Singlet stripe phases in the planar t-J model

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The dimensional crossover of coupled t-J ladders to a planer model is examined using a mean-field approach with coupling constants determined by numerical diagonalization. Having a finite spin gap, uncoupled ladders belong to the Luther-Emery class in one-dimensional fermion systems, leading to a different crossover from coupling chains. For a wide region around $J/t \gtrsim 1$ the hole-hole correlations in a single ladder are found to be predominantly charge-density-wave type, but an attraction between hole pairs on adjacent ladders leads to a stripe phase. A quantum-mechanical melting of the hole lines at $J/t \lesssim 1$ leads to a Bose condensate of hole pairs, i.e., a superconducting phase.

Although there are many aspects of the planar t-J model that are by now well established, such as the existence of a region of $d_{x^2-y^2}$ pairing at low doping and moderate J/t ratios[1] and the occurrence of some form of phase separation (PS) at larger values,[2] $J/t \gtrsim 1$, there are also many unresolved issues. Most importantly a clear physical picture is lacking which would interrelate and give insight into features such as the very rapid suppression of long-range antiferromagnetic (AF) order with doping, the absence of long-range incommensurate antiferromagnetism (ICAF), the anomalous boundary of the PS regime extending down to values $J/t \sim 1$ (e.g., see Putikka, Luchini, and Rice and Prelovšek and Zotos[3]), and of course the presence of $d_{x^2-y^2}$ pairing. Similarly the phenomenological nearly AF liquid models studied by Moriya, Takahashi, and Ueda,[4] and by Monthoux, Pines and co-workers[5] can explain the high-T_c values but only if there is an extended critical regime with very large enhancements of the staggered susceptibility which for some unspecified reasons do not crossover to long-range magnetic order (for a review of these issues see Ref. 6). In this report we shall address these points by studying the dimensional crossover from ladders to planes in the t-J model.

We start with t-J ladders rather than chains. Both are one dimensional but nonetheless behave very differently — a point which alone emphasizes the subtlety of these issues. The properties of t-J chains are well known. They form Tomonaga-Luttinger liquids upon hole doping with correlation exponents $K_\rho \approx \frac{1}{2}$ for $J/t \lesssim 1$.[7] The dominant or longest-range correlations are incommensurate magnetic correlations and there is no sign of pairing. Coupling such chains together to make a crossover to a planar model would seem to lead to ICAF phases contrary to both experiments and to studies of the planar t-J model. Note that a sequence commensurate-AF $\rightarrow$ ICAF $\rightarrow$ paramagnetism appears elsewhere, most notably as the electron/atom ratio is changed in the Cr alloys.[8] So why is the physics different here?

Recently it has been discovered that the properties of t-J ladder systems can be very different depending on the width of the ladders. Ladders made from an even number of chains when undoped (i.e., $S{=}\frac{1}{2}$ AF Heisenberg ladders) have spin-liquid ground states with a finite spin gap.[9] Upon doping the spin gap remains finite and the only modes in the low-energy sector are collective density modes of hole pairs.[10] It follows that a description of the low-energy physics in terms of the effective Boson model introduced by Efetov and Larkin[11] to describe the Luther-Emery (LE) class of one-dimensional (1D) systems will apply. An explicit demonstration of the spin gap and the power-law behavior of the density-density and pairing correlations in the closely related two-chain Hubbard model was given recently by Noack, White, and Scalapino[12] using a density-matrix renormalization-group method. At low energies two-chain t-J ladders show the key properties of LE systems.

Therefore coupling ladders will show quite a different crossover to a planar model compared to coupling chains, pointing to unexpected subtleties in the magnetic order in this extreme quantum system. Most importantly, the crossover to a region of singlet superconductivity (SSC) in the planar model would be smoother than starting with chains, since spin excitations already have a finite gap at the starting point as in the SSC region. We shall apply the dimensional crossover theory of Efetov and Larkin[11] to the case of coupled two-chain t-J ladders and examine the competition between two ordered phases:

charge-density-wave (CDW) and SSC phases. We will then examine the nature of the CDW phase more carefully, and finally discuss the transition to the SSC phase briefly.

First we review the properties of single two-chain ladders in the t-J model which has the standard form,

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

with $\tilde{c}_{i\sigma} = c_{i\sigma}(1 - n_{i,-\sigma})$, etc. The undoped ladder is a spin liquid with a spin gap $\simeq J/2$.[9] The planar Heisenberg model has a ground-state with long-range AF order. Therefore the crossover from weakly coupled ladders to the isotropic planar limit is not smooth and a critical interladder coupling strength exists separating spin-liquid and AF ordered regions. Pairing in the planar t-J model at low doping leads to propose that a smooth crossover can occur at finite doping although this key assumption remains unproven.

Upon doping the results of Lanczos diagonalization studies show that the spin gap remains but changes discontinuously due to the introduction of new states associated with breaking up hole pairs into two separated charged spin-$\frac{1}{2}$ quasiparticles.[10] Doped ladders fall into the LE class of 1D Fermion models. The density-density and pair-pair correlation functions fall off with power law and the exponents are determined by the parameter K_ρ whose value is given by $K_\rho = \pi\rho(\kappa D/2)^{1/2}$ where ρ is the electron density, κ is the compressibility and D is the Drude weight.[13] The Drude weight is calculated by evaluating the dependence on a phase shift of the boundary conditions (BC) of the ground-state energy for a $2\times L$ ladder with two holes. In calculating the compressibility κ, care must be taken since the energy of a finite ladder with periodic BC's depends sensitively on whether an AF spin arrangement along the chains is frustrated or not, e.g., two holes in 2×8 is frustrated, while two holes in 2×7 is not. We calculate κ from the ground-state energies of unfrustrated ladders with periodic BC's (zero holes in 2×8, two holes in 2×7, and four holes in 2×8) and determine the PS boundary by the condition $\kappa \to \infty$, as shown in Fig. 1(a). Further points on PS boundary line were determined with open BC's to avoid frustration effects. Note the critical value for $(J/t)_{\rm PS} (\approx 2.2)$ is considerably larger than that reported for the 2D case $(J/t)_{\rm PS} \simeq 1$.[3] The corresponding values of K_ρ are shown in Fig. 1(b). The value $K_\rho = 1$ separates a predominantly CDW region ($K_\rho < 1$) from the region ($K_\rho > 1$) where SSC correlations dominate. We note that $K_\rho \approx 0.5$ for $J/t \sim 0.3$ which agrees with the results of Noack, White, and Scalapino[12] who used a density-matrix renormalization-group method to directly calculate the correlation functions of a Hubbard ladder.

Next we consider the effect of turning on the interaction between the ladders so as to crossover to the 2D or planar limit. Efetov and Larkin discussed within a mean-field (MF) treatment the competition between SSC and CDW phases when a weak coupling between 1D LE systems is switched on.[11] The corresponding MF transition

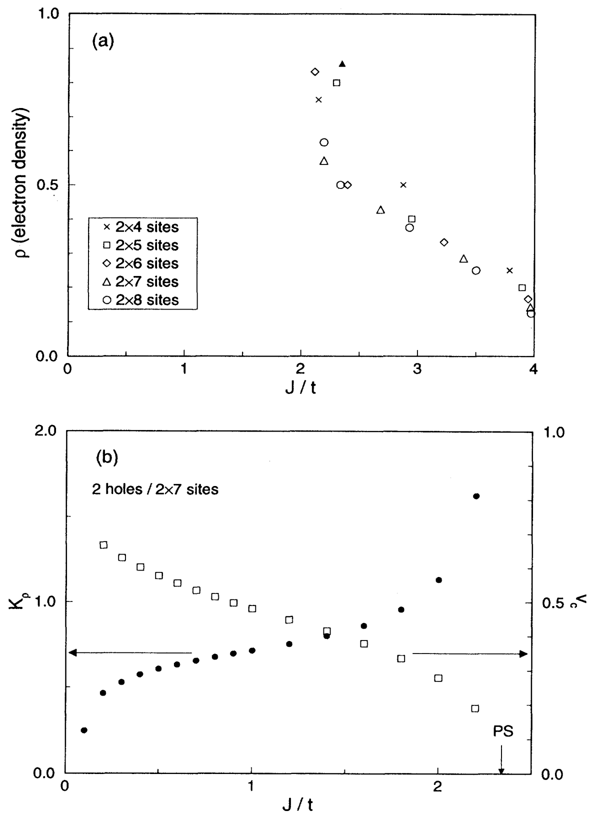

FIG. 1. (a) Phase separation boundary of t-J ladders. Open BC's are used. ▲ is determined by the data for two holes/2×7, $4/2\times8$, and $0/2\times8$ with periodic BC's as discussed in the text. (b) Correlation exponent parameter K_ρ and charge velocity v_c. The compressibility used here is calculated from the data for unfrustrated systems with periodic BC's.

temperatures T_c^α (α: SSC or CDW) is determined by the condition

$$1 = W^\alpha \int \mathrm{d}R\, \mathrm{d}\tau\; G^\alpha(R,\tau). \tag{2}$$

For α=SSC, W^α is twice the pair-hopping amplitude, $2t_{\rm eff}$, and G^α is the pairing correlation function. This formula is derived in the limit of weak interladder coupling and the crossover to the planar limit with isotropic coupling involves an uncontrolled extrapolation of the MF approximation. Nonetheless as noted earlier, various studies of the planar t-J model show evidence of d-wave pairing and encourage us to postulate a smooth crossover from the limit of weakly coupled ladders. Our approach will be to estimate the W^α-coupling strengths at the isotropic limit and use them to obtain the MF values of T_c^α from Eq. (2). A recent study of a four-chain ladder by Poilblanc, Tsunetsugu, and Rice[14] with two holes shows an energy splitting in the singlet sector between states with even and odd parities with respect to the mirror symmetry that exchanges two-chain ladders and we set $W^{\rm SSC}$ equal to this splitting (see Fig. 2). In Fig. 3 we show $T_c^{\rm SSC}$ from Eq. (2) using K_ρ and v_c values from Fig. 1(b).

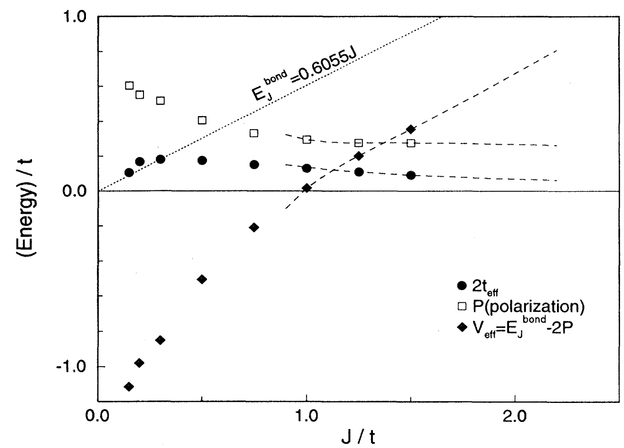

FIG. 2. Interaction between two pairs of holes determined by using data in Ref. 14. $V_{\rm eff}$ is the effective attraction between adjacent ladders. The dashed lines are extrapolated values.

In the second case, α = CDW, two possibilities are to be distinguished, namely $W^{\rm CDW} < 0$ and $W^{\rm CDW} > 0$ corresponding to attractive and repulsive interactions between hole pairs on adjacent ladders. In the case of attractive interactions the MF ground-state would be a stripe phase similar to those discussed previously in the Hartree-Fock calculations of the Hubbard model.[15] $W^{\rm CDW}$ has an attractive magnetic contribution consisting of one less broken bond, $E_J^{\rm bond}=-0.6055J$. However separated hole pairs gain energy by a polarization process through virtual hopping which we estimate roughly to be, $P=\Delta E^{2L}-\Delta E^{4L}-E_J^{\rm bond}$, where ΔE^{nL} is the energy difference between zero- and two-hole ground states for n-chain ladders (for n = 4 we take the average of even and odd parity). The magnetic and polarization contributions are plotted in Fig. 2 and show a change from repulsion to attraction when $J/t \gtrsim 1$. This value is an underestimate we believe, since we have omitted the polarization corrections to the attractive term. Equation (2) with $G^{\rm CDW}$ as the Fourier component of the density-density correlation function gives a MF $T_c^{\rm CDW}$ shown in Fig. 3. We see at once that it dominates for $J/t \gtrsim 1$, leading us to conclude that there can be a wide parameter region of stability of the CDW phase up to phase separation at $J/t \gtrsim 2.2$. In the region $J/t \lesssim 1$ where interladder interactions are repulsive one should also consider the possibility of a crystalline ordering of hole pairs, but we believe such a crystalline order would suppressed by quantum fluctuations.

The key question in the CDW phase is the relative stability of the spin liquid [short-range resonating-valence bond (RVB)] and the compressible spinon liquid. To see this competition, we compare ground-state energies of two static hole configurations at hole doping δ = 0.25, since the kinetic energy is not important at large J/t where the CDW phase is favored. One is a CDW with lines of holes separating three-chain spin ladders and the second has alternating two-chain and four-chain spinladders (see Fig. 4). Both configurations have an equal number of broken magnetic bonds (three per hole) so we can directly compare them. The energies per site for two-, three-, and four-chain ladders quoted in Table I were obtained by extrapolating the results of Lanczos diagonalizations to infinite ladders. The direct comparison of the energies of an RVB spin liquid with two- and four-chain ladders and a spinon fluid with three-chain ladders shows a small energy gain for the former of $\approx 6\times10^{-3}J$/site or $\approx$ 1% of the magnetic energy.

The CDW phase is therefore stabilized at large J/t in such a way that singlet spin liquids are formed between the hole stripes, and gains a magnetic energy associated with large quantum fluctuations. We will call this the *singlet stripe (SST) phase*. On the other hand, the ICAF fluctuations are accordingly suppressed.

Following this line of reasoning leads us to a phase diagram with an intermediate parameter range $1\lesssim J/t\lesssim 2.2$ in which SST phases are stable. This range is bounded by true PS at larger J/t and SSC with $d_{x^2-y^2}$ pairing at smaller values. This form is close to that proposed by Prelovšek and Zotos[3] on the basis of the hole-hole corre-

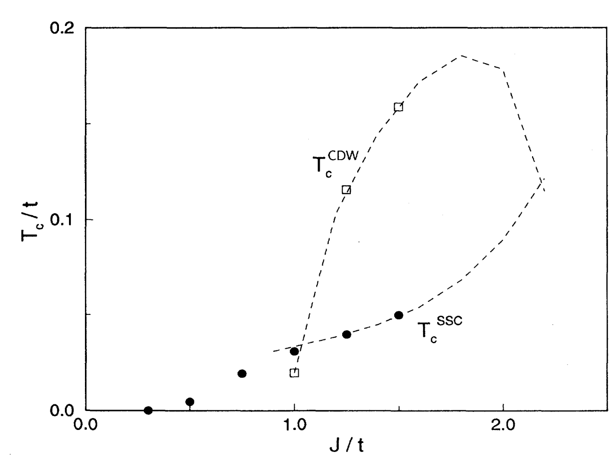

FIG. 3. The mean-field transition temperatures. The dashed lines are extrapolated values.

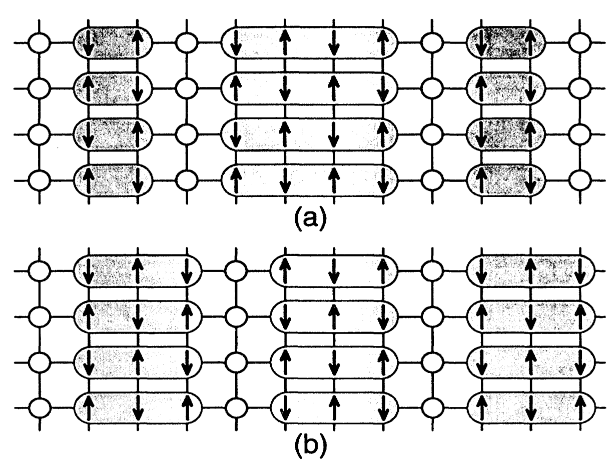

FIG. 4. Stripe phases. (a) Mixture of two-chain ladders and four-chain ladders. (b) Three-chain ladders.

TABLE I. Ground-state energies per site for the Heisenberg ladders with three and four legs. Shown are the energies for a finite ladder with length L=4, 6, and 8 and the extrapolated value for an infinite ladder.

L	$E_g(3\times L)/J$	$E_g(4\times L)/J$	$E_g(2\times L)/J$
4	−0.62751	−0.64152	
6	−0.61036	−0.62606	
8	−0.60568	−0.62210[a]	
∞	−0.601	−0.622	−0.578[b]

[a]Reference 14.
[b]Reference 9.

lations in small clusters. The key difference is that here we would have an inhomogeneous phase which is a pure CDW and the spins in the intervening regions between hole lines form spin liquids. This is the essence of the SST phase. The existence of SST phases gives an explanation for the issues raised earlier namely the anomalous PS line, the absence of long-range ICAF order, and the existence of $d_{x^2-y^2}$ pairing as a precursor to the SST phase at large J/t values.

Another point we would like to make concerns the anisotropic form of the SST phase. An isotropic arrangement of the hole lines is of course possible and may well be preferable. This would correspond to hole lines $\parallel x$ and $\parallel y$ axes or in other words a singlet square (SSQ) arrangement. The relative stability of SST and SSQ phases can be addressed using variational Monte Carlo calculations and will require further study. It is clear that small energy differences can determine the relative stability of different SST and SSQ configurations and a complex phase diagram with different patterns depending on the doping δ and the residual interactions can result. Also the energy differences to the ICAF stripe phases[15] will be very small too. The point that we want to make is that when we look at inhomogeneous phases there is good reason to believe that the SST or SSQ phases have lower energy because as shown earlier in Table I, if one breaks up a plane the magnetic energy favors the formation of spin liquid phases. Another way of viewing the competition between SST (or SSQ) and ICAF phases is that the spin gap in the magnon spectrum should remain finite even when one includes the induced interaction across the hole lines. If the magnon energy were to go negative at some $\mathbf{q}$ vector then an ICAF phase would result. The stability of SST (or SSQ) phases require that the magnon energy remains finite leading to a spin gap and finite range spin correlations.

In conclusion we have examined the crossover between coupled t-J ladders and the 2D limit of a t-J plane as the interladder coupling is increased. Isolated ladders in the parameter range $J/t \approx 1$ have predominantly repulsive correlations between hole pairs leading to longer range CDW correlations but at the same intermediate parameter range the force between hole pairs on adjacent ladders is attractive. This combination of attraction and repulsion we propose stabilizes the SST (or more generally SSQ) phases. In the fermion MF treatment these SST (or SSQ) phases have combined d-wave RVB pairing and CDW ordering. In that sense they are a form of supersolid. As the ratio J/t is lowered the attraction between hole pairs on adjacent ladders is reduced, the quantum fluctuations of the hole lines are enhanced and at end we have a quantum melting of the CDW ordering but not of the d-wave RVB pairing leading to a d-wave superconducting state.[16] Finally we speculate that the observation of a spin gap in underdoped cuprates could result from residual CDW fluctuations which may also be precursors to true SST (or SSQ) phases.

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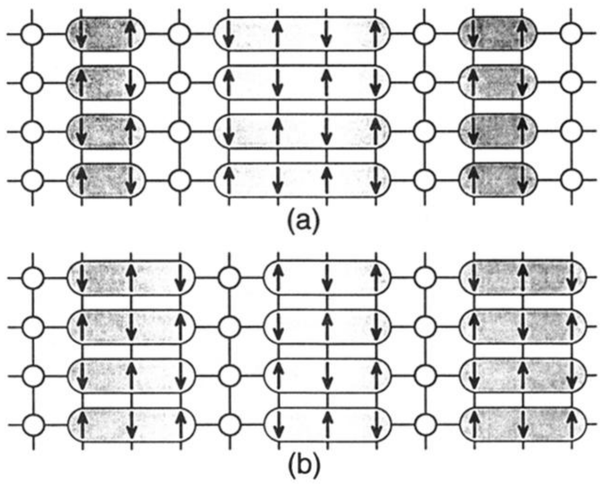

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