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Numerical Study of the Pairing Correlation of the t-J Type Models

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We reported that the pair-pair correlation function of the two-dimensional t-J model does not have long-range d-wave superconducting correlations in the interesting parameter range of $J/t \leq 0.5$. The power-Lanczos method is used under the assumption of monotonic behavior. This assumption has been well checked in the two-dimensional t-J and attractive Hubbard model. Here we re-examine this criterion of monotonic behavior of the pairing correlation function for the one-dimensional and two-leg t-J ladder where other accurate numerical results are available. The method seems to be working well.

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I. Introduction

It has been shown that several essential physical properties of the high temperature superconducting (HTSC) cuprates can be described by the two-dimensional (2D) t-J model [1, 2], such as the single hole dispersion relation [3], non-Fermi liquid behavior [4], and phase separation [5]. One of the critical issues is whether the model gives large enough pairing correlation to quantitatively explain the high T_c. We reported part of the numerical results on this issue in Ref. [6] which concludes that the 2D t-J is unlikely to explain the superconductivity in the physically interesting region of electron density n_e and coupling constant J/t from the studies on the pair-pair correlation function and the two-hole binding energy [7].

The criterion to evaluate the pairing correlation of the 2D t-J model used in Ref. [6, 8] is to apply the power-Lanczos (PL) method [9] on the variational trial wave functions. We denote the initial trial wave function as $|PL0\rangle$ and the one improved by one Lanczos iteration as $|PL1\rangle$. We calculate the change of the pairing correlations of $|PL1\rangle$ and $|PL0\rangle$ for various variational parameters. If we assume the behavior of the long-range pairing correlations which is monotonic through the Lanczos or power iteration, then the one whose pairing correlation is least changed gives the correct results of the ground state. It is extremely difficult to prove this criterion by the present computing power in 2D, we could only provide more examples to support it. In a previous paper we have checked the validity of the criterion of the 2D attractive Hubbard model [6]. Here we will show the results of the one-dimensional (lD) t-J model and 2-leg t-J ladders.

The t-J model is:

$$H = -t \sum_{\langle i,j \rangle \sigma} (\tilde{c}^{\dagger}_{i\sigma} \tilde{c}_{j\sigma} + h.c.) + J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j), \tag{1}$$

where $\tilde{c}^{\dagger}_{i\sigma} = c^{\dagger}_{i\sigma}(1 - n_{i\,-\sigma})$, and $\langle i,j \rangle$ denotes the nearest neighbors i and j.

For the 1D case, we study the pairing correlation function in the spin-gap region of the phase diagram, i.e., large $J(> 2)$ and low electron density [10, 11]. Here we use the correlated spin-singlet pair (CSP) wave function as $|PL0\rangle$. The CSP wave function is defined as

$$|CSP\rangle = P_d \prod_{i>j} \left[\frac{L}{\pi} \sin \left(\frac{\pi}{L} (r_i - r_j) \right) \right]^{\nu} \left[\sum_{n=1}^{\infty} h^{n-1} b^{\dagger}_n \right]^{Ne/2} |0\rangle, \tag{2}$$

where $h = 2t/J$. N_e is the total number of electrons, P_d is the projection operator that forbids two particles occupying the same site and the operator $b^{\dagger}_n = \sum_i c^{\dagger}_{i\uparrow} c^{\dagger}_{i+n\downarrow} - c^{\dagger}_{i\downarrow} c^{\dagger}_{i+n\uparrow}$. The variational parameter ν control the long-range correlations. In Fig. 1 we show the pairing correlation function of the $|PL0\rangle$ and $|PL1\rangle$ with $J/t = 2.8$. In order to check the ansatz of monotonic behavior, we choose a small lattice of 24 sites with 4 electrons which can be exactly diagonalized by Lanczos iteration. As it clearly show that the one with $\nu = 0.1$ has the stablest long-range correlation which

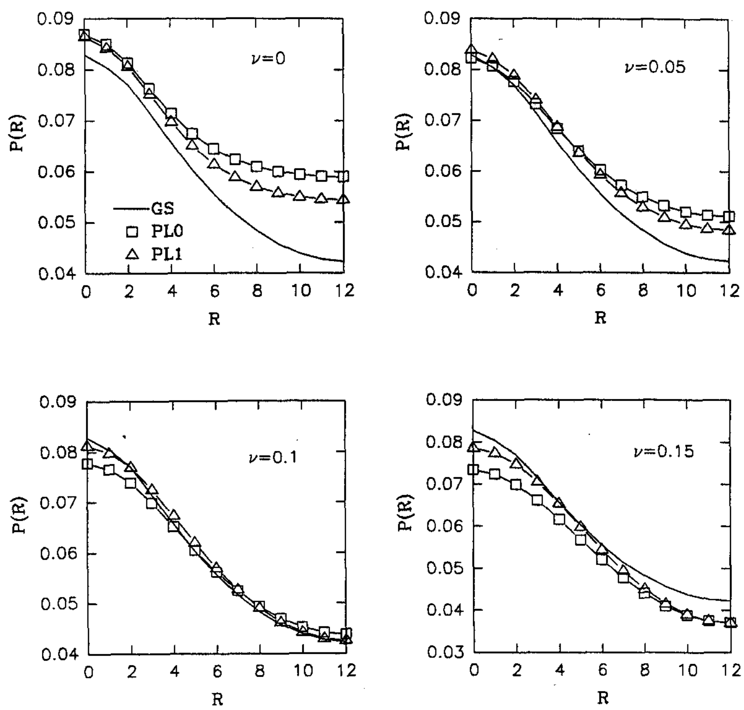

FIG. 1. Pairing correlation function $P(R)$ for various trial wave function (PL0) and their PL1 results, together with the exact data (GS) for $J/t = 2.8$ of 4 electrons in a 24-site chain.

is also very close to the value of the exact ground state. For smaller ν the long-range correlation decrease while the larger ones increase. The results for this 1D case are consistent with our ansatz.

For the ladders discussed here, the leg-leg and rung-rung t and J are assumed to be identical. In the variational level of the $2 \times L_x$ t-J ladder, the trial wave function used here is [12, 13]:

$$|\Phi(\Delta,\nu)\rangle = \prod_{i<j} \left\{ \frac{L}{\pi} \sin(\frac{\pi}{L}(x_i - x_j) \right\}^{\nu} \cdot P_d \prod_{k} (\tilde{u}_k + \tilde{v}_k c^{y}_{k,"} c^{y}_{i\ k,\#})|0\rangle \tag{3}$$

with $\tilde{v}_k/\tilde{u}_k = \Delta_k/(\epsilon_k + \sqrt{\epsilon_k^2 + \Delta_k^2})$, $\Delta_k = \Delta(\cos k_x - 2\cos k_y)$ and $\epsilon_k = (2\cos k_x + \cos k_y) - \mu$. Δ is the d-wave superconducting order parameter and μ is the chemical potential. The operator P_d enforces the constraint of no double occupancy. We take $t = 1$ in this paper. In the 2-leg ladder case, the rung-rung pairing correlation $P(R) = \langle \Delta^{y}_{i} \Delta_{i+R} \rangle$ is measured, where $\Delta_j = (c_{j,2;\#} c_{j,1;"} - c_{j,2;"} c_{j,1;\#})$.

For the 1D and ladder cases, because the correlation functions decay exponentially or in power law with respect to the distance R, rather than being flat plateaus in two dimensions, it is difficult to define the "stable" correlation of the trial wave functions with different parameters Δ and ν. Thus we define the deviation $D(\Delta,\nu)$ to quantify the difference between the $|PL0\rangle$ and $|PL1\rangle$ wave functions. The wave function with minimal D is the one having stable correlation. It is defined as

$$D = \frac{1}{N} \sum_{R, 2} \{(P_1(R) - P_0(R))/P_0(R)\}^2 \tag{4}$$

where $P_0(R)$ and $P_1(R)$ are the rung-rung pairing correlations for $/PL0\rangle$ and $/PL1\rangle$ wave functions, respectively. Note that this is not the only way to define the deviation. We tried some other reasonable definitions of deviation and the results are consistent. Fig. 2 shows the wave function

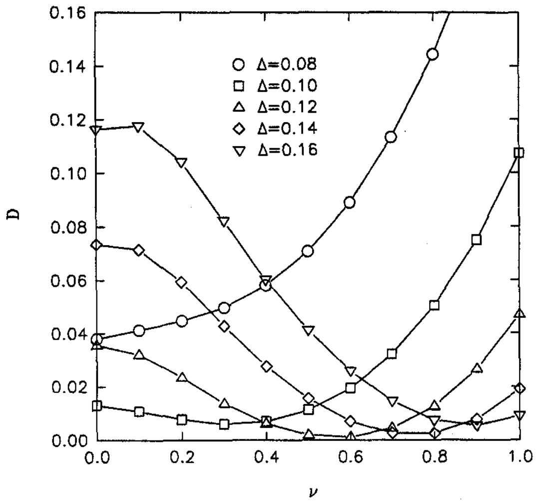

FIG. 2. Deviation $D(\Delta,\nu)$ for a 2×8 t-J ladder, $J/t = 1$.

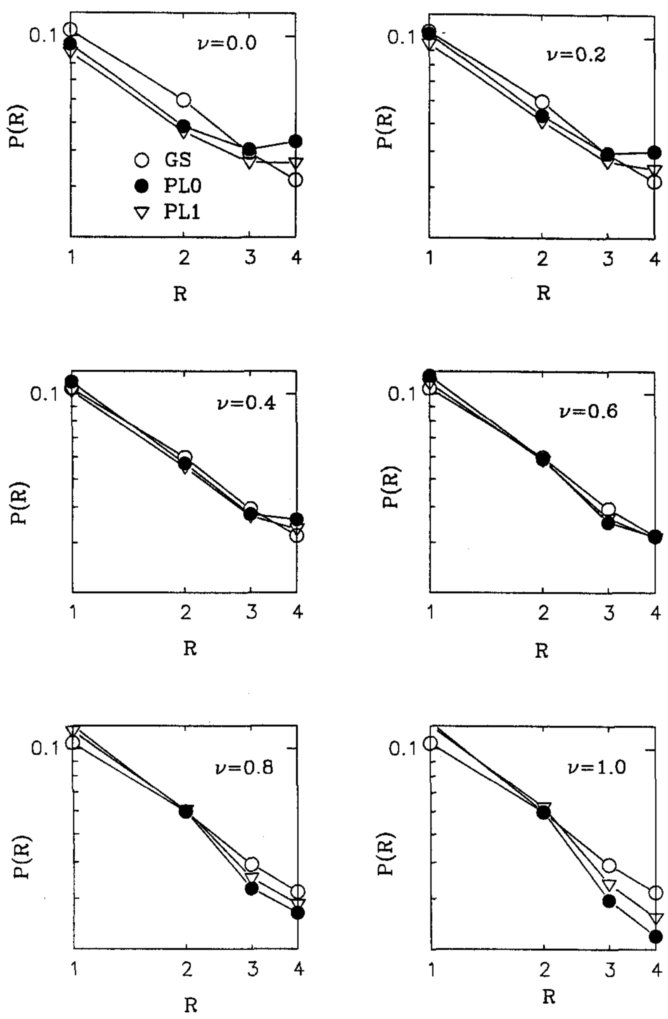

FIG. 3. Pairing correlation function $P(R)$ for trial wave functions with $\Delta = 0.12$ and various ν and their PL1 results, together with the exact data for $J/t = 1$ of 12 electrons in a 2×8 ladder.

with minimal deviation of 12 electrons $(6 \uparrow$ and $6 \downarrow)$ in the 2×8 ladder and $J/t = 1$. The wave function with minimal deviation is $\Phi(\Delta = 0.12,\ \nu = 0.6)$. Fig. 3 shows $P_0(R)$ and $P_1(R)$ of the trial wave functions and the exact results of the system. The "sandwich" behavior of the long range part $(R = 3,\ 4)$ is clear.

Since 2×8 is too small to see the long rang behavior of the pairing correlation, we did the similar analysis on 2×30 system, which the DMRG results are available for comparison [14]. We tried 24 $\uparrow$ and 24 $\downarrow$ electrons in 2×30 ladder with $J/t = 1.0$. The best one (minimal deviation) is $\Delta = 0.16$ and $\nu = 0.3$, while the trial wave function with lowest energy is $\Delta = 0.24$ and $\nu = 0.1$, whose pairing correlation is evidently overestimated. The pairing correlations obtained with three different sets of parameters are compared with the DMRG data from [14] in Fig. 4.

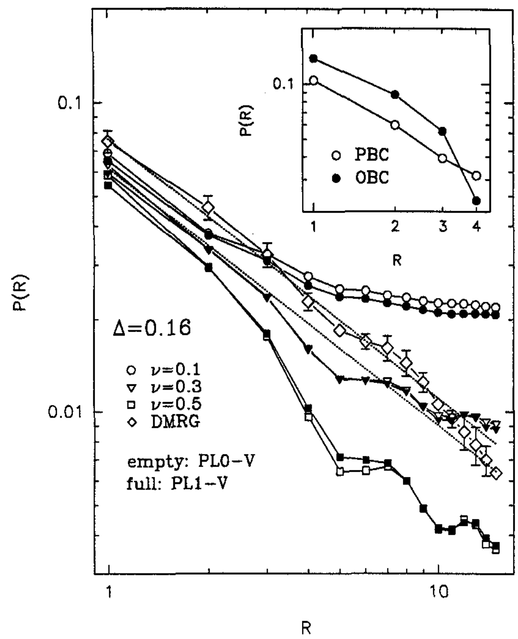

FIG. 4. Similar to Fig. 2, but for 48 electrons in a 2×30 ladder. The dot lines shows the power law fitting. The inset shows the 2×8 exact results for the different boundary conditions.

It can be seen that the slopes in the log-log plot, that is, the exponents of the power law decay, of the trial wave function (-0.835) with minimal D and the DMRG data (-0.840) are very close. The differences of amplitudes and slopes of the long tails between these two may come from the different boundary conditions of DMRG (open boundary condition, OBC) and power-Lanczos method (periodic boundary condition, PBC). In fact, we have seen similar difference between OBC and PBC by solving the 2×8 ladder with 12 electrons and $J/t = 1$ exactly, which is shown in the inset of Fig. 4.

In summary, from the study of 1D and 2-leg ladder t-J models, there are more evidences to support the "least deviation" criterion used to determine the superconductivity of the 2D t-J model. It seems that the pure 2D t-J model doesn't give enough amplitude of pairing correlation for realistic parameter values. Since there are a number of evidences that the 2D t-J model is a fairly good model for HTSC, it seems the model should not be excluded just due to the negative result with respect to the d-wave pairing correlation. It is possible that we can keep the good properties of the 2D model and enhance the superconductivity by some reasonable modification, for example, adding the interlayer hopping term [16].

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