Pairing Correlations on \( t-U-J \) Ladders

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Pairing correlations on generalized \( t-U-J \) two-leg ladders are reported. 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 onsite Coulomb interaction is reduced from infinity. Moreover, the pairing correlations are larger on a \( t-U-J \) ladder than on a \( t-J_{\text{eff}} \) ladder in which \( J_{\text{eff}} \) 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 point to the importance of the charge transfer nature of the cuprate systems.

Various \emph{ab initio} quantum chemistry calculations as well as model Hamiltonian studies have been used to determine the electronic properties of Cu-oxide clusters. 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 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 (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. 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 and \( t-J \) models. Here we will study a generalized \( t-U-J \) model which includes both an onsite 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.

The basic one-band Hubbard model is characterized by a one-electron nearest-neighbor hopping \( t \) and an onsite Coulomb interaction \( U \).

\[
H = \sum_{\langle ij \rangle, \sigma} -t \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \tag{1}
\]

Here \( c_{i\sigma}^\dagger \) creates an electron with spin \( \sigma \) 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 leads to the \( t-J \) Hamiltonian

\[
H = \sum_{\langle ij \rangle, \sigma} -t \left( c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + J \sum_{\langle ij \rangle} \left( S_i S_j - \frac{n_{i\uparrow} n_{j\downarrow}}{4} \right) - \frac{J}{4} \sum_{i, \delta \neq \delta', \sigma} \left( c_{i+\delta, \sigma}^\dagger c_{i, \sigma} c_{i+\delta', -\sigma} c_{i, -\sigma} - c_{i, \sigma}^\dagger c_{i, -\sigma} c_{i+\delta', -\sigma} c_{i+\delta, \sigma} \right), \tag{2}
\]

with \( J = 4t^2/U \) and \( \delta, \delta' \) 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 cuprates 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, when \( U \) is large, \( J \sim 4t^2/U \) decreases as \( U \) increases rather than saturating at a value set by the charge-transfer gap. That is,
in strong coupling, the three-band Hubbard model gives

\[ J = 4 \left( \frac{t_{pd}^2}{\Delta_{pd}} \right)^2 \left[ \frac{1}{U} + \frac{1}{\Delta_{pd}} \right] \]  

(3)

with \( t_{pd} \) the Cu \((d_{x^2-y^2})\) - O(pσ) hopping, \( \Delta_{pd} \) the Cu-O site energy difference and \( U \) the Cu Coulomb energy. There are in fact further contributions to Eq. (3) from O-O hopping terms, as well as modifications due to O and Cu-O Coulomb interactions. However, the basic point is that when \( U \) is large compared to the Cu-Cu hopping \( t_{pd}^2/\Delta_{pd} \), 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 a finite onsite Coulomb repulsion arising from the restriction of no double occupancy. The suppression of double occupancy reduces the mobility of the pairs, missing the physics associated with the partial occupation of the O sites surrounding a Cu.

To address these limitations, we will study a \( t-U-J \) model in which there is a finite Coulomb interaction and an effective exchange term \( J \). In the limit in which \( J \rightarrow 0 \), this is just the one-band Hubbard model while in the limit \( U/t \gg 1 \), this goes over to the \( t-J \) model \( ^{[3]} \) The DMRG calculations reported here have been carried out on open ended ladders (up to \( 2 \times 48 \) 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

\[ D(\ell) = \langle \Delta_{i+\ell} \Delta_i \rangle \]  

(4)

for a doped (8 holes) \( 2 \times 32 \) ladder. The operator

\[ \Delta_i \equiv c_{i+\ell,\uparrow}^\dagger c_{i,\downarrow}^\dagger - c_{i,\uparrow}^\dagger c_{i+\ell,\downarrow}^\dagger \]  

(5)

creates a singlet pair on the \( i \)th 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 \( i \)th rung and a singlet pair is destroyed on one of the legs at \( i+\ell \) has an opposite sign indicating the \( d_{x^2-y^2} \) 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.

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 will 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 \( \Delta_i \) and \( \Delta_{i+\ell} \) have only a partial overlap to the state in which a pair is added at the \( i \)th 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.

\[ D(\ell) \]  

(6)

versus \( U \) for \( J = 0.25 \). Here \( D \) reaches a maximum for \( U \simeq 6 \).
FIG. 2. (a) The rung-rung singlet pairing correlation function $D(\ell)$ versus $\ell$ 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 $J = 0.25$.

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 $J = 0.25$ has a spin gap $\Delta_s = 0.22$ corresponding to an effective exchange $J_{\text{eff}} \approx 2\Delta_s = 0.44$. 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

$$E_{pb} = 2E_{0}(1) - E_{0}(2) - E_{0}(0)$$  \hspace{1cm} (7)

with $E_{0}(n)$ the ground-state energy with $n$ holes. We find $E_{pb}$ is equal to 0.34 for the $t$-$U$-$J$ model with $U = 6$ and $J = 0.25$. For the $t$-$J_{\text{eff}}$ ladder with $J_{\text{eff}} = 0.44$, 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 $t_{\text{eff}}$ of a hole pair from the dependence of $\epsilon_p(\ell_x) = E_{0}(2) - E_{0}(0)$ on the length of the ladder for ladders with $\ell_x$ up to 48. In ladders with open boundary conditions, $\epsilon_p(\ell_x)$ varies as

$$\epsilon_p(\ell_x) = \epsilon_p(\infty) + t_{\text{eff}} \frac{\pi^2}{(L_{\text{eff}} + 1)^2}$$  \hspace{1cm} (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. Fig. 4 shows the results for the $t$-$U$-$J$ and the $t$-$J_{\text{eff}}$ models. The effective hopping, given by the slope divided by $\pi^2$, is $t_{\text{eff}} = 0.99$ for the $t$-$U$-$J$ ladder and $t_{\text{eff}} = 0.39$ for the $t$-$J_{\text{eff}}$ 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 $t-U-J$ 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 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.

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 (1) an additional exchange coupling reflecting the exchange path in which there is a virtual double occupancy on the oxygen rather than the Cu and (2) 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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