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Superconductivity in ladders and coupled planes

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We discuss an electronic model consisting of two chains or planes, each described by a t-J model, coupled by t'-J' interactions between them. For $J' \sim J$ or larger we show the presence of a spin-gap and hole-pair formation upon doping. The model exhibits superconducting pairing correlations away from half filling. We support our claims by numerical studies of the spin gap, the binding energy of holes, and the pairing correlations of finite clusters. The hole-pairing operator is a spin singlet with one member of the pair in each chain or plane. Our model belongs to the universality class of the $U<0$ Hubbard model with $|U| \gg t$. We argue that this model may be physically realized by doping the orthorhombic compound $(VO)_2P_2O_7$.

The V^{4+} compound $(VO)_2P_2O_7$ consists of weakly coupled arrays of one-dimensional metal oxide ladders.[1] The transition metal sites on these ladders are bridged by oxygen atoms, and in the nominal insulating state, the spin-$\frac{1}{2}$ moments on the transition metals are coupled by a superexchange interaction mediated by these oxygens. In this paper we examine a simple model for such a ladder which consists of two t-J chains with t'-J' couplings forming the rungs between them. Results for both an insulating half filled ladder and a doped ladder are obtained. At half filling we determine the dependence of the spin gap on J'/J. For the doped system with $J' \sim J$ or larger, and t' small compared to J', the added holes tend to occupy adjacent sites on a rung forming localized pairs which exhibit superconducting correlations when t is larger than J. We also generalize this analysis to the case of two planar t-J clusters coupled by t'-J' vertical links. We argue that this model has superconducting or charge-density-wave (CDW) long-range order at zero temperature and finite doping.[2]

The model Hamiltonian we will study for the ladder consists of two t-J chains with t'-J' coupling rungs (Fig. 1),

$$H = J\sum_{\mathbf{i}} \mathbf{S}_{\mathbf{i}}\cdot\mathbf{S}_{\mathbf{i}+\hat{\mathbf{x}}} + J'\sum_{\mathbf{i}} \mathbf{S}_{\mathbf{i}}\cdot\mathbf{S}_{\mathbf{i}+\hat{\mathbf{y}}} - t\sum_{\mathbf{i},s} (\bar{c}^{\dagger}_{\mathbf{i},s}\bar{c}_{\mathbf{i}+\hat{\mathbf{x}},s} + \text{H.c.}) - t'\sum_{\mathbf{i},s} (\bar{c}^{\dagger}_{\mathbf{i},s}\bar{c}_{\mathbf{i}+\hat{\mathbf{y}},s} + \text{H.c.}) \,. \quad (1)$$

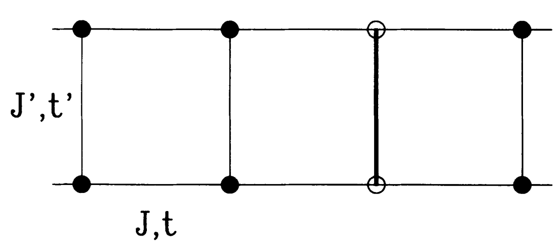

FIG. 1. Schematic definition of the t-J-t'-J' model on a ladder. Dots represent sites of the t-J chains which are in interaction through vertical links with couplings J',t'. Solid dots are occupied sites while open dots denote holes. A tight bound state of two holes is shown.

Here the chains run along the x axis and the rungs connect site $\mathbf{i}$ with $\mathbf{i}+\hat{\mathbf{y}}$. $\bar{c}_{\mathbf{i},s}$ are *hole* destruction operators with spin s at sites $\mathbf{i}$. We will consider ladders with periodic boundary conditions in the x direction. The rest of the notation is standard and the generalization to two coupled t-J planar clusters with t'-J' vertical links between them is straightforward.

In order to gain some physical insight into the nature of the correlations which may occur, it is useful to consider the large J' limit. In this case the ground state at half filling consists, in leading order, of a set of spin singlets on each rung of the ladder. Naturally, there is a spin gap in the spectrum of order J' which corresponds to creating a triplet on one of the rungs. When the system is doped with holes, it is energetically favorable to break as few of the singlet rungs as possible. Thus, when a pair of holes is added, the system will minimize its energy by breaking just one spin-singlet rung forming a hole-pair bound state (see Fig. 1) with a pair binding energy varying as $\sim J'$. Additional hole pairs can bind on other rungs. The hole pairs are spin singlets and in this strong coupling picture correspond to a pair-field operator[3]

$$\Delta_{\mathbf{i}} = \frac{1}{\sqrt{2}} (\bar{c}_{\mathbf{i},\uparrow}\bar{c}_{\mathbf{i}+\hat{\mathbf{y}},\downarrow} - \bar{c}_{\mathbf{i},\downarrow}\bar{c}_{\mathbf{i}+\hat{\mathbf{y}},\uparrow}) \,. \quad (2)$$

For two coupled planes the "physics" and pairing operator are the same. In addition, in this case Δ is *invariant* under a rotation in the planes of $\pi/2$. The residual interaction between pairs and between spins will determine the various phases of the model and the type of long-range order. In this framework, recently discussed by Imada[4] for a dimerized t-J-J' model, it is the spin-spin correlations that lead to an effective attraction between the holes rather than an explicit hole-hole attractive interaction.

The existence of hole pairs in the Hamiltonian of Eq. (1) is a nontrivial feature that is difficult to obtain in purely two-dimensional (2D) systems without the complication of phase separation. The t-J-t'-J' ladder which we have studied can exhibit both spin-gap and singlet-pairing correlations in certain parameter regimes. In this model, the pairs are formed due to the anisotropy between J' and J, with $J' > t'$, rather than from the explicit introduction of an attractive interaction. What is the influence of the perpendicular hopping t'? Consider the case of two holes on a 2×2 cluster with t' and J' being the dominant interactions. If t' is larger than $\frac{3}{8}J'$, the holes are *not* localized on one rung. Thus, here we will take t' fixed at a small value compared with J'. Actually if a one-band Hubbard model with couplings t, t', and U is used instead of the t-J-t'-J' model, one cannot achieve $J'>t'$. Thus the parameter regime analyzed here is not contained in the one-band Hubbard model on a ladder which does not have an obvious limit with a superconducting phase. For example, when $t'/t\rightarrow\infty$ the model decouples into N vertical links described only by a hopping term (like a two site $U=0$ Hubbard model) and there is no pair formation.

The mobility of the hole pairs depends on the parameter t^2/J'. In the subspace of pairs it can be easily shown that the effective Hamiltonian is equal to a negative-U model[4] with $|U|\sim J'$. If the density of holes corresponds to quarter filling, then, the ground state at small t for two coupled planes will consist of a checkerboard of hole singlets and spin singlets. Replacing hole singlets by doubly occupied sites and spin singlets by empty sites, this resembles the ground state of the negative-U Hubbard model at half filling which is known to be superconducting for $D\geq2$ (although degenerate with a CDW).[5,6] From this analogy it is clear that the model described by Eq. (1) will have a superconducting ground state at $T=0$ in an appropriate region of parameter space. Actually, the t'-J' links that induce hole binding when J' is large can be thought of as "negative-U centers".[4,7,8] If J' is large, then the model will have a critical temperature where superconductivity disappears with $T_c\sim t^2/J'$. At higher temperatures $T\sim J'$ pairs will be dissociated. In this respect this model resembles a Bose condensation of pairs whose size is of order one lattice spacing in the vertical direction while the distance between pairs is larger and depends on the hole concentration, the ratio J/t and other possible in-plane interactions.

The preceding discussion has been based on the limit where J' is the largest scale and it is important to find if this assumption can be relaxed. For that purpose we have studied this model numerically using Lanczos techniques to calculate the ground-state properties of half filled insulating $2\times N$ ladders with $N=4$, 6, 8, 10, and 12; doped ladders with up to $N=8$ rungs, and half filled and doped coupled planes with 8 and 10 sites per plane. First, let us study the existence of a spin gap in the system. We have analyzed the case of zero and two holes in the model given by Eq. (1). Figures 2(a) and 2(b) show the difference between the triplet and singlet ground-state energies, $\Delta S_0=E(0,1)-E(0,0)$, $\Delta S_2=E(2,1)-E(2,0)$ in the subspace of zero (half filling) and two holes, respectively, where $E(n,S)$ is the ground-state energy of the model with n holes and total spin S, of ladders of various lengths N. Extrapolating the spin gap of the undoped ladder versus $1/N$ we can conclude that the critical ratio for the opening of the gap is $J'/J|_c\sim0.4$–0.5 or smaller, and thus the assumption $J'\gg J$ is not necessary. Evidence for such a spin gap is seen[1] in the temperature dependence of the magnetic susceptibility of $(VO)_2P_2O_7$. Our numerical studies are not accurate enough to show if indeed a *finite* J' is necessary to open the gap of if this occurs immediately for a nonzero J'/J. It would be interesting to perform a Monte Carlo study of the undoped model (where they are feasible) to find this critical ratio. We obtain similar results for the ladder doped with two holes (here we have set $t'/t=0.1$) and for two *planes* in interaction [in this case we cannot make a finite-size scaling but the shape of the curve in Fig. 2(b) suggest that the gap also opens for $J'\sim J$].

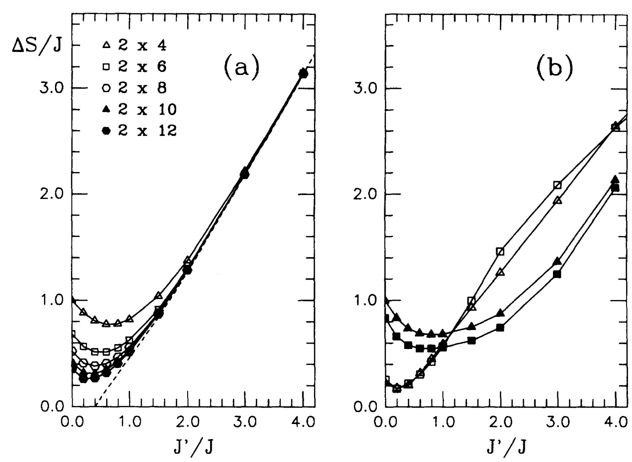

FIG. 2. (a) Spin gap (defined in the text) for the undoped ladder as a function of J'/J for different lattice sizes. The dashed line is the $1/N$ extrapolation to the bulk limit. (b) Spin gap (defined in the text) for different lattices as a function of J'/J. ▲ and ■ denote results for the undoped coupled planes with 8 and 10 sites per plane, respectively. △ and □ indicate results for the case of two holes, $J=0.4$, $t=1$, $t'=0.1$ for the 2×8 ladder and 8 sites coupled planes, respectively.

In the doped case, it is interesting to study the two-hole binding energy $\Delta E=E(2,0)+E(0,0)-2E(1,1/2)$, which is shown in Fig. 3. Here, as expected, for large J'/J the pair-binding energy approaches $\Delta E\sim-\frac{3}{4}J'$ corresponding to the two holes being strongly localized on one rung of the ladder breaking only one spin singlet. However, note that $\Delta E<0$ even for $J'\sim J$ or smaller. The results for the coupled planes do not differ qualitatively from the ladder. The presence of a spin gap and the pairing of holes seems to be a robust property of these models and both appear to be correlated. We have checked explicitly that there is *no* phase separation in our model by adding one more pair of holes to the clusters. This can be easily understood since at large J' the energy gained by putting pairs on adjacent rungs is of order J^2/J' while the kinetic energy lost is order t^2/J'. Thus, if $t>J$ the model will not phase separate.

After checking that pairs are properly formed we study the existence of superconducting correlations. Consider, e.g., the case of quarter filling ($\langle n\rangle=0.5$) with $J=0.4$, $t=1$, $t'=0.1$, and varying J'. We have examined the equal-time pair-field correlation function

$$C(m)=\frac{1}{N}\sum_{\mathbf{i}}\langle\Delta_{\mathbf{i}}^{\dagger}\Delta_{\mathbf{i}+m}\rangle\,. \tag{3}$$

Here $\Delta_{\mathbf{i}}$ is the singlet pair-field operator given by Eq. (2) and $\langle\;\rangle$ denotes an expectation value in the ground state.

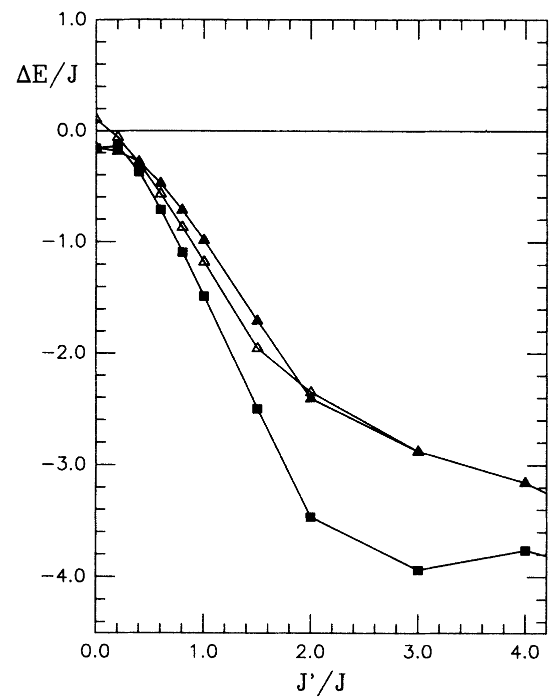

FIG. 3. Binding energy (defined in the text) as a function of J'/J. ▲, △, and ■ denote results for the 2×8, 2×6, and 8 sites coupled planes, respectively.

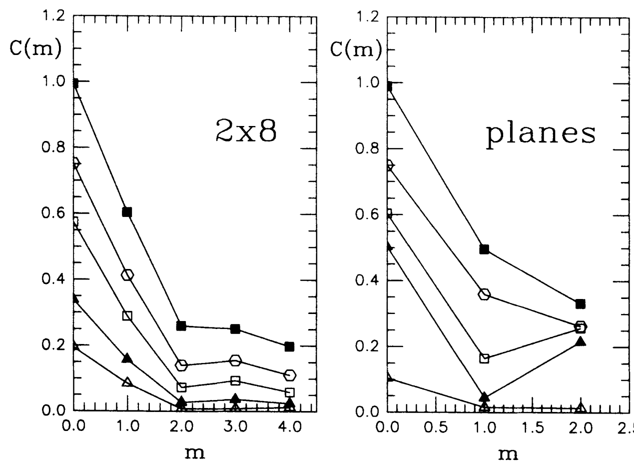

FIG. 4. (a) Pairing correlation function $C(m)$, as defined in the text, as a function of distance for different values of J'/J on a 2×8 ladder. The couplings are $J=0.4$, $t=1.0$, and $t'=0.1$. △, ▲, □, ○, and ■ denote results for $J'=0.01$, 0.4, 1.6, 4, and 40, respectively. The number of particles corresponds to quarter filling, i.e., there are eight electrons in the figure. (b) Same as (a) but for two planes of 8 sites each, in interaction.

Figure 4 shows $C(m)$ vs m for an eight rung ladder and also for planes in interaction. At the maximum distance allowed in our small clusters the correlation function is enhanced by increasing J' showing that a tendency towards superconductivity is being developed.[9] This correlation at $J'\sim0$ is negligible. The physical properties of two coupled chains or two coupled planes seem very similar. We again observed that results for different ladders $2\times N$ show small finite-size effects. For *low* doping of holes the phase diagram of the model will consist of antiferromagnetic correlations below the critical ratio $J'/J|_c$ similar to those of the t-J model near half filling. Above the critical ratio the model exhibits superconducting pair-field correlations. Based on the analogy with the negative-U model in 2D, we believe that T_c corresponds to a Kosterlitz-Thouless transition[5] having performed pairs above T_c, at least at large J'/J.

Can such a model be physically realized? As mentioned before there are materials like $(VO)_2P_2O_7$ whose structure is that of a spin-$\frac{1}{2}$ Heisenberg model on a ladder with superexchange interactions mediated by intermediate oxygens.[1] Our analysis provides information on the spin gap of the insulating state of this material. If it were possible to dope such ladders, our results suggest that interesting pairing and CDW correlations may occur.[10] However, note that we have not included the Coulombic repulsion between holes on neighboring sites explicitly in the calculation. Also we do not know if the condition $t'<J'$ will be satisfied in the doped ladder.

Summarizing, we have analyzed a model in which strong spin-spin correlations give rise to a spin gap and an effective attractive interaction between holes. In the insulating state, the spin gap is observable in the temperature dependence of the magnetic susceptibility of $(VO)_2P_2O_7$. In the doped case, our calculations suggest the possibility of pairing or CDW correlations.

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[1]D. C. Johnston *et al.*, Phys. Rev. B **35**, 219 (1987); J. Bonner *et al.*, *ibid.* **27**, 248 (1983); see also E. Dagotto and A. Moreo, *ibid.* **38**, 5087 (1988); **44**, 5396(E) (1991); L. Hubert and A. Caillé, *ibid.* **43**, 13 187 (1991); K. Hida, J. Phys. Soc. Jpn. **60**, 1347 (1991).

[2]A preliminary version of this work was reported by E. Dagotto, in Proceedings of the International Meeting on Computational Physics for Condensed Matter Phenomena, Osaka, 1991, edited by M. Imada (unpublished).

[3]Similar ideas have been discussed recently in the context of the Hubbard model by N. Bulut, D. Scalapino, and R. Scalettar (unpublished); see also R. Fye *et al.* (unpublished).

[4]M. Imada, J. Phys. Soc. Jpn. **60**, 1877 (1991); see also M. Ogata, M. Luchini, and T. M. Rice, Phys. Rev. B **44**, 12083 (1991).

[5]A. Moreo and D. Scalapino, Phys. Rev. Lett. **66**, 946 (1991); R. Scalettar *et al.*, *ibid.* **62**, 1407 (1989).

[6]In our approach a strong singlet is formed because the length of the lattice in the c direction is of only one lattice spacing. If more layers (L) were added and keeping J' as the dominant interaction, the model would reduce to a bundle of Heisenberg chains which are known to be gapless when $L \rightarrow \infty$. Then, our model, Eq. (1), superconducts when the number of layers is small enough such that a spin gap exists.

[7]P. W. Anderson, Phys. Rev. Lett. **34**, 953 (1975).

[8]Other models have been presented in the literature where tunneling of hole *pairs* between the Cu-O layers plays an essential role. See J. M. Wheatley *et al.*, Phys. Rev. B **37**, 5897 (1988); J. C. Phillips (unpublished). However, in these approaches the pairs are already *preformed* in each plane while in the present model the pairs are formed across a link (rung) between the planes (chains).

[9]We have observed that at quarter filling the superconducting state is degenerate with a CDW state as in the case of the attractive Hubbard model at half filling. However, away from these fillings superconductivity dominates in both models.

[10]Another interesting but more speculative scenario considering the cuprate $YBa_2Cu_3O_{6+x}$ has recently been discussed (see Ref. 2). In this case there are two CuO_2 planes in the unit cell with $J'/J = \frac{1}{40}$ probably outside the range of validity of our model. [See J. Jorgensen, Phys. Today **44** (6), 35 (1991), and references therein; A. Fernandes, J. Santamaria, S. Bud'ko, O. Nakamura, J. Guimpel, and I. Schuller (unpublished); Y. Le Page *et al.*, Phys. Rev. B **36**, 3617 (1987); see also J. M. Tranquada *et al.*, *ibid.* **40**, 4503 (1989). The coupling J' between the Cu-O layers of the unit cell should not be confused with the coupling between double layers which governs the Néel temperature and is much smaller.] If a new material with oxygen atoms between the two Cu-O layers of the unit cell could be prepared, then the superexchange constants would be similar ($J' \sim J$) and our model could apply.