Pairing Correlations on t-U-J Ladders

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We find that the pairing correlations on the usual t-U Hubbard ladder are significantly enhanced by the addition of a nearest-neighbor exchange interaction J. Likewise, these correlations are also enhanced for the t-J model when the on-site Coulomb interaction is reduced from infinity. Moreover, the pairing correlations are larger on a t-U-J ladder than on a t-J_{eff} ladder in which J_{eff} has been adjusted so that the two models have the same spin gap at half filling. This enhancement of the pairing correlations is associated with an increase in the pair-binding energy and the pair mobility in the t-U-J model and points to the importance of the charge-transfer nature of the cuprate systems.

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Various *ab initio* quantum chemistry calculations as well as model Hamiltonian studies have been used to determine the electronic properties of Cu-oxide clusters [1–6]. In particular, these calculations have provided parameters for simpler, effective one-band Hubbard and t-J models which have then been used to study many-body correlations in larger systems. However, both the one-band Hubbard and the t-J models differ in an essential manner from the high T_c cuprates which are known to be charge-transfer insulators [7] in their undoped state. Thus, the one-band Hubbard model at half filling is characterized by a Mott-Hubbard gap which is set by U and in the t-J model, U is taken to infinity with the constraint of no double occupancy. Therefore, while Coulomb fluctuations associated with double occupancy of a site are controlled by U in the Hubbard model, U also determines the strength of the exchange coupling. In the Hubbard model as U increases beyond the bandwidth, J decreases as $4t^2/U$. Although J is an independent parameter in the t-J model, U is infinite in this model, suppressing charge fluctuations.

While we believe that the basic pairing mechanism arises from the exchange correlations, the charge-transfer nature of the cuprates can play an essential role in the doped systems where it allows for a more flexible arrangement between J and U than reflected in either the one-band Hubbard or t-J models. To explore this, we have carried out density-matrix renormalization group [8] (DMRG) calculations of the pairing correlations on two-leg t-U-J ladders. Ladders are known to provide model systems which exhibit various phenomena similar to those of the cuprates [9]. In particular, when doped away from half filling they are known to have power-law pairing correlations which have opposite, $d_{x^2-y^2}$-like, signs between the rung-rung and rung-leg correlations. These correlations have previously been investigated for both Hubbard [10,11] and t-J models [12,13]. Here we study a generalized t-U-J model which includes both an on-site Coulomb repulsion U and a nearest-neighbor exchange J. While both Hubbard and t-J ladders show pairing correlations when doped, we find that these correlations can be significantly enhanced in a model with both U and J. We argue that, in fact, a t-U-J model is appropriate for a charge-transfer material [7].

The basic one-band Hubbard model is characterized by a one-electron nearest-neighbor hopping t and an on-site Coulomb interaction U.

$$H = \sum_{\langle ij\rangle,\sigma} -t(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}) + U\sum_i n_{i\uparrow}n_{i\downarrow}. \quad (1)$$

Here $c^\dagger_{i\sigma}$ creates an electron with spin σ on site i and $\langle ij\rangle$ sums over nearest-neighbor sites. As is well known, when U/t is large, a strong coupling expansion [14] of Eq. (1) leads to the t-J Hamiltonian

$$\begin{aligned} H = \sum_{\langle ij\rangle,\sigma} -t(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}) + J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\mathbf{S}_j - \frac{n_i n_j}{4}\right) \\ - \frac{J}{4}\sum_{i,\delta\neq\delta',\sigma}(c^\dagger_{i+\delta,\sigma}c^\dagger_{i,-\sigma}c_{i,-\sigma}c_{i+\delta',\sigma} \\ - c^\dagger_{i+\delta,-\sigma}c^\dagger_{i,\sigma}c_{i,-\sigma}c_{i+\delta',\sigma}) \end{aligned} \quad (2)$$

with $J = 4t^2/U$ and δ, δ' are vectors separating nearest-neighbor sites. Here there is an important restriction that no site can have two fermions. Typically in Eq. (2), t and J are treated as independent parameters and for doping near half filling the latter three-site term is dropped. Now, while these effective models both describe certain aspects of the cuprate's system, they lack the flexibility to describe an important feature that arises from the charge-transfer nature of these materials. Specifically, in the insulating state the one-band Hubbard model at large U has a Mott-Hubbard gap set by U rather than a charge-transfer gap set by the difference in the oxygen and copper sites' energies. Furthermore, for a one-band Hubbard model, when U is large, $J \sim 4t^2/U$ so that the exchange interaction becomes negligible for large U. However, when the planar O is included in a three-band Hubbard model [15] with a Cu($d_{x^2-y^2}$)-O($p\sigma$) hopping t_{pd}, one finds in strong

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coupling that

$$J = 4\left(\frac{t_{\mathrm{pd}}^2}{\Delta_{\mathrm{pd}} + U_{\mathrm{pd}}}\right)^2\left[\frac{1}{U_{\mathrm{d}}} + \frac{2}{2\Delta_{\mathrm{pd}} + U_{\mathrm{p}}}\right]. \quad (3)$$

Here Δ_{pd} is the Cu-O site energy difference and U_{d}, U_{p}, and U_{pd} are the Cu, O, and Cu-O Coulomb interactions, respectively. In this case, when U_{d} becomes large J remains finite, saturating at a value set by the charge-transfer gap and the O and Cu-O Coulomb interactions. There are in fact further contributions to Eq. (3) from O-O hopping terms which Eskes and Jefferson [16] have shown are important in obtaining a quantitative estimate of the exchange interaction. In addition, there are in fact various ways to construct effective single-band Hubbard models which take into account the Cu-O charge excitations [17–19]. However, the basic point which we want to make here, illustrated by Eq. (3), is that when U_{d} is large compared to the effective Cu-Cu hopping, the exchange remains finite rather than going to zero. Likewise, in the t-J model, while J/t can be set to a physical value, one has in effect an infinite on-site Coulomb repulsion arising from the restriction of no double occupancy. The suppression of double occupancy reduces the mobility of the pairs [20], missing the physics associated with the partial occupation of the O sites surrounding a Cu.

Thus it is of interest to consider a generalized t-U-J model in which there is both a finite Coulomb interaction U and an effective exchange term J. In the limit in which $J = 0$, this is just the one-band Hubbard model while in the limit $U/t \gg 1$, this goes over to the t-J model [21]. Since the doped two-leg ladder exhibits $d_{x^2-y^2}$-like pairing correlations which can be reliably calculated using DMRG techniques, we have a controlled way of investigating the interplay of U and J in determining the pairing response.

The DMRG calculations reported here have been carried out on open ended ladders (up to 2×48 sites) keeping up to 800 states, so that the maximum weight of the discarded density matrix eigenvalues is 10^{-6}. We first examine the rung-rung pair-field correlation function

$$D(\ell) = \langle \Delta_{i+\ell} \Delta_i^\dagger \rangle \quad (4)$$

for a doped (eight holes) 2×32 ladder. The operator

$$\Delta_i^\dagger = c_{i1,\uparrow}^\dagger c_{i2,\downarrow}^\dagger - c_{i1,\downarrow}^\dagger c_{i2,\uparrow}^\dagger \quad (5)$$

creates a singlet pair on the ith rung and $\Delta_{i+\ell}$ destroys it on the $(i + \ell)$th rung. A similar calculation in which a singlet pair is created on the ith rung and a singlet pair is destroyed on one of the legs at $i + \ell$ has an opposite sign indicating the $d_{x^2-y^2}$-like structure of the pairing. Because of the finite length of the ladder, we have kept $\ell \leq 12$, with the measurements made in the central portion of the ladder, in the plots of $D(\ell)$. In this region the effects of the open ends are negligible.

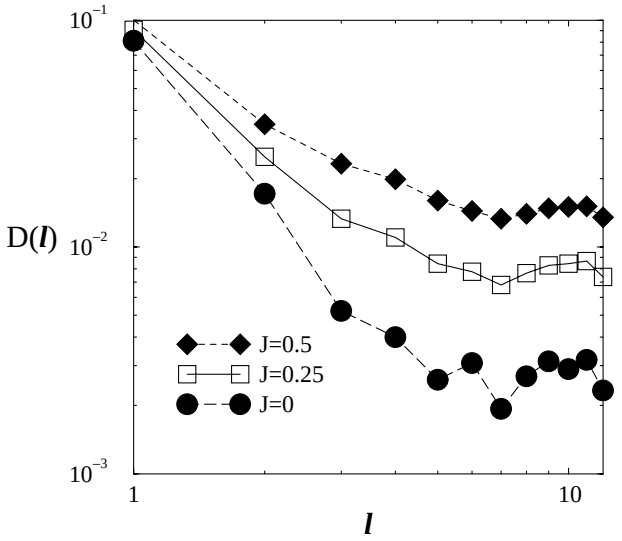

FIG. 1. The rung-rung singlet pairing correlation function $D(\ell)$ versus ℓ on a doped 2×32 ladder with $\langle n \rangle = 0.875$ for $U = 6$ and various values of J.

In Fig. 1 we show the effect of adding an additional exchange term J to a Hubbard model with $U = 6$. Here and in the following we measure energy in units of t. As seen, the addition of J clearly enhances the pairing. In all of the plots it is important to recognize that the pair has an internal structure so that $\Delta_i^\dagger$ and $\Delta_{i+\ell}$ have only a partial overlap to the state in which a pair is added at the ith rung or removed from the $i + \ell$ rung, and the basic size of $D(\ell)$ is reduced by the square of this overlap. As seen in Fig. 1, adding an additional exchange strongly enhances the pair-field correlations.

Similarly, in Fig. 2a we examined the effect of U on the pairing correlations of a t-U-J ladder with $J = 0.25$. For $U \gg 1$, we have the usual t-J result. As U initially decreases, there is again a significant enhancement of the pairing correlations, but eventually as U decreases below the bandwidth, the pairing correlations are reduced. This is also shown in Fig. 2b, where we have plotted

$$\bar{D} = \sum_{\ell=8}^{12} D(\ell) \quad (6)$$

versus U for $J = 0.25$. Here $\bar{D}$ reaches a maximum for $U \simeq 6$.

One would, of course, expect that the pairing correlations would depend on the total effective exchange interaction, both the explicit "J" exchange and the additional exchange associated with a finite U. Thus, in the t-U-J model, as U initially increases, the effective exchange increases and then as U exceeds the bandwidth its contribution to the exchange decreases as $4t^2/U$. However, there is more to this than just the enhancement of the exchange interaction which can be seen by comparing the two models. A half-filled Hubbard ladder with $U = 6$ and $J = 0.25$

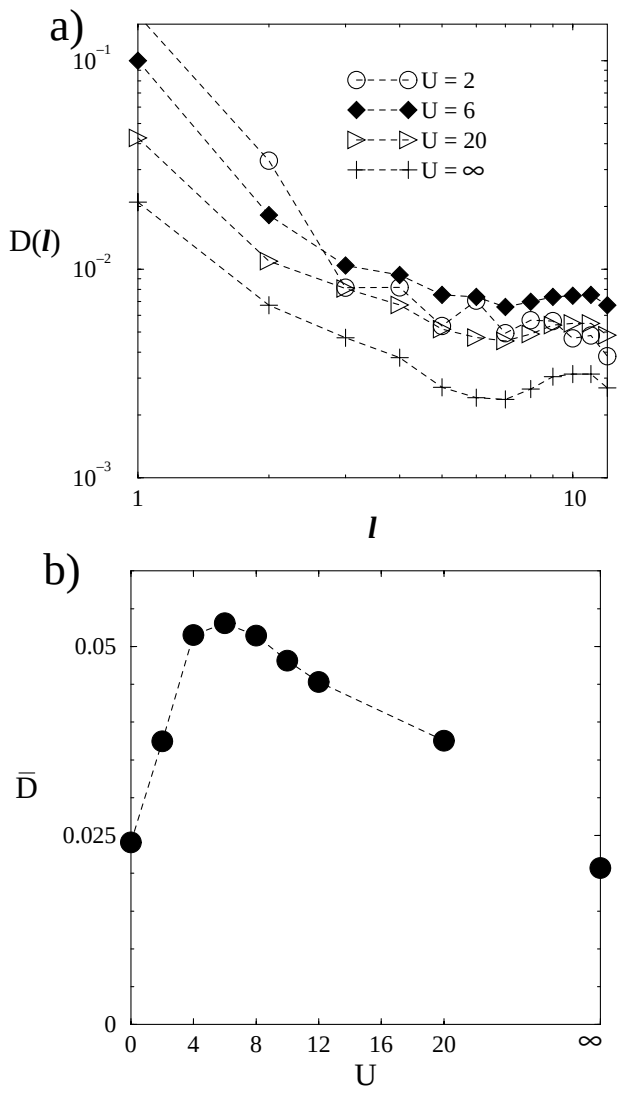

FIG. 2. (a) The rung-rung singlet pairing correlation function $D(\ell)$ versus ℓ on a doped ladder with $\langle n\rangle = 0.875$ for $J = 0.25$ and various values of U. (b) The partial singlet pairing correlation function sum $\bar{D}$ as a function of U for a doped ladder with $\langle n\rangle = 0.875$ and $J = 0.25$.

has a spin gap $\Delta_s = 0.22$ corresponding to an effective exchange [22] $J_{\rm eff} \approx 2\Delta_s = 0.44$. Using this value for the exchange in a t-J model we have calculated the pair-field correlation function $D(\ell)$ in Fig. 3 and compared it with the pair-field correlations found for the corresponding t-U-J model. Although both of these models have the same spin gap at half filling, it is clear that the t-U-J ladder has significantly stronger pairing correlations.

In order to understand the reasons for this, we have calculated the pair-binding energy and the pair mobility for both these models. The pair-binding energy is

$$E_{\rm pb} = 2E_0(1) - E_0(2) - E_0(0) \qquad (7)$$

with $E_0(n)$ the ground-state energy with n holes. We find $E_{\rm pb}$ is equal to 0.34 for the t-U-J model with $U = 6$ and

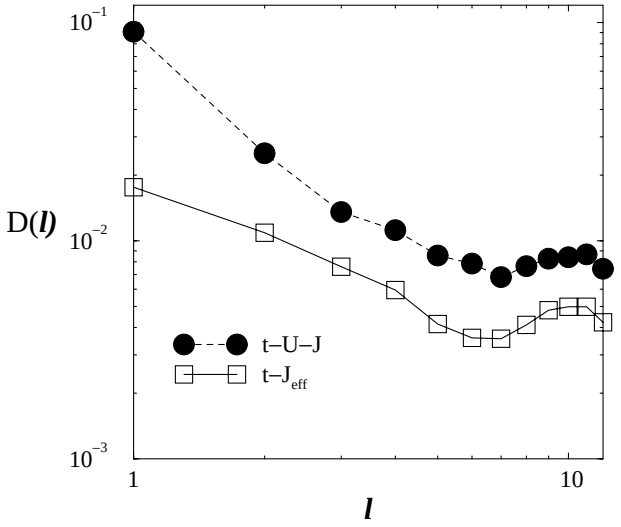

FIG. 3. Comparison of $D(\ell)$ versus ℓ for a t-U-J model (full circles) with $U = 6$ and $J = 0.25$ with a t-U model (open squares) which has the same spin gap at half filling.

$J = 0.25$. For the t-$J_{\rm eff}$ ladder with $J_{\rm eff} = 0.44$, adjusted so that the two models have the same spin gap at zero doping, the pair-binding energy is 0.23. We have also calculated the effective hopping $t_{\rm eff}$ of a hole pair from the dependence of

$$\epsilon_p(L_x) = E_0(2) - E_0(0) \qquad (8)$$

on the length of the ladder for ladders with L_x up to 48. In ladders with open boundary conditions, we expect that the pair behaves like a particle in a box and hence $\epsilon_p(L_x)$ varies as

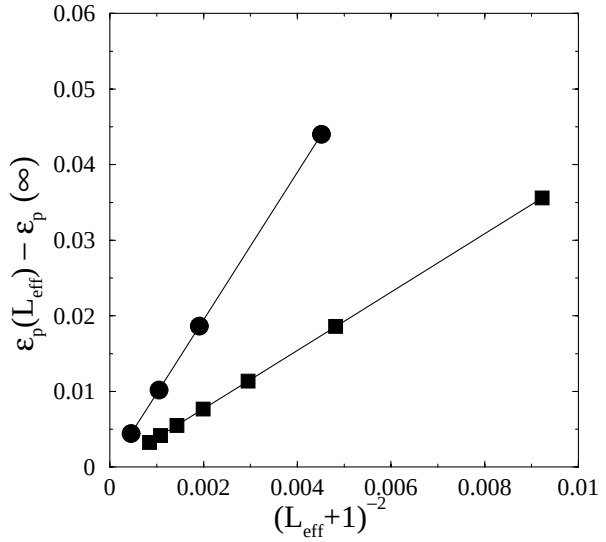

FIG. 4. Hole pair energy ϵ_p versus $(L_{\rm eff} + 1)^{-2}$ for the t-U-J model with $U = 6$ and $J = 0.25$ (circles) and the corresponding t-J model with $J = 0.44$ (squares). The solid lines are least mean square fit of Eq. (9).

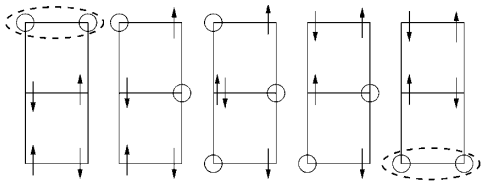

FIG. 5. Illustration of a pair transfer process involving a set of intermediate states. The state in the center has a doubly occupied site. This transfer process cannot occur in the t-J model but it does contribute to the pair hopping in the t-U-J model.

$$\epsilon_p(L_x) = \epsilon_p(\infty) + t_{\text{eff}} \frac{\pi^2}{(L_{\text{eff}} + 1)^2}, \qquad (9)$$

where the effective length differs from the actual ladder length L_x because of end effects. For large enough systems, the difference $L_{\text{eff}} - L_x = \delta L$ tends to a constant and is considered as a fitting parameter [20]. Figure 4 shows the results for the t-U-J and the t-J_{eff} models. The effective hopping, given by the slope divided by π^2, is $t_{\text{eff}} = 0.99$ for the t-U-J ladder and $t_{\text{eff}} = 0.39$ for the t-J_{eff} ladder.

The enhancement of the effective pair hopping which occurs when U is finite can be understood as arising from virtual states involving doubly occupied sites. An example of this is illustrated in Fig. 5. Here a pair of holes on the top rung hops to the bottom rung via a set of intermediate states. In this sequence, the second intermediate state, shown in the middle of the figure, has a doubly occupied site. In the t-J model this would not be allowed, leading to a reduction in the effective pair hopping. This effect not only enhances the pair-field correlations on the t-U-J ladder, but we believe it also would act to reduce the stripe stiffness in the 2D t-J problem. This would favor a $d_{x_2-y_2}$-pairing state over the striped state we have typically found in DMRG calculations on n-leg t-J ladders [23].

Thus we conclude that the charge-transfer nature of the cuprates can be more appropriately described using a t-U-J model. Furthermore, this model exhibits enhanced pairing correlations due to (i) an additional exchange coupling reflecting the exchange path in which there is a virtual double occupancy on the oxygen rather than the Cu and (ii) an enhanced pair hopping allowed by a finite value of U which reflects the alternate paths for electron transfer in the charge-transfer system.

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