d-Wave Pairing Correlation in the Two-Dimensional t-J Model

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The pair-pair correlation function of the two-dimensional t-J model is studied by using the power-Lanczos method under the assumption of monotonic behavior. In comparison with the results of the ideal Fermi gas, we conclude that the 2D t-J model does *not* have long-range d-wave superconducting correlation in the interesting parameter range of $J/t \leq 0.5$. Implications of this result are also discussed. [S0031-9007(98)06835-5]

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It is believed that the two-dimensional (2D) t-J model is a reasonable starting point to understand the physical properties of the high temperature superconducting (HTSC) cuprates [1,2]. One of the critical issues is whether the model has enough ingredients to quantitatively explain the high T_c. Here we shall report a numerical study to address this issue.

The 2D t-J model on a square lattice is

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

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. Using the experimental results of HTSC, we expect the physical interesting value of J/t to be about 0.4 and that superconductivity should occur for electron density n_e greater than 0.7.

The first indication about the superconductivity of the t-J model is to determine if the two holes would form a bound state by the exact diagonalization study on small lattices [3]. However, the attractive potential among doped holes is not a sufficient condition for superconductivity. The long-range pair-pair correlation should be a better indicator. The pair-pair correlation function is defined as

$$P_{s \text{ or } d}(R) = \frac{1}{N_s} \sum_i \langle \Delta^{\dagger}_i \Delta_{i+R} \rangle, \tag{2}$$

where $\Delta_i = c_{i\uparrow}(c_{i+\hat{x}\downarrow} + c_{i-\hat{x}\downarrow} \pm c_{i+\hat{y}\downarrow} \pm c_{i-\hat{y}\downarrow})$. $+$ and $-$ represent s and $d_{x^2-y^2}$ pairing states, respectively. N_s is the number of sites.

White *et al.* [4] studied the one-band Hubbard model and suggested that at low temperatures the pair-field susceptibility $\chi_d = \sum_R P_d(R)$ is enhanced in the $d_{x^2-y^2}$ channel and is small for others. Other convincing results are from variational Monte Carlo studies [5]. Although it did not provide quantitative values for T_c, the magnitude of pair-pair correlation varies with the hole density in a similar way as T_c of HTSC. The prediction of the dominance of d-wave pairing, instead of s-wave, in the t-J model is also quite encouraging.

However, these results are not quite consistent with a recent report by Zhang *et al.* They studied the 2D one-band [6] and three-band Hubbard models [7] by using the constrained path Monte Carlo (CPMC) method. They concluded that for $U/t > 4$ the long-range pair-pair correlation vanishes. It becomes quite important to have a careful numerical study of the pairing correlation in the 2D t-J model for larger lattices. In this paper we show that it is likely that there is no long-range $d_{x^2-y^2}$ pair-pair correlation at all for the *two-dimensional* t-J model in the physical parameter range ($J/t \leq 0.5$).

In the variational level, the optimal state of the 2D t-J model for a range of parameters is the $d_{x^2-y^2}$ resonating-valence-bond (RVB) trial wave function:

$$|\text{RVB}\rangle = P_d \prod_k (\tilde{u}_k + \tilde{v}_k c^{\dagger}_{k,\uparrow} c^{\dagger}_{-k,\downarrow}) |0\rangle, \tag{3}$$

with $\tilde{v}_k/\tilde{u}_k = \Delta_k/(\epsilon_k + \sqrt{\epsilon_k^2 + \Delta_k^2})$, $\Delta_k = \Delta(\cos k_x - \cos k_y)$, 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. This wave function with the form of a projected BCS wave function is known to be superconducting [5].

It is well known that the variational calculation usually overestimates the effect of superconductivity of the true ground state. For the t-J model the energy is dominated by the nearest neighbor interaction. Hence it naturally leads to large Δ in the variational calculation. Heeb and Rice [8] suggested that to examine the true pairing correlation, it might not be a good idea to use the lowest variational energy as a criterion in selecting the parameters of the trial function. They modified the function Eq. (3) with parameters that they believe can separate the short- and long-range parts of the correlations. They found the critical $J_c \simeq 0.44$ for the onset of superconducting

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long-range order for $n_e = 42/50$. Here we modify their idea with a more systematic approach and provide a more rigorous analysis.

One of the ways to eliminate the bias induced by the trial wave function is to project the trial function onto the true ground state of the system. Recently we have shown that the ground state energy and many other properties might be obtained accurately by using a particular ground state projection method, the power-Lanczos method [9,10], which is a hybrid of the power method and the variational Lanczos method. In the power method it can be easily shown that if a trial wave function $|\Psi\rangle$ is not orthogonal to the ground state, $(W - H)^m|\Psi\rangle$ is proportional to the ground state wave function as the power m approaches infinity. W is an appropriately chosen constant to make the ground state energy the largest eigenvalue of the W-H matrix. However, in practice, due to the Fermion sign problem, the power cannot be too large. A better way is to improve the trial function $|\Psi\rangle$ by using the first order Lanczos method, i.e., to use $|\mathrm{PL1}\rangle = (1 + C_1 H)|\Psi\rangle$ and then apply the power of W-H. C_1 is a new variational parameter. The results described below are either calculated by $|\Psi\rangle$, denoted by PL0-V, or by $(W\text{-}H)^m|\mathrm{PL1}\rangle$ denoted as PL1-Pm. $m = 0$ is the variational result, PL1-V, of the $|\mathrm{PL1}\rangle$ state.

Clearly, if the trial function is a very good representation of the ground state, the various correlation functions calculated in PL0-V should be almost the same as in PL1-Pm. On the other hand, if the trial function is biased in the wrong way, results of PL1-Pm will be very different from PL0-V and it will correct the bias [9,10]. This is demonstrated in Fig. 1.

The averaged value, P_d^{avg}, of the long-range part ($R > 3$) of $P_d(R)$ is plotted as a function of powers in Fig. 1 for $\Delta = 0.64$ which gives the lowest variational energy. The electronic density is $n_e = 42/50$ and $J = 0.7$. The value of P_d^{avg} is suppressed substantially from the VMC or PL0-V result when the power is increased. Clearly the optimized trial function has grossly overestimated the strength of the long-range pair-pair correlation. As noted above, this is due to the choice of a large Δ to optimize the short-range pairing.

Although the result in Fig. 1 is not yet converged, we could see that the long-range pair correlation changes *monotonically* as the wave function approaches the ground state. A clearer demonstration of this monotonic behavior is shown in Fig. 2.

P_d^{avg} is plotted as a function of powers in Fig. 2 for three different values of Δ: open circles are for $\Delta = 0.18$, full circles for 0.22, and triangles for 0.26. P_d^{avg} remains almost unchanged for $\Delta = 0.22$. For Δ larger than 0.22, the pair correlation always decreases with power. And the opposite is true for Δ smaller than 0.22. Since P_d^{avg} for $\Delta = 0.22$ hardly changes as the state gets closer and closer to the ground state, it is natural to assume that this is the ground state result. Moreover, if this is a good criterion to determine the ground state value, then we really need only to calculate PL0-V, PL1-V, and PL1-P2. There is no need to go to larger powers and the minus sign problem is avoided. The same result would be obtained if we examine $P_d(R)$ for the largest R instead of using P_d^{avg}.

In addition to Δ, μ is also a variational parameter in the RVB wave function. Just like Δ, which is not the real superconducting order parameter, μ is not the real chemical potential as in the simple mean field equations. In the discussion in the previous paragraph, μ is chosen to be consistent with the Fermi surface of the ideal Fermi gas. For example, $\mu = -0.4$ for $n_e = 42/50$. If P_d^{avg} is the true ground state value, then, just like Δ, no matter what initial values of μ we use for the trial wave function, the converged result would remain the same. In other words, different sets of (Δ, μ) will converge to the same final P_d^{avg}. This important consistency check has been verified. For example, for $n_e = 42/50$, we obtain $P_d^{\mathrm{avg}} = 0.0245(4)$ for $\Delta_{J=1} = 0.4$ and $\mu = -0.4$;

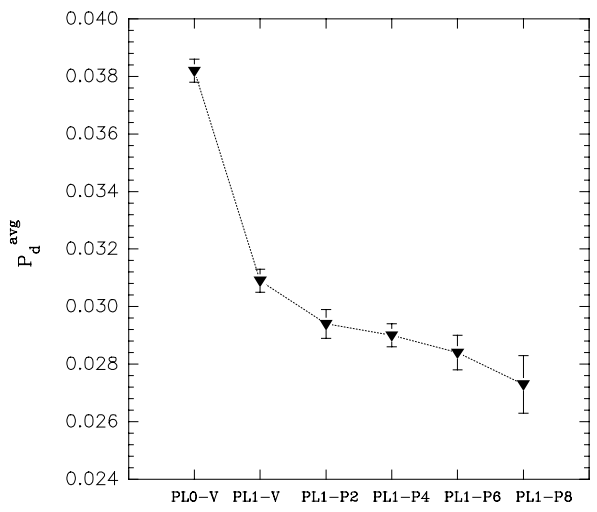

FIG. 1. Power dependence of the long-range pairing average P_d^{avg} for $n_e = 42/50$, $\Delta = 0.64$, and $J = 0.7$.

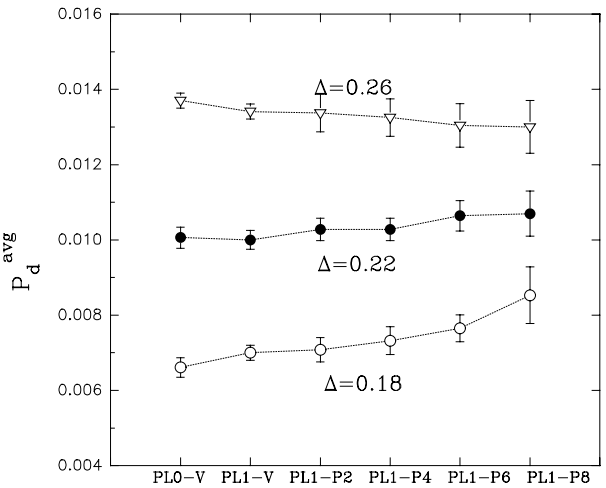

FIG. 2. Power dependence of the long-range pairing average P_d^{avg} for several trial wave functions with different Δ for $n_e = 42/50$ and $J = 0.7$.

$P_d^{\rm avg} = 0.0238(4)$ for $\Delta_{J=1} = 0.34$ and $\mu = -0.6$; and $P_d^{\rm avg} = 0.0238(3)$ for $\Delta_{J=1} = 0.24$ and $\mu = -0.8$.

So far by using the ground state projection method, we have shown that the long-range pair correlation $P_d^{\rm avg}$ approaches the ground state value monotonically. This basic assumption is used to choose parameters to best represent the ground state value of $P_d^{\rm avg}$ instead of determining variational parameters according to the lowest energy criterion. Unfortunately there are no exact calculations for the 2D t-J model with large lattices to test our assumption. However, the method could be tested in the study of the pairing correlation for the 2D attractive and repulsive Hubbard models.

It is known that the 2D attractive Hubbard model has long-range s-wave pairing correlation. The on-site pairing correlation, $\Delta_i = c_{i\uparrow}c_{i\downarrow}$, for several U is shown in Fig. 3. We consider the electron density at $4/64$ which is solved exactly. The figure shows that the energy-optimizing trial wave functions (full circles) always overestimate the pairing correlation in comparison with the exact results (open squares). And the results obtained by our power-Lanczos method (open triangles) are in much better agreement.

We have examined the long-range d-wave pairing correlation for the 2D repulsive Hubbard model. Our result agrees with Zhang *et al.* [6] that the long-range pairing correlation is vanishingly small.

The success for the attractive and repulsive Hubbard models further support our method. The method allows us to calculate the ground state $P_d^{\rm avg}$ for large lattices. In Fig. 4, $P_d^{\rm avg}$ is plotted as a function of electron density for 82 and 122 sites with $J = 0.5$. The PL0-V and PL1-V results for the trial wave functions with $\Delta_{\rm opt}$ optimizing the variational energies are also shown in the insets of Fig. 4 for 82 sites. It is clear that $P_{d,{\rm opt}}^{\rm avg}$ is substantially reduced by PL1. And the variational values are an order of magnitude greater than the ground state values.

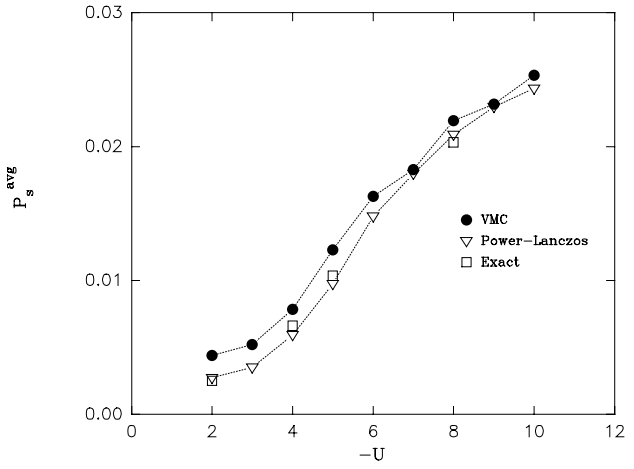

FIG. 3. Pairing correlation as a function of U for $n_e = 4/64$. Full circles are results evaluated from the energy-optimizing trial wave functions, open squares are for exact results, and open triangles are results based on our method.

Further, the $P_d^{\rm avg}$ for $J = 0.5$ can be compared with that of the ideal Fermi gas (IFG). The error bars denote the range of values for different degenerate states of the IFG. The nonzero $P_d^{\rm avg}$ is obviously a finite size effect. Since $P_d^{\rm avg}$ for $J = 0.5$ are smaller than that of the IFG we can easily conclude that there is no long-range d-wave pairing correlation for $J = 0.5$.

In Fig. 5 we show $P_d^{\rm avg}$ for different densities and J for 82 sites. The dotted line is the result of the IFG. It can be seen that $P_d^{\rm avg}$ is larger than the IFG values only for $J \geq 0.6$, which is considerably larger than the physical value of $J = 0.3$ or 0.4. The large values observed for $J \geq 0.6$ could be due to the phase separation [10]. For $J \leq 0.5$ not only $P_d^{\rm avg}$ seems to be too small to give large T_c for the HTSC materials, the maximum $P_d^{\rm avg}$ is at the hole density $x_h = 1 - x_e \sim 10\%$. This disagrees with experiments which have optimal doping at $x_h \sim 15\% \sim 20\%$. For $J \geq 0.6$, the values of x_h are very close to the critical hole densities of phase separation [10]. It is possible that for large J the $P_d^{\rm avg}$ measured actually indicates electron clustering near phase separation rather than superconductivity.

Our result that there is no long-range d-wave pairing correlation for $J \leq 0.5$ is actually consistent with the exact numerical results for the two-hole binding energy. It is known that binding two holes is a necessary condition for the occurrence of superconductivity. In Fig. 6 the binding energy of two holes for various J is plotted as a function of the inverse of N_s which is the cluster size. The results of 32 sites are obtained by Leung [11] and 26 sites by Poilblanc [12]. It shows that two holes do not bind together unless $J > 0.8$. Because of the different cluster

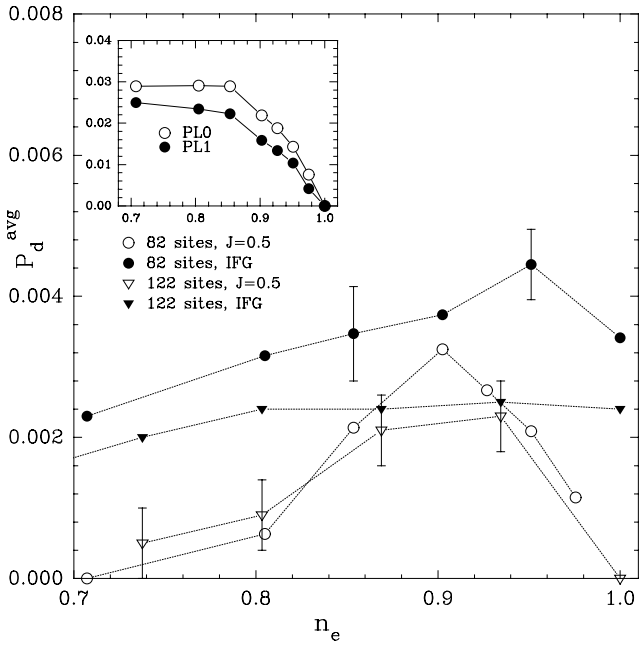

FIG. 4. $P_d^{\rm avg}$ for $J/t = 0.5$ and ideal Fermi gas for 82 and 122 sites. The PL0 and PL1 results of energy-optimizing $\Delta_{\rm opt}$ for 82 sites are shown in the inset.

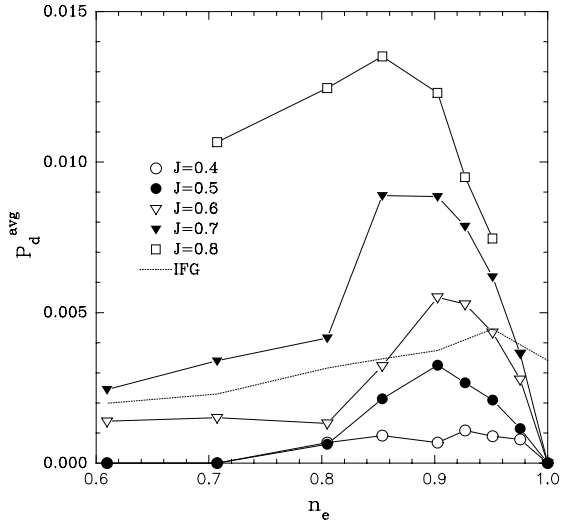

FIG. 5. P_d^{avg} for 82 sites for different density and J.

shapes, the data are not quite on a straight line. However, even taking into account the deviation, the result is still consistent with the absence of hole binding for $J \leq 0.5$.

In summary, based on a simple observation that the long-range d-wave pairing correlation changes monotonically when the state approaches the ground state, we assume that the ground state value can be determined by choosing parameters that do not optimize the variational energy but keep the correlation value unchanged when we project the wave function onto the ground state. As a consistency check we show that different sets of values of parameters, Δ and μ, produce the same correlation value. This method has also been successfully tested for the 2D attractive and repulsive Hubbard models. The result that the long-range d-wave pairing correlation is nonzero only for $J \geq 0.6$ is consistent with the finite size analysis of exact results for small clusters. It is also consistent with the result obtained in a completely different analysis that the phase separation boundary occurs only for $J \geq 0.6$.

Since there are a number of evidences that the 2D t-J model is a fairly good model for HTSC, the negative result with respect to the d-wave pairing correlation reported above is quite disturbing. There are several possibilities to explain this discrepancy.

The first thing one can point to is the possible contribution of next-nearest neighbor hopping and next-next-nearest neighbor hopping, t' and t'', respectively. We found that the superconductivity is not enhanced by adding the t' term even though we have tuned the parameters to have the Fermi surface passing through the van Hove singularity at 15% hole density.

Another possibility is that due to other interactions such as electron phonon the effective J/t might be larger than 0.6. However, in this case, it is more likely we will have phase separation. The doping dependence of T_c is also inconsistent with experiments. The interlayer tunneling model proposed by Anderson [13] certainly expects the absence of pairing in our pure 2D model. A more exotic possibility might be that the true ground state symmetry is not d-wave but a time-reversal-broken order parameter [14,15].

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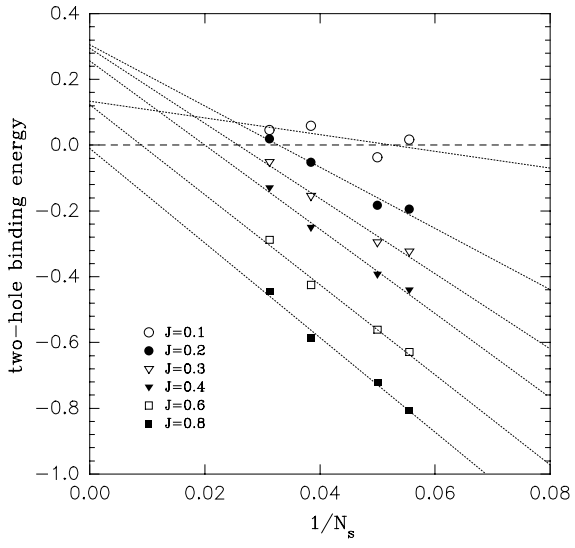

FIG. 6. Two-hole binding energies as a function of the inverse of cluster size for different J.

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