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t-J model studied by the power Lanczos method

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The initial trial wave function used in a simple ground-state projection method, the power method, is systematically improved by using Lanczos algorithm. Much faster convergence to the ground state achieved by using these wave functions significantly reduces the effect of the fermion sign problem. The results for the ground state of the two-dimensional *t-J* model are presented. The density correlation function for the *t-J* model at small *J* shows a surprisingly good agreement with that of a system of noninteracting hard-core bosons.

Recently we have studied ground-state properties of the *t-J* model in one[1] and two dimensions[2] by using a simplified Green-function Monte Carlo (GFMC) method,[3] the power method. In this method the ground-state wave function of a Hamiltonian H is obtained by applying large powers of the operator W-H to a trial wave function, where W is a constant. In fermionic systems when the power becomes large same configurations with opposite signs will be generated if a Monte Carlo (MC) algorithm is used. It causes very large error bars in numerical values. This is the famous *sign* problem[3,4] occurred in MC simulations of fermionic systems. In one dimension the phase of the wave function can be fixed to rid of the sign problem, power method is very successful for all possible electronic densities.[1] In two dimensions only at low electronic density the sign problem is not severe and the converged ground state is obtained.[2] At high density the sign problem makes the power method ineffective to study this interesting region for high-temperature superconductors.

The freedom to choose the trial wave function is one of the special properties of the ground-state projection method. A trial function chosen inappropriately would require a lot of computer time to converge to ground state. Sometimes the sign problem makes the convergence impossible. It is imperative to have a good trial function to reduce the number of negative terms which increases with the power.

In the last several years variational MC method has been widely used to study the *t-J* model.[5–7] Several innovative wave functions have been proposed for the ground state. Some of them tested by the power method are not as close to the ground state as one would have anticipated. There were few methods[8] that we can use to systematically improve the trial wave function. Recently Heeb and Rice[9] proposed to use Lanczos[10] iteration to obtain better wave functions. The effectiveness of the method is demonstrated by studying the two-dimensional antiferromagnetic Heisenberg model. Along the same idea, in the study of L_iH molecule, Caffarel *et al.*[11] obtained lower energies by analyzing results of GFMC method in a generalized Lanczos scheme.

Although Lanczos method[10] is best known in searching for wave functions of small clusters, the method itself is quite general. Starting with a wave function $|\phi_0\rangle$, we can generate a tridiagonal matrix by using the recurrence relation[9]

$$\begin{aligned} H|\phi_0\rangle &= a_0|\phi_0\rangle + b_1|\phi_1\rangle \ , \\ H|\phi_n\rangle &= a_n|\phi_n\rangle + b_n|\phi_{n-1}\rangle + b_{n+1}|\phi_{n+1}\rangle \ , \end{aligned} \tag{1}$$

where $n=1,2,\ldots$, etc. The matrix elements, a_n and b_n, are related to the moments of the Hamiltonian. For example, $a_0=\langle\phi_0|H|\phi_0\rangle$ and $b_1=\sqrt{\langle\phi_0|(H-a_0)^2|\phi_0\rangle}$. When n increases, the lowest eigenvalue of the tridiagonal matrix approaches the ground-state energy. And the eigenfunction of this lowest eigenvalue gets closer to the ground-state wave function. It is straightforward to show that in successive iteration the eigenstates have the form

$$|\Psi_1\rangle = |\phi_0\rangle + C_1\frac{1}{N}H|\phi_0\rangle \tag{2}$$

and

$$|\Psi_2\rangle = |\phi_0\rangle + C_1'\frac{1}{N}H|\phi_0\rangle + C_2'\frac{1}{N^2}H^2|\phi_0\rangle \ , \tag{3}$$

etc. These functions form the basis in Krylov subspace.[12] The C's are calculated from the matrix elements, a_n and b_n, by diagonalizing the matrix.

Heeb and Rice[9] propose to calculate the matrix elements, a_n and b_n, by using the Monte Carlo technique. The C's are then determined. However, in this method the values of the matrix elements must be calculated very accurately. A small error will produce large uncertainty in the eigenvalues and in C's. Here we choose an alternative. We treat C's as the variational parameters. The wave function with the optimal energy is the eigenfunction with the lowest eigenvalue. This is more efficient and sometimes more accurate than diagonalizing the matrix.[9,11]

The result of this variational Lanczos algorithm is

that we have a sequence of wave functions, $|\phi_0\rangle, |\Psi_1\rangle, |\Psi_2\rangle, \ldots$, etc., with lower and lower energy. Besides the statistical fluctuation associated with the MC technique, the same result as the Lanczos method will be obtained. The fact that this method does not need very large memory space to store all the configurations as in the usual Lanczos method is one of its biggest advantages. But there is a practical difficulty with this approach of getting the ground state. Each time the Hamiltonian H is applied to a particular configuration the number of new configurations generated is of order of, N, the size of the cluster. It is impractical to do any calculation with $|\Psi_n\rangle$ for $n \geq 3$ for a cluster of 64 sites or greater. A more efficient way to obtain the ground state is to use $|\Psi_1\rangle$ or $|\Psi_2\rangle$ as the trial wave functions in the power method. We shall refer to this as the power-Lanczos (PL) method. If the starting trial function before the power method is applied is $|\Psi_n\rangle$ we shall call it PLn. PL0 is the same as the usual power method. For the reason discussed above we shall only consider PL1 and PL2 in this paper.

Once the optimal wave functions $|\Psi_1\rangle$ and $|\Psi_2\rangle$ are determined, we can proceed to calculate quantities such as $\langle\Psi_1|(W-H)^p|\Psi_1\rangle/\langle\Psi_1|\Psi_1\rangle$, where p is the power. It is sufficient to choose the constant W to be zero in the t-J model. The procedure to carry out this part is the same as the power method.[1]

We use several different forms of $|\phi_0\rangle$ to study the t-J Hamiltonian. The familiar Gutzwiller wave function[13] (GWF) is just the wave function for an ideal Fermi gas excluding configurations with doubly occupied sites. Another function proposed by Hellberg and Mele[6] and used by Valenti and Gros[7] in two dimensions (2D) was shown to be close to the ground state at low density.[2] This function, which we shall call HMVG, is basically of the same form as GWF, i.e., a Slater determinant for up-spin electrons and one for down-spin electrons. In addition to these two determinants, it has a long-range correlation part between all the particles, $\Pi_{i<j}|\mathbf{r}_i-\mathbf{r}_j|^\nu$ (while for nearest-neighbor particles we choose $\nu=0$). Besides these two functions we also use the projected BCS state or the resonating-valence-bond state[5,14] with either s-wave or d-wave symmetry for the gap order parameter.

The energy, $E=\langle H^{2p+1}\rangle/\langle H^{2p}\rangle$, as a function of power p, is plotted in Fig. 1 for 10 particles in a 4×4 lattice. Here we consider $J=2t$ and GWF is chosen to be the initial trial function $|\phi_0\rangle$. The open triangles are the result of Lanczos algorithm for different orders of iteration. These results are obtained exactly using the usual Lanczos method described briefly in Eq. (1). The variational energy of GWF is about 5% above the ground-state energy. This difference is reduced to about 0.3% by using the second-order wave function. The solid circles, squares, and triangles are the results of PL0, PL1, and PL2 by using $|\phi_0\rangle$, $|\Psi_1\rangle$, and $|\Psi_2\rangle$, respectively. For $|\Psi_1\rangle$ of Eq. (2), we choose C_1 to be 0.8. We have $C_1'=1.72$ and $C_2'=0.72$ in $|\Psi_2\rangle$ of Eq. (3). Clearly, when the power becomes large enough, all these three algorithms would produce ground-state energy. For comparison, we also calculated the energy exactly without using

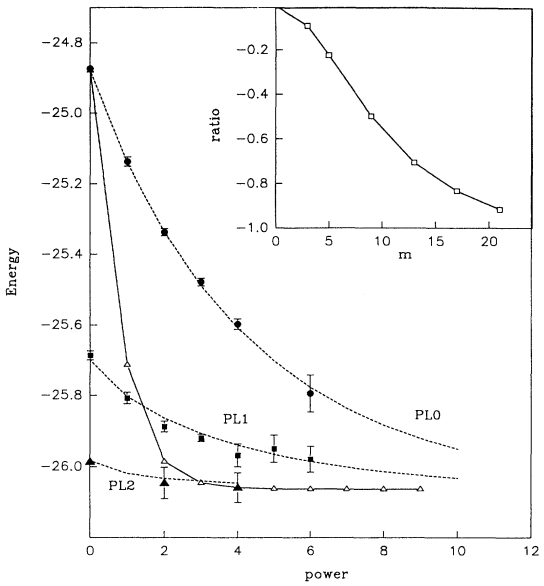

FIG. 1. Energy as a function of power for 10 electrons in a 4×4 cluster. GWF is the trial function used for $J=2t$. The solid circles, squares, and triangles represent results for PL0, PL1, and PL2, respectively. The dashed lines represent exact results without using Monte Carlo technique. Open triangles are the exact results obtained from each order of Lanczos iteration. In the inset ratio of contributions from negative terms and contributions from positive terms as a function of the power m in $\langle(-H)^m\rangle$.

the MC technique in PL0, PL1, and PL2. They are shown by the dashed lines. The excellent agreement between exact and MC calculations reaffirms the stability of MC technique.

The relatively large error bar at powers greater than 4, in Fig. 1, is mainly due to the fermion sign problem. The effect of this sign is studied by calculating the ratio of contributions from negative and positive terms in the quantities $\langle(-H)^m\rangle$. It is shown in the inset of Fig. 1. This ratio is about the same for different PL's. At large powers the negative terms make it very time consuming to get good statistics.

The data for PL0 and PL1 are obtained by averaging 10–20 independent groups, N_g. Each group usually consists of 1000–2000 starting configurations, N_c. The configurations are chosen by sweeping the lattice. Each starting configuration would produce several hundred branches, N_b, in the evaluation of powers of H. For a system of N_e electrons, we estimate the number of determinants or its ratio calculated in PL$_n$ with pth power is about $N_g\times N_c\times N_e^n\times(N_e+\alpha\times N_b)$, where α is a fraction of p. For a system with N_e of the order of 10^2, the calculation in PL2 without power is at least several times longer than PL1 with power even without taking into account the effort in optimizing the $|\Psi_2\rangle$. This is out of reach with our computing resources. In order to demonstrate that more laborious calculation of PL2 without power can be easily replaced by more efficient calcula-

tions of PL1 with power, we shall only consider clusters with 26 and 42 electrons.

In Figs. 2(a) and 3(a) energy as a function of power is plotted for 26 and 42 electrons, respectively, in an 8×8 lattice for $J=0.1t$. VGHM function with $\nu=0.04$ is used as $|\phi_0\rangle$ and its variational energy is about 3% above the ground-state energy for $\langle n\rangle=\frac{26}{64}$, but more than 5% for $\langle n\rangle=\frac{42}{64}$. The situation is improved substantially in PL1 when $|\Psi_1\rangle$ of Eq. (2) is used. $C_1=1.33$ in Fig. 2(a) and 1.49 in Fig. 3(a). The effect of the negative sign is larger when the density is increased from $\langle n\rangle=\frac{26}{64}$ to $\frac{42}{64}$. The variational energies of $|\Psi_2\rangle$ are represented by the solid triangles in Fig. 2, where $C_1'=2.66$ and $C_2'=1.77$, and in Fig. 3 where $C_1'=2.95$ and $C_2'=2.18$. As discussed above, PL1 with power takes less time than this variational PL2 calculation, yet it obtained the same or better energy. The important-sampling idea used in the power method is necessary to overcome the excess time requirement of the Lanczos approach.

Besides the energy we also calculate the equal-time correlation functions, in particular, the spin and density structure factors, $S(\mathbf{k})$ and $N(\mathbf{k})$, respectively. These structure factors are plotted along the Γ-X-M-Γ direction in the Brillouin zone in Figs. 2(b) and 2(c) for $\langle n\rangle=\frac{26}{64}$ and in Figs. 3(b) and 3(c) for $\langle n\rangle=\frac{42}{64}$. Open circles represent the variational result of $\mathrm{VGHM}_{\nu=0.04}$, and open squares are for PL1 without power. Open triangles are results of PL1 with power equal to 6 for $\langle n\rangle=\frac{26}{64}$ and power equal to 5 for $\langle n\rangle=\frac{42}{64}$. The solid lines connecting triangles are guides for the eyes. The results have changed markedly between the initial variational wave function and the first-order Lanczos wave function. The situation seems to get worse when the density $\langle n\rangle$ increases, even though the VGHM wave function still has the best variational energy at $J=0.1t$. This points out a possible deficiency in using the trial wave function VGHM to understand ground states of the t-J model at high electronic density. For comparison, we also show the results of GWF as dotted lines. GWF clearly does not reflect the correlation of the ground state. So far we have not yet found a wave function that would have energy within 5% of the ground state.

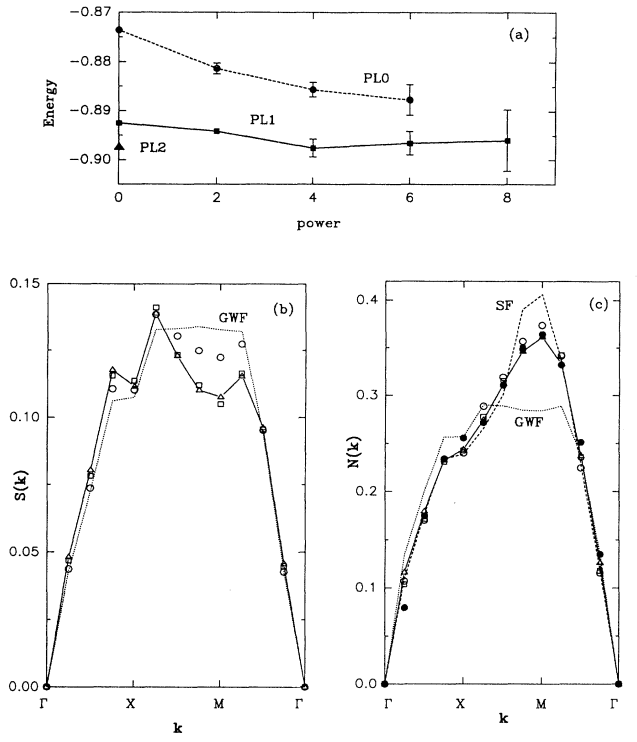

FIG. 2. (a) Energy as a function of power for $\langle n\rangle=\frac{26}{64}$ and $J=0.1t$ calculated using PL0, PL1, and PL2 algorithms. $C_1=1.33$ in $|\Psi_1\rangle$, $C_1'=2.66$, and $C_2'=1.77$ in $|\Psi_2\rangle$. (b) Spin structure factor $S(\mathbf{k})$ and (c) density structure factor $N(\mathbf{k})$ in the k space along Γ-X-M-Γ directions. Open circles represent variational results using VGHM function with $\nu=0.04$. Open squares are results of PL1 without power. Open triangles are PL1 results at power equal to 6. Solid circles represent results of noninteracting hard-core bosons. Dotted line is the variational results of GWF. Results of SF are represented by the dashed line.

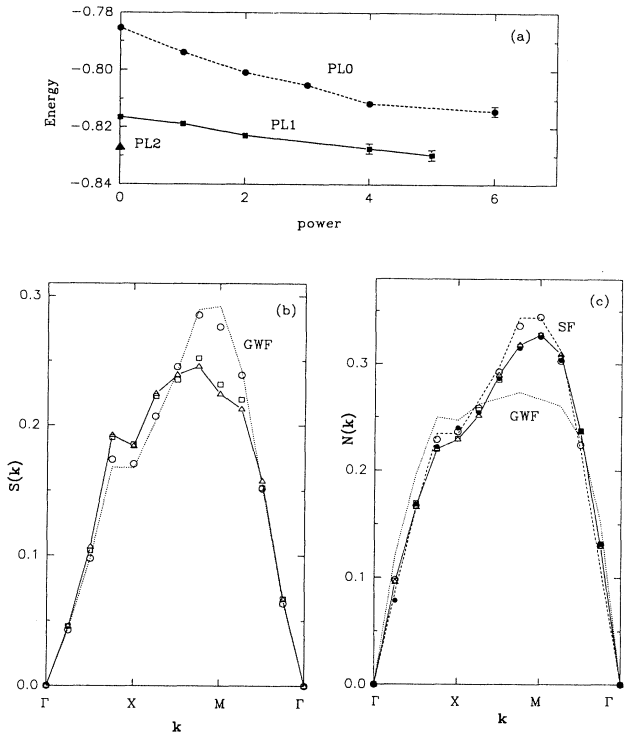

FIG. 3. (a) Energy as a function of power for $\langle n\rangle=\frac{42}{64}$ and $J=0.1t$ calculated using PL0, PL1, and PL2 algorithms. $C_1=1.49$ in $|\Psi_1\rangle$, $C_1'=2.95$, and $C_2'=2.18$ in $|\Psi_2\rangle$. (b) Spin structure factor $S(\mathbf{k})$ and (c) density structure factor $N(\mathbf{k})$ in the k space along Γ-X-M-Γ directions. Open circles represent variational results using VGHM function with $\nu=0.04$. Open squares are results of PL1 without power. Open triangles are PL1 results at power equal to 5. Solid circles represent results of noninteracting hard-core bosons. Dotted line is the variational results of GWF. Results of SF are represented by the dashed line.

Recently we have shown that many results of the t-J model at low electronic density are qualitatively consistent with the prediction of the Tomonaga-Luttinger liquid[15] in one dimension. The cusps or peaks at $\mathbf{k}=2\mathbf{k}_F$ in $S(\mathbf{k})$ are enhanced over the variational results of VGHM. $N(\mathbf{k})$ has a maximum at $\mathbf{k}=(\pi,\pi)$. But we cannot[16] identify in $N(k)$ the characteristic wave vector $2k_F^{\mathrm{SF}}$ associated with spinless fermions (SF) as claimed by Putikka *et al.*[17] using the high-temperature expansion. There is another fact against the ideal SF. Unlike one dimension the energy of the t-J model in the limit of vanishing J is lower than SF by about 12 and 6 % for $n=\frac{26}{64}$ and $\frac{42}{64}$, respectively. Here we try to understand $N(k)$ from a different point of view.

One way to treat the constraint of no double occupancy in the t-J model is to write the fermion operator as a product of a hard-core boson and a fermion operator. In this slave-boson approach[18] the fermion operator represents spin degree of freedom and the boson is for charge degree of freedom. We may expect the charge correlation to be similar to that of a system of noninteracting hard-core bosons in the limit of vanishing J. In one-dimensional hard-core bosons and spinless fermions are equivalent, but they are not in two dimensions.

The ground-state correlation function of a system of noninteracting hard-core bosons is calculated by using the power method. The trial wave function is of the form of Jastrow type.[19] Details of this calculation will be presented elsewhere. Results of density correlation are represented by the solid circles in Figs. 2(c) and 3(c). They almost lie on top of the triangles representing the result of PL1, except[20] at very small k. A similar result[21] has been found for the infinite-U Hubbard model for small clusters. On the other hand, $N(\mathbf{k})$ of SF as shown by the dashed lines in Figs. 2(c) and 3(c) is not as close to the result of t-J model. The fact that hard-core bosons have almost the same density-density correlation as the charges in the t-J model does not by itself prove the separation of spin and charge. But this and other evidences[2,16,17] make the idea[22] of separation of charge and spin in the t-J model more plausible.

In conclusion, we have presented an algorithm that utilizes the advantages of two very powerful techniques, the Lanczos and the power methods. On the one hand, the variational Lanczos improves the trial function to accelerate the convergence to the ground state in the power method so the effect of fermion sign problem is reduced. Unlike the commonly used fixed-node method,[23] our results are not overwhelmingly influenced by the initial choice of trial functions. On the other hand, the important sampling used in the power method can achieve the same results as the pure Lanczos approach but with much more efficiency. This benefit would become more important when the number of electrons increases. A surprising result has been found. The density-density correlation obtained at small J is very close to that of a system of noninteracting hard-core bosons, and it is not the same as that of spinless fermions.[17]

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