Superconductivity in a quasi-one-dimensional spin liquid

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The single-rung t-J ladder is analyzed in a mean-field theory using Gutzwiller renormalization of the matrix elements to account for strong correlation. The spin-liquid (resonance valence bond) state at half-filling evolves into a superconducting state upon doping. The order parameter has a modified d-wave character. A lattice of weakly coupled ladders should show a superconducting phase transition.

There is a striking difference between the properties of a chain and a ladder (double chain) antiferromagnetic (AF) $s=\frac{1}{2}$ Heisenberg model. Whereas the chain has power-law decay of the AF correlations, the ladder has a purely exponential decay and a finite energy gap in the spin-excitation spectrum, i.e., a spin gap (see for example Ref. 1). If, as is the case for other spin-gap systems, the spin gap persists to finite doping, then the possibilities for superconducting fluctuations are greatly enhanced in ladder systems.[2] Recently we pointed out that compound $Sr_2Cu_4O_6$ offers the possibility of realizing a lattice of weakly coupled ladders.[3,4] This compound is a member of the homologous series $Sr_{n-1}Cu_{n+1}O_{2n}$, which differ from known high-T_c cuprates through the presence of a parallel array of line defects in the CuO_2 planes. In this letter we examine the properties of undoped and lightly doped ladders described by a t-J model within a mean-field approximation which uses a Gutzwiller renormalization factor to approximate the local constraint. Superconducting correlations of a modified d-wave symmetry are predicted. The system of weakly coupled chains offers an interesting example of a short-range resonance valence bond (RVB) state in a system intermediate between 1 and 2 dimensions.[5]

The basic model we apply is the t-J model on the ladder with the Hamiltonian

$$\mathcal{H}=-\sum_{i,s}[t_x\sum_{a=1,2}c^{\dagger}_{i+1,a,s}c_{i,a,s}+t_y c^{\dagger}_{i,1,s}c_{i,2,s}+\text{H.c.}]+\sum_{i}[J_x\sum_{a=1,2}\mathbf{S}_{i+1,a}\cdot\mathbf{S}_{i,a}+J_y\mathbf{S}_{i,1}\cdot\mathbf{S}_{i,2}]\ , \tag{1}$$

where i runs over all rungs and a over the two legs, 1 and 2. The constraint $\sum_s c^{\dagger}_{i,a,s}c_{i,a,s}\le 1$, projecting out all the doubly occupied states on each site, is implied. We examine this model within the mean-field theory used by Zhang *et al.* for the two-dimensional (2D) square lattice.[6] The constraint is taken into account approximately by a Gutzwiller-type renormalization of the coupling constant along the chain,

$$\langle c^{\dagger}_{i+1,a,s}c_{i,a,s}\rangle=g_{tx}\langle c^{\dagger}_{i+1,a,s}c_{i,a,s}\rangle_0\ ,$$

and

$$\langle\mathbf{S}_{i+1,a}\cdot\mathbf{S}_{i,a}\rangle=g_{Jx}\langle\mathbf{S}_{i+1,a}\cdot\mathbf{S}_{i,a}\rangle_0\ ,$$

and analogous g_{ty} and g_{Jy} on the rungs with $\langle\cdots\rangle$ and $\langle\cdots\rangle_0$ the expectation values in the projected and unprojected state, respectively. These g factors are determined by the ratio of the probabilities of the matrix elements in the projected and unprojected states.[6] The renormalized coupling constants are then defined by $\tilde{J}_\alpha=J_\alpha g_{J\alpha}$ and $\tilde{t}_\alpha=tg_{t\alpha}$.

Using the fermion representation for the Heisenberg term in (1), we introduce two types of mean fields, $\chi_x=\langle c^{\dagger}_{i+1,a,s}c_{i,a,s}\rangle_0$ and $\Delta_x=\langle c_{i+1,a,\downarrow}c_{i,a\uparrow}\rangle_0$, and $\chi_y=\langle c^{\dagger}_{i,1,s}c_{i,2,s}\rangle_0$ and $\Delta_y=\langle c_{i,1,\downarrow}c_{i,2\uparrow}\rangle_0$, a bond and pairing mean field, respectively. The t-J model is then reduced to a renormalized Hamiltonian with the constraint released

$$\mathcal{H}_{\text{MF}}=\sum_{\mathbf{k},s}\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k},s}c_{\mathbf{k},s}-\sum_{\mathbf{k}}[\Delta^{*}_{\mathbf{k}}c_{\mathbf{k}\downarrow}c_{-\mathbf{k}\uparrow}+\text{H.c.}]+\frac{3N}{4}\sum_{\alpha=x,y}f_\alpha\tilde{J}_\alpha(|\chi_\alpha|^2+|\Delta_\alpha|^2)\ , \tag{2}$$

where $f_x=2$ and $f_y=1$ and N is the number of lattice sites. The summation over $\mathbf{k}$ is restricted to $-\pi<k_x\le\pi$ and k_y equals to 0 (bonding) or π (antibonding). In (2)

$$\varepsilon_{\mathbf{k}}=-2\sum_\alpha f_\alpha(\tilde{t}_\alpha+\tfrac{3}{4}\tilde{J}_\alpha\chi_\alpha)\cos k_\alpha-\mu\ ,$$
$$\Delta_{\mathbf{k}}=\frac{3}{2}\sum_\alpha f_\alpha\tilde{J}_\alpha\Delta_\alpha\cos k_\alpha\ , \tag{3}$$

with μ as the effective chemical potential. We calculate the Gutzwiller renormalization factors by including the correlations of the probability between the two nearest-neighbor sites,[7] which improves the approximation of Ref. 6. They are given by

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$$g_{t\alpha}=2n\delta/[n(1+\delta)+4\chi_\alpha^2]\,,$$
$$g_{J\alpha}=4n^2/[n^2(1+\delta)^2+8\delta^2(|\Delta_\alpha|^2-|\chi_\alpha|^2) +16(|\Delta_\alpha|^4+|\chi_\alpha|^4)]\,, \quad (4)$$

where n is the electron density and $\delta=1-n$ is the hole-doping concentration.

The mean-field Hamiltonian has to be solved self-consistently together with the mean-field-dependent Gutzwiller renormlization factors. Additionally, the chemical potential is chosen to give the correct electron concentration, $n=1-\delta=\langle \hat{n}_i \rangle_0$. Numerical solutions of these mean fields as a function of doping concentration are plotted in Fig. 1 for realistic parameters, $t_x=t_y$ and $J_x=J_y=0.3t_x$. Within this mean-field treatment the excitations are described by the effective quasiparticle Hamiltonian obtained by standard Bogolyubov transformation of $\mathcal{H}_{\rm MF}$, $\mathcal{H}_{\rm eff}=\sum_{\mathbf{k},\sigma=1,2}E_{\mathbf{k}}\gamma^\dagger_{\mathbf{k}\sigma}\gamma_{\mathbf{k}\sigma}$ with the spectrum $E_{\mathbf{k}}^2=\varepsilon_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2$. The quasiparticles define the ground state by the condition $\gamma_{\mathbf{k},\sigma}|\Phi_0\rangle=0$. For finite $\Delta_{\mathbf{k}}$ these excitations have always a finite gap.

We begin at half-filling where this system reduces to a Heisenberg ladder. This case was considered by various groups for different couplings along the chains J_x and rungs J_y.[1,8,9] In the limit $J_y \gg J_x > 0$ the ground state consists essentially of singlet dimers on each rung leading to a spin-liquid (singlet) ground state. The lowest spin (triplet) excitation is obtained by replacing one singlet by a triplet dimer with an excitation energy $\sim J_y - J_x$. By numerical diagonalization and dimer mean-field treatments it was demonstrated that the spin-liquid ground state persists even for $J_x \sim J_y$ with a spin gap of $0.4-0.6J$ for $J=J_x=J_y$.[8,9]

The mean-field solution at half-filling independent of the coupling constants satisfies the relation $\Delta_x\Delta_y+\chi_x\chi_y=0$. This state is similar to the d-wave RVB in the square lattice, where the pairing mean fields Δ_α differ by a phase π in x and y direction. It is also identical to the Affleck-Marston flux phase[10] with half integer flux quanta as follows from a SU(2) symmetry.[6] Upon doping, the flux phase and the d-wave RVB state differ. In the case of the square lattice, the d-wave RVB state is found to have lower energy than the staggered flux phase.[11] We expect the similar result for the ladder, and will not discuss the flux phase here.

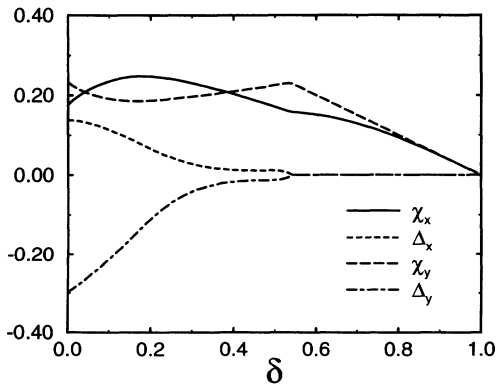

FIG. 1. The mean fields as a function of the doping concentration for $J_x=J_y=J=0.3t$.

Turning to the spin excitation (singlet-triplet) we find that it is not well described by the simple quasiparticle Hamiltonian $\mathcal{H}_{\rm eff}$ given above. The spin gap is generally too large ($\approx 2J$ for $J_x=J_y$). Additionally the excitation energy has several minima at the momenta $\mathbf{q}=(0,0)$, $(0,\pi)$, $(\pi,0)$, and (π,π), while in the theories mentioned above the only minimum lies at $\mathbf{q}=(\pi,\pi)$.[8,9]

We can remedy this flaw in our treatment partially by taking the residual interaction among quasiparticles into account. Most easily the spectrum of the spin excitations can be obtained from the dynamical (transverse) spin susceptibility, $\chi(\omega,\mathbf{q})=\langle\langle S^-_{-\mathbf{q}},S^+_{\mathbf{q}}\rangle\rangle_\omega$. We use the equation of motion to determine $\chi(\omega,\mathbf{q})$ on the level of RPA including the residual interaction. In Fig. 2 we show the spectrum $\mathrm{Im}\chi(\omega,\mathbf{q})$ at $\mathbf{q}=(\pi,\pi)$ for both the simple mean-field and the random phase approximation (RPA) corrected result with $J_x=J_y$. The RPA shows a sharp excitation peak at $\approx 0.15J_x$ and a broad continuous spectrum between about $2J_x-3J_x$ which is the strongly suppressed remainer of the continuous excitation spectrum of $\mathcal{H}_{\rm eff}$. The analysis of the full $\mathbf{q}$ dependence shows that the minimal excitation is obtained at $\mathbf{q}=(\pi,\pi)$. The corresponding binding energy is rather large bringing the excitation gap down to a value of $0.15J_x$ which is only slightly smaller than the one found in other calculations ($\approx 0.5J_x$).[8,9]

As a consequence of the local constraint the singlet dimer on a rung is a coherent superposition of pair states in the bonding $[c^\dagger_{i+,s}=(c^\dagger_{i,1,s}+c^\dagger_{i,2,s})/\sqrt{2}]$ and the antibonding $[c^\dagger_{i-,s}=(c^\dagger_{i,1,s}-c^\dagger_{i,2,s})/\sqrt{2}]$ state, i.e., avoiding double occupancy the rung state

$$(1/\sqrt{2})(c^\dagger_{i+\uparrow}c^\dagger_{i+\downarrow}-c^\dagger_{i-\uparrow}c^\dagger_{i-\downarrow})|0\rangle$$

gains the maximal exchange energy. In other words, the splitting of the bonding and antibonding band, which would appear in a band-structure description, is absent in the presence of the local constraint so that they are equally filled at half-filling.

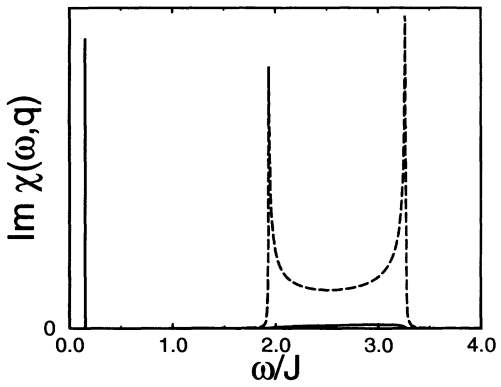

FIG. 2. The spectrum of the spin excitations for $J_x=J_y=J=0.3t$ and $\mathbf{q}=(\pi,\pi)$. The solid line denotes the exciton spectrum obtained from RPA and the dashed line the mean-field quasiparticle spectrum neglecting the interaction among the quasiparticles. The sharp exciton mode at $\omega\approx 0.15J$ contains practically all weight of the excitation spectrum.

To get an intuitive understanding of the properties of this sharp excitation found in RPA let us consider the problem in the strong-coupling limit, $J_y \gg J_x$. In the mean field a triplet excitation creates two quasiparticles which may be considered as spinons freely moving and destroying each one singlet dimer. The energy loss is $3J_y/2$, neglecting the kinetic energy contribution. These two quasiparticles can form a triplet dimer on a rung with the lower energy J_y. Thus, there exists an effective attraction between them leading to a bound exciton state within the quasiparticle excitation gap. This interaction has only an attractive triplet channel if one of the two quasiparticles is in the bonding and the other in the antibonding band. Furthermore, the kinetic energy of the triplet dimer is given by $\tilde{J}_x \cos q_x$ which is lowest at $q_x = \pi$. Hence, we interpret the sharp excitation in the RPA calculation for $J_x = J_y$ as an exciton with lowest energy at $\mathbf{q} = (\pi, \pi)$ and the reduced continuum above $\sim 2J_x$ as a spinon continuum (Fig. 2).

Upon doping holes the two quasiparticle bands which are degenerate at half-filling split. The antibonding band is raised and the bonding band slightly lowered relative to the chemical potential. As holes are doped the kinetic energy can be lowered if they occupy preferentially the antibonding band. In this way the antibonding band is gradualy emptied down to a critical doping δ_c, where eventually only the bonding band is occupied. The loss of antibonding electrons leads to a gradual decrease of the pairing amplitude Δ_α which disappears eventually at δ_c. The long tail of finite Δ_α down to δ_c may be an artifact of our approximation.

The behavior of Δ_α yields a monotonic decrease of the quasiparticle excitation gap described by $\mathcal{H}_{\text{eff}}$. On the other hand, the spin-excitation band formed by the triplet exciton is shifting nonmonotonically with doping leading to an *increase* in the spin gap at small doping (see Fig. 3, for coupling constants $t_x = t_y = t$ and $J_x = J_y = J = 0.3t$). With the shift of the Fermi levels in the antibonding band the optimal relative momentum q_x for a triplet exciton of two quasiparticles deviates gradually from π. Since $q_x = \pi$ yields the strongest attraction this deviation weakens the interaction and decreases the binding energy.

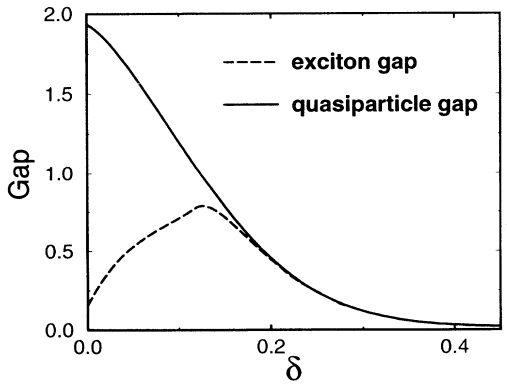

FIG. 3. The spin gap as a function of the doping concentration for $J_x = J_y = J = 0.3t$. The solid line denotes the bottom of the quasiparticle spectrum and the dashed line the gap of the exciton state.

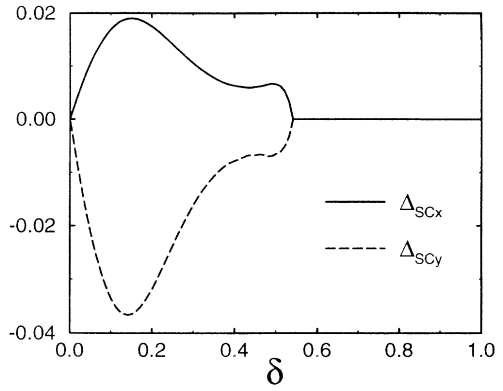

FIG. 4. The superconductivity order parameter versus the doping concentration for $J_x = J_y = J = 0.3t$.

The resulting increase of the spin gap for small doping shows that here hole doping suppresses antiferromagnetic correlation and stabilizes a spin-liquid state. Also results of exact diagonalization confirm this tendency.[12]

The BCS superconductivity order parameter is given by the pairing mean field multiplied by the Gutzwiller renormalization factor $g_{t\alpha}$ as shown in Ref. 6. In Fig. 4 we show the two components of $\Delta_{SC\alpha} = \Delta_\alpha g_{t\alpha}$. There is a phase difference of π between Δ_{SCx} and Δ_{SCy}, reminding one of d-wave pairing, although d-wave is a misnomer in this low-symmetry system.

In summary, our mean-field theory of the t-J ladder model gives a description of the doped spin-liquid system. The spin-liquid state persists for a finite-doping region away from half-filling and seems even to become more stable with weak doping. Although mean field is certainly not a good concept for quasi-1D systems, we have seen that qualitatively reasonable results are obtained. We may expect that weak interchain (intraplanar and interplanar) coupling would lead essentially to a 3D situation stablizing the mean-field solution. The superconductivity obtained in this theory is intimately connected with the existence of a spin-liquid state (see also in Refs. 2 and 13). Considering their energy scales we observe that at light doping the spin gap is by far larger than the superconducting pair-correlation energy. Beside the triplet exciton mode discussed here we expect in the doped region a low-lying collective (sound) mode in connection with the superconducting order will occur.[14]

Our result suggests that also for chains extended in y direction having 4, 6, or a larger even number of parallel chains would qualitatively be very similar. Although the spin gap must be diminished with growing system size, as recent mean-field calculations show,[9] the concept of the doped spin-liquid system is still applicable. In this sense the superconducting state would continuously tend to a real d-wave state, if we would extend the lattice in y direction approaching in this way the 2D square lattice.

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