other fundamental models of interacting electrons in two dimensions. For the Hubbard model in two dimensions, the momentum-space DMRG method reproduces accurately the exact diagonalization results of ground-state energies on a 4×4 lattice and yields new upper bounds of ground-state energies on an 8×8 lattice. [S0163-1829(96)52416-1]

The real-space density-matrix renormalization-group (DMRG) method, which was proposed by White[1] in 1992, is a powerful method for studying ground-state properties of interacting electrons or spins. It has been successfully applied to various one-dimensional (1D) quantum models, such as the spin Heisenberg model,[1,2] the Kondo lattice model,[3] the Hubbard model,[4] and other models.[5] However, in 2D its application is still not satisfactory.[6] In this paper we generalize the DMRG method to momentum space. We hope this may enlarge the range of application of the DMRG method and provide an accurate numerical method for studying interacting electrons in 2D. We shall take the Hubbard model as an example to show how the DMRG method works in momentum space. The properties of the Hubbard model have been extensively studied in both one and two dimensions, and so this provides a good background for comparing the momentum-space DMRG method with other methods.

The DMRG method is a diagonalization technique which attempts to use a small number of states, say m states, to expand the ground state (or some low-energy excitation states) accurately. In conventional numerical renormalization-group (RG) methods, one keeps the m lowest-energy eigenstates of a block Hamiltonian.[7–9] In the DMRG method, however, one keeps the m most probable basis states in describing the ground state of a larger block, called a superblock. A superblock contains two blocks, a system block and an environment block. In a DMRG iteration, one diagonalizes the Hamiltonian of the superblock, finds out the reduced density matrix for the system block from the ground state of the superblock, truncates the Hilbert subspace by keeping the m largest eigenstates of the density matrix, adds one or more sites to the system block to form a new superblock, and then repeats the above procedure until the desired result is obtained.

There are two approaches in constructing a superblock, an infinite-lattice approach and a finite-size approach. In the infinite-lattice approach, the environment block is generally chosen as the space reflection of the system block. In the finite-size approach, on the other hand, the size of the superblock is fixed and the environment block is chosen as the remaining part of the lattice for a given system block. The infinite-lattice approach allows the size of the superblock to be flexible and can be used to study directly the thermodynamic limit. The finite-size approach is, however, more accurate in calculating quantities for a finite-lattice system. In White's original paper, two sites are added to a superblock each time, one to the system block and the other to the environment block. This way of constructing a superblock preserves the reflection symmetry and avoids some problems caused by odd-size lattices if the infinite-lattice approach is used in 1D. However, it is generally more efficient in computation if one adds just one site to the system block and no site to the environment block when the finite-size approach is used.

The DMRG method satisfies the variational principle because it uses a small physical subspace to approximate the full Hilbert space and no unphysical states enter the truncated Hilbert subspace. Thus the ground-state energy obtained using this method is always an upper bound for the true value. The error for the ground-state energy decreases as the number of retained states is increased. The truncation error is generally smaller than the true error of the result.

The Hubbard model is defined by the Hamiltonian

$$H=-t\sum_{\langle ij\rangle\sigma} c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_{i} n_{i\uparrow}n_{i\downarrow}, \tag{1}$$

where $\langle ij\rangle$ means summation over nearest neighbors. In momentum space, it reads

$$H=\sum_{k\sigma} \epsilon_k c_{k\sigma}^{\dagger}c_{k\sigma}+\frac{U}{N}\sum_{k_1,k_2,k_3} c_{k_1\uparrow}^{\dagger}c_{k_2\uparrow}c_{k_3\downarrow}^{\dagger}c_{k_1-k_2+k_3\downarrow}, \tag{2}$$

with N the lattice size. Here the periodic boundary condition is assumed. Each momentum k point has four degrees of freedom, i.e., $\{|0\rangle,\ c_{k\uparrow}^{\dagger}|0\rangle,\ c_{k\downarrow}^{\dagger}|0\rangle,\ c_{k\uparrow}^{\dagger}c_{k\downarrow}^{\dagger}|0\rangle\}$. In the RG iteration, generally a k point with these four states can be added to a system block to form a new system block. However, in our calculation we treat the spin degree of freedom as an extra spatial coordinate and a momentum-spin point $(k\sigma)$, which has only two degrees of freedom $\{|0\rangle,\ c_{k\sigma}^{\dagger}|0\rangle\}$, as a basic unit which is added to a system block. In this case, the spin rotation symmetry is broken, but the total number of degrees of freedom of a superblock is reduced and more states can be retained at each truncation of Hilbert subspace. This can reduce truncation errors and save computer time.

For convenience in the discussion below, we label a superblock as $(A \bullet B)$, where $\bullet$ represents a momentum-spin point $(k\sigma)$ which has just been added to the system block, A represents the collection of all the momentum-spin points in the system block excluding the point $(k\sigma)$, and B represents the collection of all the momentum-spin points in the environment block. There are many ways of ordering k points in a system. In calculation, one should test a few possibilities of orders of k points and choose the one which gives the lowest ground-state energy.

The Hubbard interaction is local in real space. However, it is nonlocal in momentum space; it contains terms which link two or more k points in momentum space. The summation in the second term of (2) contains N^3 terms. They can be grouped into the terms which are defined purely in each subblock and the terms containing interactions among A, $\bullet$, and B. To evaluate matrix elements of the Hamiltonian, we find it is very useful to define the following composite operators of electrons: in block A,

$$a_0(p\sigma)=c_{p\sigma}\delta_{(p\sigma)\in A},$$

$$a_1(p\sigma)=\sum_q a_0^\dagger(q\sigma)a_0(p+q\sigma),$$

$$a_2(p)=\sum_q a_0^\dagger(q\uparrow)a_0(p+q\downarrow), \tag{3}$$

$$a_3(p\sigma)=\sum_{q_1q_2} a_0^\dagger(q_1\overline{\sigma})a_0(q_2\overline{\sigma})a_0(p+q_1-q_2\sigma)\delta_{(p\sigma)\notin A},$$

$$a_4(p)=\sum_q a_0(q\downarrow)a_0(p-q\uparrow),$$

where $\overline{\sigma}=-\sigma$; in block B, the corresponding operators can be obtained by changing (a,A) into (b,B). They are the basic operators whose matrix elements are kept and updated in our DMRG iterations. The total number of these composite operators is $6N$ at each subblock. Using these composite operators, the Hamiltonian (2) can be rewritten as $H=H_\bullet+H_A+H_B+H_{A\bullet}+H_{B\bullet}+H_{AB}+H_{A\bullet B}$, where $H_\bullet=\epsilon_k n_{k\sigma}$, H_A is the same as the Hamiltonian (2) with $c_{k\sigma}$ replaced by $a_0(k\sigma)$,

$$H_{A\bullet}=\frac{U}{N}\{n_{k\sigma}a_1(0,\overline{\sigma})+c_{k\sigma}^\dagger a_3(k\sigma)+a_3^\dagger(k\sigma)c_{k\sigma}\},$$

$$H_{AB}=\frac{U}{N}\sum_p\left\{\sum_{\sigma'}\left[\tfrac{1}{4}a_1(p\sigma')b_1(-p\overline{\sigma'})+b_0^\dagger(p\sigma')a_3(p\sigma')\right.\right.$$
$$\left.\left.+(a\leftrightarrow b)\right]+a_4^\dagger(p)b_4(p)-b_2(p)a_2^\dagger(p)\right\}+\text{H.c.},$$

$$H_{A\bullet B}=\frac{U}{N}c_{k\sigma}^\dagger\sum_p\{a_1(k-p\overline{\sigma})b_0(p\sigma)-\tilde{a}_2(p-k)b_0(p\overline{\sigma})$$
$$+\sigma b_0^\dagger(p\overline{\sigma})a_4(k+p)+(a\leftrightarrow b)\}+\text{H.c.},$$

and H_B and $H_{B\bullet}$ can be obtained from H_A and $H_{A\bullet}$ by changing a into b. In $H_{A\bullet B}$, $\tilde{a}_2(p)=a_2^\dagger(p)$ if $\sigma=\uparrow$ or $a_2(p)$ if $\sigma=\downarrow$.

The breaking of lattice symmetries in truncating basis states is an unavoidable source of errors in the DMRG method. It is also the main difficulty in using the DMRG method in real space in 2D. In real space, the translation symmetry, i.e., the momentum conservation, is broken in the DMRG method. In momentum space, however, this symmetry is preserved. This symmetry property is undoubtedly very useful. Combined with two other conserved quantities, the number of up spins $N_\uparrow$ and the number of down spins $N_\downarrow$, it can be used to block diagonalize the Hamiltonian. Not only can this save computer time, but also it allows us to keep many more eigenstates in the truncation of Hilbert space as the number of nonzero matrix elements is now significantly reduced. Basis states at each block can be classified by three quantum numbers $(N_\uparrow,N_\downarrow,P)$ with P the total momentum. For the composite operators defined in (3) it can be shown that their matrix elements are nonzero only when the difference between the momentum of the initial state and that of the final state is p.

In the DMRG method, the basis states for both the system block A and the environment block B are incomplete. If the Hamiltonian contains terms with interactions between A and B, the matrix elements of these terms will be less accurately approximated after the truncation of the Hilbert space compared with the matrix elements of other terms which are defined purely within each block. In 1D in real space one can choose A and B so that no interactions exist between A and B, i.e., $H_{AB}=H_{A\bullet B}=0$, if all terms in the Hamiltonian are local in space. In real space in 2D or in momentum space in any dimension, however, interaction terms between A and B always exist no matter how A and B are constructed. Thus in general results obtained by the DMRG method in real space in 2D or in momentum space in any dimension will not be as accurate as, for example, the ground state energy of the 1D spin-1 Heisenberg model that White and Huse obtained using the real-space DMRG method.[2]

In momentum space, different size lattices have different k points. Thus in using the DMRG method in momentum space, the size of the lattice needs to be fixed at the beginning. This means that only the finite-size approach of the DMRG method can be used in momentum space. To use the finite-size approach, however, one needs first to build up a series of initial system blocks and the corresponding environment blocks. As the infinite lattice approach of the DMRG is not applicable in this case, we shall use the conventional RG method[8,9] to build up the initial system and environment blocks. The steps in building up the initial system blocks (similarly for the environment blocks) are as follows: (1) Start from a small system block A_1, which can be handled without truncation of basis states. (2) Add a new $(k\sigma)$ point to A_1 to form a new system block A_2. (3) Diagonalize the Hamiltonian in the Hilbert space spanned by A_2. (4) Truncate the Hilbert space by retaining m lowest energy eigenstates, but restrict the number of states retained at each $(N_\uparrow,N_\downarrow,P)$ subspace not more than a small integer n. Here n is a variational parameter which should be determined so that the final result for the ground-state energy is minimized. In our calculations, we find that $n=1$ or 2 generally gives the best result for the ground-state energy for 8×8 systems with 1000 states retained. The reason for limiting the number of retained states at each $(N_\uparrow,N_\downarrow,P)$ sub-

TABLE I. Comparison of the ground-state energy per site obtained using the DMRG method in momentum space with that obtained in real space at half-filling on a 16-site chain.

	Momentum space		Real space (Ref. 11)	
m	$U=1$	$U=4$	$U=1$	$U=4$
400	-1.02925	-0.51316	-1.02958	-0.575896
600	-1.02944	-0.53574	-1.02969	-0.575900
800	-1.02952	-0.53724	-1.02972	-0.575901
1000	-1.02958	-0.54562		
1200	-1.02959	-0.55218		

space is to prevent the retained states from being centralized in a few $(N_\uparrow,N_\downarrow,P)$ subspaces in A_2. Otherwise, some of the $(N_\uparrow,N_\downarrow,P)$ subspaces in A_2, which may make a substantial contribution to the final ground-state energy, may be neglected in the DMRG iterations later. (5) Replace A_2 by A_1 and repeat steps 2–5 until all the initial system blocks required are established.

All $(N_\uparrow,N_\downarrow,P)$ subspaces that a system block can have are determined purely by the $(k\sigma)$ points the block contains. In the above initialization step, in fact, not all $(N_\uparrow,N_\downarrow,P)$ subspaces in a system (or environment) block need be considered. If a subspace with the quantum numbers $(N_{1,\uparrow},N_{1,\downarrow},P_1)$ in a system (environment) block cannot find a subspace with the quantum numbers $(N_{2,\uparrow},N_{2,\downarrow},P_2)$ in the corresponding environment (system) block such that $(N_{1,\uparrow}+N_{2,\uparrow},N_{1,\downarrow}+N_{2,\downarrow},P_1+P_2)$ is equal to the quantum numbers of the ground state required, then this $(N_{1,\uparrow},N_{1,\downarrow},P_1)$ subspace in the system (environment) block will make no contribution to the ground state and can be ignored.

After the above initialization step, the *finite-size approach of the DMRG method* will be used to find out the eigenvalue and eigenfunction of the ground state for a given filling factor and momentum. Now m largest eigenstates of the *density matrix* are retained at each truncation of Hilbert space and the number of retained states at each $(N_\uparrow,N_\downarrow,P)$ subspace will no longer be limited.

We have evaluated ground-state energies of the Hubbard model in both 1D and 2D using this momentum-space DMRG method. In most of our calculations 1000 states are retained at each truncation of basis states. The number of states retained at each $(N_\uparrow,N_\downarrow,P)$ subspace on average is small. Our results are much better than those obtained by the conventional RG method.[9] For a ten-electron system with $U=4$ (the energy is measured in units of t, i.e., $t=1$) in 2D, for example, the momentum-space DMRG result for the ground-state energy with 1000 states kept is -19.57, which is much lower than the conventional RG result with even 3000 states kept, -18.541 (Ref. 9) (their relative errors with respect to the exact diagonalization result[10] are 0.05% and 5%, respectively).

Table I compares the ground-state energies obtained by the DMRG method in momentum space with those obtained in real space[11] at half-filling in 1D. The ground-state energies obtained by the DMRG method are lower in real space than in momentum space if the same number of states is kept, which means that in 1D the DMRG method works better for the Hubbard model in real space than in momentum space. This is not surprising because the Hubbard interaction is a local interaction and at half-filling all electrons are localized in space as a result of a Mott insulator transition.

Table II compares the momentum-space DMRG results with the exact diagonalization and the quantum Monte Carlo results on 2D square lattices. The largest lattice we have studied so far is 12×12. Compared with the exact results on a 4×4 lattice, we find that the DMRG results are very accurate when U is small. The relative error for the DMRG result with $U=2$ is 3×10^{-4}. The momentum-space DMRG method works better in the weak-coupling limit because the single-particle basis state used here is the plane-wave state. When $U=0$, the ground state is a filled Fermi sea of noninteracting electrons; the momentum-space DMRG method gives the exact result for the ground state even when only one state is kept. For large U, the DMRG results are not as good as in the weak-coupling limit. However, they are still comparable with those obtained by the projected quantum

TABLE II. Comparison of the ground-state energy obtained using the DMRG method with $m=1000$ with the exact results on 4×4 lattices (Exact), the cluster diagonalization results on 6×6 lattices (CD), and the projected quantum Monte Carlo (QMC) and the stochastic diagonalization (SQ) results on 2D square lattices with N electrons.

$L_x\times L_y$	U	N	Exact (Ref. 10)/CD (Ref. 12)	DMRG	QMC (Ref. 13)	SQ (Ref. 13)
4×4	2	16	-18.01757	-18.012		
4×4	4	14	-15.74459	-15.673		
4×4	4	16	-13.62185	-13.571	-13.6	-13.59
4×4	8	16	-8.46887	-8.263	-8.48	
6×6	4	26	41.49	41.108	41.98	40.77
8×8	4	10		-34.325	-34.3	-34.31
8×8	4	18		-54.394	-54.6	-54.37
8×8	4	26		-66.098	-66.8	-66.05
12×12	4	18		-64.107		

Monte Carlo and the stochastic diagonalization methods. Both the DMRG method and the stochastic diagonalization method satisfy the variational principle (the projected quantum Monte Carlo method does not satisfy the variational principle due to the important sampling), and the results obtained from these two methods give upper bounds of ground-state energies. On an 8×8 lattice, the ground-state energies obtained by the DMRG method are systematically lower (and hence better) than the stochastic diagonalization results. The DMRG results therefore provide new upper bounds for the ground-state energies of the Hubbard model on these lattices.

In 1D, no exact diagonalization results are available for the 16-site Hubbard model, but the results obtained with the real-space DMRG method are very accurate.[11] If we use the best result for the ground-state energy of the 1D 16-site Hubbard model obtained by the real-space DMRG method as the true value of the ground-state energy, we estimate that the relative error for the ground-state energy obtained by the momentum-space DMRG method with $m=1000$ is 5% when $U=4$, which is higher than the corresponding value in 2D. Thus the momentum-space DMRG method works better for the Hubbard model in 2D than in 1D. Physically this is because the contribution of the kinetic energy term to the ground state, which is rigorously treated in the momentum-space DMRG method, is larger in 2D than in 1D.

The above discussion for the momentum-space DMRG method has been focused mainly on the Hubbard model. However, it can be easily generalized to apply to several other physically interesting models, such as the Anderson lattice model and the interacting fermion model with nearest-neighbor Coulomb potentials. For the Anderson lattice model, the composite operators defined in (3) can be used without modification. In other cases we need to generalize the definitions of the composite operators in (3) [for example a_3 in (3) should be defined as

$$a_3(p\sigma)=\sum_{q_1q_2\sigma'} V(q_1-q_2)a_0^{\dagger}(q_1\sigma')a_0(q_2\sigma') \times a_0(p+q_1-q_2\sigma)\,\delta_{(p\sigma)\notin A}$$

for a general electron-electron interacting model $\Sigma V(q-q')c^{\dagger}_{q\sigma}c_{q'\sigma}c^{\dagger}_{q''+q'\sigma'}c_{q''+q\sigma'}]$ and introduce some new composite operators of electrons. For an arbitrary interacting fermion model with a Coulomb-type potential, the number of composite operators required is generally of order N^2, which will limit the application of the momentum-space DMRG method to small lattices. However, if $V(q-q')$ can be factorized as a sum of products of a function of q and a function of q', i.e., $V(q-q')=\Sigma_l^n f_l(q)g_l(q')$, it can be shown that the total number of composite operators required can be reduced to the order of the system size N. In that case a 12×12 or even larger lattice system is accessible by the momentum-space DMRG method with presently available computer facilities. The Hubbard model is obviously a factorizable potential, with $f_1=g_1=1$ and $n=1$. The nearest-neighbor Coulomb potential is also a factorizable potential: $V(q-q')\sim\cos(q-q')=\cos q\cos q'+\sin q\sin q'$. For this nearest-neighbor Coulomb potential, the total number of composite operators needed is $5N$ in 1D and $7N$ in 2D if fermions are spinless.

In conclusion, we have generalized successfully the DMRG method to momentum space and studied ground-state properties of the Hubbard model. Our results show that the momentum-space DMRG method is a powerful numerical method for studying the Hubbard model in 2D. There is no reason to believe that this is the only model for which the momentum-space DMRG method can work. For any finite ranged potential, if it is factorizable, we believe that the momentum-space DMRG should work even better than for the Hubbard model.

The numerical calculations reported here were performed on a HP735/99 workstation. In the DMRG iteration, all intermediate data were stored in a hard disk. For the calculation on an 8×8 (12×12) lattice with 1000 states kept the computer memory space needed is 36 (45) Mb in RAM and 200 (500) Mb in hard disk.

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