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 energy, spin and charge correlation functions are calculated for the ground states of the two-dimensional $t-J$ model. Results for an $8 \times 8$ cluster with 42 and 26 electrons 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 non-interacting hard-core bosons.
Recently we have studied ground-state properties of the $t - J$ model in one\textsuperscript{1} and two dimensions\textsuperscript{2} by using a simplified Green function Monte Carlo (GFMC) method\textsuperscript{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\textsuperscript{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\textsuperscript{1}. In two dimensions only at low electronic density the sign problem is not severe and the converged ground state is obtained\textsuperscript{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\textsuperscript{5,6,7}. 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 that we can use to systematically improve the trial wave function. Recently Heeb and Rice\textsuperscript{8} proposed to use Lanczos\textsuperscript{9} iteration to obtain better wave functions. The effectiveness of the method is demonstrated by studying the two-dimensional antiferromagnetic Heisenberg model. A few years earlier,
Caffarel et al. have also used a variation of the Lanczos algorithm to study \( L_i H \) molecule.

Although Lanczos method 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 tri-diagonal matrix by using the recurrence relation

\[
H |\phi_0\rangle = a_0 |\phi_0\rangle + b_1 |\phi_1\rangle \\
H |\phi_n\rangle = a_n |\phi_n\rangle + b_n |\phi_{n-1}\rangle + b_{n+1} |\phi_{n+1}\rangle
\]

(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 tri-diagonal 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

\[
|\Psi_1\rangle = |\phi_0\rangle + C_1 \frac{1}{N} H |\phi_0\rangle ,
\]

(2)

and

\[
|\Psi_2\rangle = |\phi_0\rangle + C_1' \frac{1}{N} H |\phi_0\rangle + C_2' \frac{1}{N^2} H^2 |\phi_0\rangle ,
\]

(3)

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

Heeb and Rice 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.
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 PL\( n \). 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 \( \frac{\langle \Psi_1 \mid (W-H)^p \mid \Psi_1 \rangle}{\langle \Psi_1 \mid \Psi_1 \rangle} \), 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 (GWF)\(^{12}\) 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 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, \( \Pi_{i<j} |r_i - r_j|^\nu \) (while for nearest-neighbor particles we choose
Besides these two functions we also use the projected BCS state or the resonating-valence-bond state\textsuperscript{5,13} with either s-wave or d-wave symmetry for the gap order parameter.

The energy, \( E = \frac{\langle H^{2p+1} \rangle}{\langle H^{2p} \rangle} \), as a function of power \( p \) is plotted in Fig.1 for 10 particles in a \( 4 \times 4 \) 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 equation 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 equation (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 equation (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 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.

In Fig. 1 we note the relatively large error bars at powers greater than 4. This is mainly due to the fermion sign problem. The effect of this sign is studied by calculating the ratio of contributions from the negative terms and contributions from the positive terms in the quantities \( \langle (-H)^m \rangle \). In the inset of figure 1 this ratio is plotted as a function of \( m \). This ratio is about the same for different PL’s. At power equal to 6 or \( m = 13 \), the negative terms are as large as seventy percent of the positive terms. It is very time consuming to get good statistics.

The data for PL0 and PL1 are obtained by averaging ten to twenty independent groups. Each group usually consists of one to two thousand starting configurations. Each starting configuration would produce several hundred
terms in the evaluation of powers of $H$. At large power we usually need to have more runs to reduce the fluctuations caused by the sign problem. The calculations are all done in workstations like HP720. For PL0, the longest calculation is about six hours for this $4 \times 4$ cluster. It takes about four to six times longer for PL1. If we had used the same number of runs for PL2 we would probably increase the CPU time by another factor of four to six. Instead, we reduced the number of runs in PL2, therefore we have a somewhat larger error at power equal to four. The amount of computer time quoted above is only for a small cluster of size $4 \times 4$. We estimate the time needed for an $8 \times 8$ cluster with same electronic density is about ten times longer. Clearly, it is quite impractical to carry out a calculation for large powers in PL2. Hence, below we shall present mostly results of PL0 and PL1 for $8 \times 8$ clusters and may be a few results of PL2 without powers.

In figure 2(a) and 3(a) energy as a function of power is plotted for 26 and 42 electrons respectively, in an $8 \times 8$ 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 equation (2) is used. $C_1 = 1.33$ in 2(a) and 1.49 in 3(a). In figure 2(a) the large error bars at power equal to 6 and 8 makes it difficult to determine the exact ground state energy. The effect of the negative sign is larger when the density is increased from $\langle n \rangle = \frac{26}{64}$ to $\frac{42}{64}$. Nevertheless, it seems quite reasonable to conclude that the ground-state energy should be within half a percent of the variational energy of $|\Psi_2\rangle$ which are represented by the solid triangles. For PL2 in Fig.2, $C'_1 = 2.66$ and $C'_2 = 1.77$, and $C'_1 = 2.95$ and $C'_2 = 2.18$ in Fig.3.

Besides the energy we also calculate the equal time correlation functions, in particular, the spin and density structure factors, $S(k)$ and $N(k)$ respectively. These structure factors are plotted along $\Gamma$-$X$-$M$-$\Gamma$ direction in the Brillouin
zone in figures 2(b) and 2(c) for $\langle n \rangle = \frac{26}{64}$ and in figures 3(b) and 3(c) for $\langle n \rangle = \frac{42}{64}$. Open circles represent the variational result of VGHM$_{v=0.04}$, 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. We note that the results 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 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.

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\cite{14} in one dimension. The cusps or peaks at $k = 2k_F$ in $S(k)$ are enhanced over the variational results of VGHM. $N(k)$ has a maximum at $k = (\pi, \pi)$. But we cannot\cite{15} identify in $N(k)$ the characteristic wave vector $2k_{SF}^F$ associated with spinless fermions (SF) as claimed by Putikka et al.\cite{16} using the high temperature expansion. 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. While the fermion operator represents spin degree of freedom, the boson is for charge degree of freedom. This is the so called slave-boson approach\cite{17}. If the separation of charge and spin indeed occurs it will be most apparent in the limit of vanishing $J$ where the dynamics is controlled by the charge hopping
or the motion of the hard-core bosons. We may expect the charge correlation
to be similar to that of a system of non-interacting hard-core bosons. In one
dimension hard-core bosons and spinless fermions are equivalent, but they are
not in two dimensions. A careful examination of the correlation function of the
hard-core bosons in a 2D lattice is needed.

We have calculated the ground-state correlation function of a system of
non-interacting hard-core bosons by using the power method. The trial wave
function is of the form of Jastrow type described in Ref. 18. Details of this
calculation will be presented elsewhere. Results of density correlation are rep-
resented by the solid circles in figure 2(c) and 3(c). They almost lie exactly on
top of the triangles representing the result of PL1, except at very small k.
A similar result has been found for the infinite-U Hubbard model for small
clusters. On the other hand, N(k) of SF as shown by the dashed lines in figure
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 make the idea of separation of charge and spin in
the t−J model much more plausible.

In summary, we have presented a new modified power method using a
systematically improved trial wave function obtained by the Lanczos method.
Even the wave function obtained by a first order iteration greatly improves the
rate of convergence to the ground state. This faster convergence significantly
reduces the effect of the fermion sign problem that has plagued fermion MC
calculations so far. For the first time very accurate ground-state results are
obtained for electronic density as high as 65% in an 8×8 cluster. A surprising
result has been found. The density-density correlation obtained at small J is
very close to that of a system of non-interacting hard-core bosons.

The power-Lanczos method presented above is in principle an exact ap-
proach to obtain the ground state. Unlike the fixed-node method, the results
are not overwhelmingly influenced by the initial choice of trial function. The numerical algorithm we have used is the simplest among many complicated GFMC methods. It is already sufficient to get very accurate results. More sophisticated approaches, such as using guiding function$^{3,22}$, would be explored in the future. Calculations for much larger clusters are feasible now.

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Figure Captions:

Fig. 1 Energy as a function of power for 10 electrons in a $4 \times 4$ cluster. GWF is the trial function used for $J = 2t$. The solid circles, squares and triangles represent results for PLO, 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 $\langle (-H)^m \rangle$.

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 $S(k)$ and (c) density structure factor $N(k)$ in the $k$ space along $\Gamma$-$X$-$M$-$\Gamma$ directions. Empty 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 non-interacting 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 $S(k)$ and (c) density structure factor $N(k)$ in the $k$ space along $\Gamma$-$X$-$M$-$\Gamma$ directions. Empty 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 non-interacting hard-core bosons. Dotted line is the variational results of GWF. Results of SF are represented by the dashed line.