Numerical renormalization group study of the 1D $t - J$ model

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Abstract

The one-dimensional (1D) $t - J$ model is investigated using the density matrix renormalization group (DMRG) method. We report for the first time a generalization of the DMRG method to the case of arbitrary band filling and prove a theorem with respect to the reduced density matrix that accelerates the numerical computation. Lastly, using the extended DMRG method, we present the ground state electron momentum distribution, spin and charge correlation functions. The $3k_F$ anomaly of the momentum distribution function first discussed by Ogata and Shiba is shown to disappear as $J$ increases. We also argue that there exists a density-independent $J_c$ beyond which the system becomes an electron solid.

71.10.+x, 71.27.+a, 75.10.Jm
I. INTRODUCTION

For a number of years, the more so since the discovery of high-$T_c$ superconductors, the study of strongly correlated electron systems has been a major theme of theoretical condensed matter physics. The $t - J$ model is one of the simplest of such models. Although high-$T_c$ cuprates are at least two-dimensional (2D) systems, it is also relevant to fully understand the one-dimensional (1D) model. The Hamiltonian for the $t - J$ model in one dimension can be written in the subspace of no doubly occupied sites as

$$H = -t \sum_{i,\sigma}(c_{i\sigma}^\dagger c_{i+1\sigma}^\dagger + c_{i+1\sigma}^\dagger c_{i\sigma}) + J \sum_i (S_i \cdot S_{i+1} - \frac{1}{4} n_i n_{i+1}),$$

where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the creation and annihilation operators for an electron at lattice site $i$ with spin $\sigma$, while $S_i$ and $n_i$ are the corresponding spin and electron number operators. This model has been solved exactly only for $J \to 0$, where it is equivalent to the $U \to \infty$ Hubbard model, and at the supersymmetric point $J = 2t$. In both cases the ground state at arbitrary density belongs to a broad class of interacting Fermi systems known as Luttinger liquids, which exhibit power-law decay of correlation functions with exponents characterized by a single parameter. Additionally, for very large $J/t$, the attractive Heisenberg interaction term dominates the kinetic energy and the model phase separates. The level of understanding of this model is derived mostly from small cluster exact diagonalizations, variational Monte Carlo methods and finite temperature Monte Carlo simulations for relatively larger system sizes. There still lurks, however, the question of whether the thermodynamic limit has been reached or not. In this paper we use the density matrix renormalization group (DMRG) method to study the ground-state properties of the $t - J$ model in the thermodynamic limit.

The text is organized as follows. In Sec. II, we review the formulation of DMRG and its extension to arbitrary band-filling. In Sec. III, we discuss our numerical results. We present ground-state static spin and charge correlation functions as well as electron momentum distribution functions. Finally in Sec. IV we summarize our results.
II. DMRG FORMULATIONS

The DMRG technique was developed by White in 1992. It leads to highly accurate results for systems much larger than those which can be solved by exact diagonalization. The DMRG allows a systematic reduction of the Hilbert space to the basis states most relevant to describe a given eigenstate (e.g. the ground state) of a large system. This is to be contrasted with previous real space renormalization techniques in which the lowest states are kept. A general iteration step of the method for open boundary conditions proceeds as follows: 

a) The effective Hamiltonian defined for the superblock $1 + 2 + 2' + 1'$ (where the block 1 and 1' come from previous iterations and 2 and 2' are new added ones) is diagonalized to obtain the ground-state wave function $|\psi>$ (other states could be also kept). 

b) The reduced density matrix of blocks $1 + 2$: $\rho_{i,i'} = \sum_j \psi_{ij}^* \psi_{i'j}$ is constructed, where $\psi_{ij} = \langle i \otimes j | \psi >$, the states $|i>$ ($|j>$) belongs to the Hilbert space of blocks 1 and 2 (1' and 2'). The eigenstates of $\rho$ with the highest eigenvalues (equivalent to the most probable states of blocks $1 + 2$ in the ground state of the superblock) are kept up to a certain cutoff. 

c) These states form a new reduced basis in which all the operators have to be expanded and the block $1 + 2$ is renamed as block 1.

d) A new block 2 is added (one site in our case) and the new superblock $(1 + 2 + 2' + 1')$ is formed as the direct product of the states of all the blocks (the blocks 1' and 2' are identical to blocks 1 and 2 respectively). The method has been successfully applied to problems such as the Haldane gap of spin-1 chains, critical exponents of spin-$\frac{1}{2}$ chains, the 1D Kondo-insulator and two-chain Hubbard model.

In our study of the 1D $t - J$ model we have used the infinite-size version of the above iteration scheme to reach the thermodynamic limit. One immediately realizes, however, there is a problem in keeping the electron density fixed in the iteration process since we insert only two sites at each iteration (which only makes the half-filling and quarter-filling cases invariant). To get around this, we construct the reduced density matrix from two ground states that bracket the desired density. To be more specific, if our desired electron density is $n$ and the current superblock lattice size is $N$, then we can always find two nearest integers
$N_1$ and $N_2$ such that $N_1 \leq nN \leq N_2$. Assuming $|\psi(N_1)\rangle$ is the ground state wavefunction of $N_1$ electrons and $|\psi(N_2)\rangle$ is that of $N_2$ electrons, we build the reduced density matrix by the following weighting procedures:

$$
\begin{cases}
\rho_{i,i'} = \rho_1 \sum_j \psi_{ij}(N_1) \psi_{i'j}^\ast(N_1) + \rho_2 \sum_j \psi_{ij}(N_2) \psi_{i'j}^\ast(N_2) \\
nN = \rho_1 N_1 + \rho_2 N_2 \\
1 = \rho_1 + \rho_2
\end{cases}
$$

(2)

It is clear that the above construction ensures the desired constant band filling at every iteration. The success of this construction inherently requires that the ground state be homogeneous. Therefore one should expect failure when the system goes into the phase separation regime. However, phase separation can still be studied using the finite size version of DMRG which does not require translational invariance. It is perhaps worthwhile to remark that in our computer program we have generally targeted three states since the ground state has two-fold degeneracy when the electron number is odd.

The correlation functions are calculated when the iteration has converged. Typically we start to measure them after the superblock size reaches 40 lattice sites. More specifically we measure the correlation between operators in the middle of the superblock. For example, the nearest-neighbor correlation is measured between sites 20 and 21 in the superblock size 40; while the second-nearest-neighbor correlation is measured between sites 20 and 22 in the next iteration (i.e when superblock size becomes 42). Similarly the third-nearest-neighbor correlation is measured between sites 20 and 23 in the superblock size 44. Thus as we iterate our procedure to increase the system size we obtain correlations over increasing distances. Finally, the desired ground-state correlations are obtained in a similar way as the reduced density matrix, e.g. the spin-spin correlation is measured in the following way

$$
S(r - r') = \rho_1 < \psi(N_1) | S(r) \cdot S(r') | \psi(N_1) > + \rho_2 < \psi(N_2) | S(r) \cdot S(r') | \psi(N_2) > .
$$

(3)

Before we discuss the numerical results, let us prove the following theorem: the eigenstates of the reduced density matrix retain their good quantum numbers when the corresponding operator of the superblock is a direct sum of the operators of its subsystems. The electron
number operator $\hat{N}$ and the total $z$-component of the spin operator $\hat{S}_z$ are two such operators. To prove such a theorem all we need to show is that the reduced density matrix is block diagonal in its good quantum operator subspace. Let us consider one subspace at a time, e.g. the electron number subspace. Then the most general form of the eigenstate of the superblock with $L$ electrons can be written as

$$|\psi(L)\rangle = \sum_{l_1+l_2=L} \sum_{\alpha,\beta} c(l_1, \alpha; l_2, \beta) |l_1, \alpha >_1 \otimes |l_2, \beta >_2,$$

(4)

where $|l_1, \alpha >_1$ stands for the basis wavefunction of block 1 with $l_1$ electrons, and $\alpha$ labels other quantum numbers, while $|l_2, \beta >_2$ represents the basis wavefunction of block 2 with $l_2$ electrons, and $\beta$ marks other quantum numbers. Thus the reduced density matrix elements have the form

$$\rho_{(l_1, \alpha); (l'_1, \alpha')} = \sum_{l_2, \beta} c(l_1, \alpha; l_2, \beta) \cdot c^*(l'_1, \alpha'; l_2, \beta).$$

(5)

However according to the construction of the wavefunction we have both $L = l_1 + l_2$ and $L = l'_1 + l_2$ leading automatically to the conclusion $l_1 \equiv l'_1$. Therefore the reduced density matrix is block diagonal in the electron number subspace. In the same way one can show that the reduced density matrix is block diagonal in the $S_z$ subspace. We emphasize that this theorem can be explicitly implemented to accelerate the diagonalization of the reduced density matrix in the subspace of its good quantum numbers.

III. NUMERICAL RESULTS

For most of the numerical results reported here we have kept 110 states in blocks 1 and $1'$, the truncation error defined as $1 - p(m)$ (where $p(m)$ is the summation of the highest $m$ eigenvalues of the reduced density matrix) is of the order of $10^{-5}$. In Table I we list some of the ground-state energies per site $E_g$ as a function of band filling $n$ and spin exchange coupling $J$. In the same table we also list the results obtained from the exact Bethe ansatz solution at $J = 2t$. As can be seen immediately from the table, our DMRG results are
highly accurate. To make it convenient for the reader we quote the coupled Bethe ansatz equations determining the ground-state energy at density $n$ and $J = 2t$:

$$\int_{-Q}^{Q} \rho(\nu) d\nu = 1 - n \quad (6)$$

$$\rho(\nu) = 2R(2\nu) + \int_{-Q}^{Q} 2R(2[\nu - \nu'])\rho(\nu') d\nu', \quad (7)$$

where $R(x)$ denotes Shiba’s function

$$R(x) = \frac{1}{4\pi} \int_{-\infty}^{\infty} d\omega \frac{e^{i\omega x/2}}{1 + e^{i\omega}}. \quad (8)$$

Then the ground-state energy is given by

$$E_g = 2t[1 - n - \pi \rho(0)]. \quad (9)$$

Since we are going to present our results in momentum space it is now opportune to discuss the way we analyse our data. First, because open boundary conditions are used in our DMRG procedure, we obviously lose translational invariance. To overcome this boundary effect we have done an average on the real space correlation functions before we do the Fourier transform into momentum space. More specifically we obtain several real-space correlation functions of the same system by starting the measurement at different superblock sizes. For example we start our real-space density-density correlation $\rho \rho(r) = \langle n_i n_{i+r} \rangle$ measurement after the superblocks reach the sizes of 40, 42, 44, 46 and 48 sites and then take the average among them. The final Fourier transform is done in the usual way:

$$\rho \rho(k) = \frac{1}{N} \sum_{l=1}^{N} \sum_{h=1}^{N} e^{ik(l-h)} \langle n_l n_h \rangle - \langle n_l \rangle \langle n_h \rangle, \quad (10)$$

where $N$ is the largest separation available in our measurement. For the results of this work we stop at a superblock size of 150 sites.

In Fig. 1(a) we plot the electron momentum distribution function for quarter filled band at $J = 0.1t$. We see that this result is almost identical to the 1$D$ infinite-$U$ Hubbard model
studied by Ogata and Shiba. This is not surprising considering the fact that the small $J$ limit of the $t-J$ model is equivalent to the strong coupling limit of the Hubbard model. Here we have both $k_F (= n\pi/2)$ and $3k_F$ anomalies as indicated by arrows in the figure. Unlike normal Fermi liquids, however, the $3k_F$ anomaly is a new feature which is related to the effect of the coupled holon and spinon representation of the normal electron. Fig. 1(b) shows the spin-spin correlation. There is a $2k_F$ anomaly reflecting the nature of the antiferromagnetic exchange among nearest-neighbor electrons. Fig. 1(c) is the density-density correlation function. Here one observes the $4k_F (= \pi)$ anomaly only.

Before discussing the effect of increasing $J$ let us remember the two competing factors in correlation effects: a) The nearest-neighbor antiferromagnetic spin exchange $J$ favors the formation of spin-singlet electron pairs on nearest-neighbor sites which in turn leads to $2k_F$ spin density wave (SDW) fluctuations. But eventually, when $J$ is large enough, there emerges a phase separation exhibiting antiferromagnetic SDW fluctuations. b) The kinetic energy $t$ term favors the delocalization of the electrons. But the Pauli principle as well as on-site repulsion promote uniform separation between electrons synonymous with $4k_F$ charge density wave (CDW) fluctuations. On the other hand the formation of bound singlet pairs due to $J$ term enhances $2k_F$ CDW fluctuations.

In Fig. 2(a) it is seen that as the antiferromagnetic exchange $J$ increases, the momentum distribution function is modified more drastically in the region $k > k_F$ where it changes from decreasing to increasing as a function of $k$. Notably the $3k_F$ feature has been washed out for larger $J$. Besides, the critical exponent at the Fermi wavevector $k_F$ seems to decrease as $J$ increases. In Fig. 2(b) we have plotted the spin-spin correlation function at quarter filling with $J/t = 0.5, 2, \text{ and } 2.5$. We see that at $J = 0.5t$ there is a clear $2k_F$ anomaly, however at $J = 2t$ this anomaly is significantly weakened. At $J = 2.5t$ the $2k_F$ anomaly seems to have completely disappeared and the maximum is located at $k = \pi = k_{AF}$. This is an indication of singlet pairing between nearest-neighbor electrons. Fig. 2(c) shows the corresponding density-density correlation. At $J = 0.5t$ there is only a $4k_F$ anomaly which indicates the system is quite uniformly distributed. However as one increases $J$ the
4k_F feature disappears and a new feature at 2k_F develops which reflects the formation of nearest-neighbor pair. At J = 2.5t the behavior near k = 0 has a tendency to flatten out. But the 2k_F feature still dominates which shows singlet pairing. Fig. 3 shows similar results for the band filling n = 0.8. Again it is seen from Fig. 3(a) that J has the largest effect on the momentum distribution function in the regime k > k_F. Fig. 3(b) is very much the same as of Fig. 2(b): as J increases the maximum in the spin-spin correlation function moves to the antiferromagnetic wavevector k_{AF} = \pi. But in Fig. 3(c) the J = 3t density-density correlation shows a clearer tendency towards phase separation near k = 0. Both 2k_F and 4k_F anomalies are seen in the density correlation at intermediate J as predicted.\[6\]

As mentioned in the previous section our DMRG procedure is not applicable to the study of the phase separated regime. But we know from other numerical calculations there exists a \textit{density-dependent} J'_c indicating the onset of a phase separation. Here we wish to argue that there exists another critical J_c (that is larger than the \textit{max[J'_c]}) beyond which the system forms an \textit{electron solid}, i.e., a phase with no hole inside but having a thin interface at which the boundary electrons can still evaporate into the vacuum (hole). This J_c should be independent of the band filling since once the \textit{electron solid} is reached there is only a single phase boundary between the hole region and the solid, and that is density independent. By definition, the first instability of such an \textit{electron solid} comes from the ability to dissolve a single hole inside. Accordingly J_c can be estimated from finite size exact diagonalizations by comparing the ground-state energy of a 2N-site Heisenberg chain with that of 2 holes in the 2N-site t – J model. This has been done by Ogata et al\[7\] on a 16-site system and by Assaad et al\[9\] with path-integral Monte Carlo simulation. Both results seem to point towards J_c \approx 3.6t. Further, Yokoyama et al\[8\] have hinted the existence of such a J_c in their recent variational Monte Carlo study of t – J model. The same thing is also implied in the work of Ammon et al\[14\].
IV. SUMMARY

We have extended the DMRG method to allow calculations at arbitrary band filling and proven a theorem regarding the reduced density matrix that could accelerate the numerical calculation. We then used the extended DMRG procedure to study the $1D t - J$ model. It is found that our procedure gives highly accurate ground-state energy and correlation functions. It is shown that the $3k_F$ anomaly first discussed by Ogata and Shiba in the electron momentum distribution disappears as $J$ is increased. It is argued that there exists a density-independent $J_c$ beyond which the system forms an electron solid.

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TABLES

TABLE I. Ground-state energies of the 1D $t - J$ model calculated using DMRG method. Exact results for the $J = 2t$ case are listed as a comparison. The last number in the brackets are the estimated value accurate at that digit.

| $< n >$ | $J/t$ | DMRG $E_g/t$ | Exact $E_g/t$ |
|--------|------|-------------|---------------|
| 0.4    | 0.5  | -0.631(8)   |               |
| 0.4    | 1.0  | -0.664(2)   |               |
| 0.4    | 2.5  | -0.803(3)   |               |
| 0.5    | 0.1  | -0.647(0)   |               |
| 0.5    | 0.5  | -0.692(0)   |               |
| 0.5    | 2.0  | -0.903(6)   | -0.9036(4)    |
| 0.5    | 2.5  | -0.988(5)   |               |
| 0.8    | 0.1  | -0.416(2)   |               |
| 0.8    | 0.5  | -0.586(7)   |               |
| 0.8    | 2.0  | -1.246(4)   | -1.2464(4)    |
| 0.8    | 3.0  | -1.698(7)   |               |
| 0.9    | 1.0  | -0.756(4)   |               |
| 0.9    | 2.0  | -1.322(3)   | -1.3223(7)    |
| 0.9    | 3.0  | -1.891(9)   |               |
FIGURES

FIG. 1. The ground state electron momentum distribution function (a), spin-spin correlation function (b), and density-density correlation (c) are plotted for quarter band filling at $J = 0.1t$.

FIG. 2. Same as that of Fig. 1 but with $J = 0.5t, 2t$ and $2.5t$.

FIG. 3. Same as that of Fig. 2 with $J = 0.5t, 2t$ and $3t$ but at band filling 0.8.
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of the reduced density matrix we can keep more states in blocks 1 and 1' and obtaining higher accuracy. Work in this direction is in progress.

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Fig. 1

(a) $n(k)$ vs. $k$

(b) $S_{S_iS_i}(k)$ vs. $k$

(c) $P_{P_iP_i}(k)$ vs. $k$

- $\langle n \rangle = 0.5$
- $J = 0.1t$
Fig. 3