

Superconductivity from doping a spin-liquid insulator: A simple one-dimensional example

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We study the phase diagram of a one-dimensional Hubbard model where, in addition to the standard nearest-neighbor hopping t , we also include a next-to-nearest-neighbor hopping t' . For strong enough on-site repulsion, this model has a transition at half filling from a magnetic insulator with gapless spin excitations at small t'/t to a dimerized insulator with a spin gap at larger t'/t . We show that upon doping this model exhibits quite interesting features, which include the presence of a metallic phase with a spin gap and dominant superconducting fluctuations, in spite of the repulsive interaction. More interestingly, we find that this superconducting phase can be reached upon hole doping the magnetic insulator. The connections between this model and the two chain models, recently object of intensive investigations, are also discussed. [S0163-1829(96)02838-X]

I. INTRODUCTION

The properties of correlated electrons confined to a double chain have recently attracted considerable attention from both the theoretical and experimental point of views.

The theoretical analyses have been mainly focused on simplified models as two chains of electrons interacting via a short-range repulsion (e.g., the Hubbard model) and coupled by a transverse hopping t_{\perp} or two t - J chains coupled both by a transverse hopping and by a transverse exchange J_{\perp} . At half filling both models are equivalent to two coupled Heisenberg chains whose ground state has been found to be a spin-liquid insulator with a gap in the excitation spectrum for arbitrary transverse coupling.¹⁻³ Away from half-filling both models describe a metal which, however, maintains a finite gap for the spin excitations. This behavior suggests the existence of electron pairs which is confirmed by the evidence that the dominant fluctuations describe $4k_F$ density waves and interchain-pairing fluctuations.²⁻⁸ The latter are expected to dominate for weak repulsion and sufficiently away from half filling or, in the t - J ladders, for strong J .

From the experimental point of view, recent measurements on ladders compounds like SrCu_2O_3 (Ref. 9) and $(\text{VO})_2\text{P}_2\text{O}_7$ (Ref. 10) confirmed the theoretical prediction of a spin gap at half filling. The transition upon doping from the spin-liquid insulator to the metal with a spin gap has also been verified experimentally in Sr-doped $\text{LaCuO}_{2.5}$.¹¹ Unfortunately no superconducting transition seems to occur down to 5 K, which is, however, not in contrast with the theoretical predictions (it would imply either that the doping is still low or that the interaction is too strong).

An important message which in our opinion arises from all the theoretical analyses of the two-chain models and which is the subject of the present work is that doping a one-dimensional (1D) spin liquid may indeed result in superconductivity also in the presence of a repulsive interaction. The goal of this paper is to show that this feature is shared not only by two-chain models but also by a wider class of 1D models which do describe a spin-liquid insulator at half filling.

Among the spin models which are known to exhibit a spin

gap in the excitation spectrum, a very simple and well-studied model is the spin-1/2 Heisenberg chain with an additional next-to-nearest-neighbor exchange:

$$\hat{H}_{JJ'} = J \sum_{i=1}^L \vec{S}_i \cdot \vec{S}_{i+1} + J' \sum_{i=1}^L \vec{S}_i \cdot \vec{S}_{i+2}. \quad (1)$$

If $J' = 0$, this model is the well-known Heisenberg model,¹² which is characterized by gapless excitations and power-law decay of the spin correlations. If $J' = J/2$, the ground state is exactly known¹³ and consists of a product of singlets among nearest-neighboring sites (dimerized state). There are two of these states, which are related among each other by the translation of one lattice constant. A finite energy gap exists between these two degenerate states and the first excited ones.¹⁴ The transition upon increasing J' from the gapless regime to the gapped dimerized state was studied using bosonization by Haldane,¹⁵ who predicted the transition to occur at $J' \approx J/6$. Successively, Nomura and Okamoto¹⁶ performed a detailed numerical investigation of the model and estimated a larger transition value of $J' \approx J/4$.

A model of interacting electrons which in a particular limit reproduces the spin model (1) is the Hubbard model with an additional next-to-nearest-neighbor hopping ($t-t'-U$ model), described by the Hamiltonian

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} \sum_{i=1}^L (c_{i\sigma}^{\dagger} c_{i+1\sigma} + \text{H.c.}) + t' \sum_{\sigma=\uparrow,\downarrow} \sum_{i=1}^L (c_{i\sigma}^{\dagger} c_{i+2\sigma} + \text{H.c.}) + U \sum_{i=1}^L n_{i\uparrow} n_{i\downarrow}, \quad (2)$$

where $c_{i\sigma}$ annihilates a spin σ electron at site i and $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$. At half filling and for $U \gg (t, t')$ this model indeed maps onto Eq. (1) with $J = 4t^2/U$ and $J' = 4t'^2/U$,

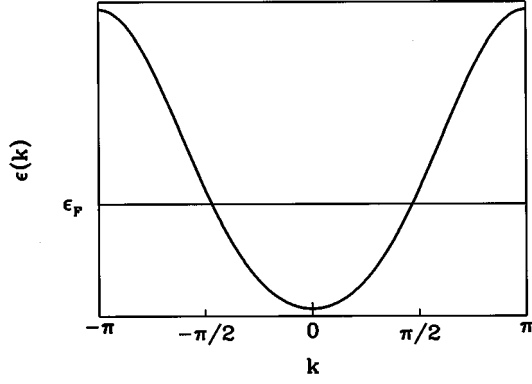


FIG. 1. Energy dispersion relation of the t - t' - U model for $t' < t/4$.

and therefore it is a good candidate to study the properties upon doping of a spin-liquid state.

In this paper we study the phase diagram of Eq. (2) by making use of the weak-coupling renormalization group (RG) and bosonization. We will show that, as a function of the parameters (electron density n , U/t , and t'/t), the phase diagram is surprisingly rich. In particular we find that also in this simple case superconductivity may arise from doping the spin-liquid insulator, even though the electron-electron interaction is repulsive. Moreover, for $t/4 < t' < t/2$ we find a transition upon doping from a magnetic insulator at half filling to a metal with dominant spin and charge density wave fluctuations and finally to a superconductor (for small U/t) or a metal with a spin gap and dominant dimer wave fluctuations (at larger U/t). Although the model is purely one dimensional, this behavior is quite suggestive especially for its similarity to the phase diagram of high- T_c superconductors.

II. MODEL

As stated in the Introduction, we are going to study the model described by the Hamiltonian (2) which, in the absence of interaction, has the energy dispersion relation

$$\epsilon(k) = -2t \cos k + 2t' \cos 2k. \quad (3)$$

Notice that the model has particle-hole symmetry if contemporary $t' \rightarrow -t'$. Let us first analyze the dispersion relation (3) which is the starting point of our perturbative analysis.

If $t' < t/4$, the band minimum is at $k=0$ (see Fig. 1). The model is then a simple one-band model, and if the interaction U is turned on, we expect a behavior qualitatively similar to the standard Hubbard model ($t'=0$). We are not going to discuss this case in much detail, since its behavior is very well known.¹⁷

If $t' > t/4$ the band minima $\pm k_{\min}$ move away from $k=0$ (which turns into a band maximum) and satisfy the relation

$$\cos k_{\min} = \frac{t}{4t'}.$$

In this case two different situations may occur (see Fig. 2).

(1) If the density is such that the chemical potential is larger than $\epsilon(0) = -2t + 2t'$, the model at low energy is ef-

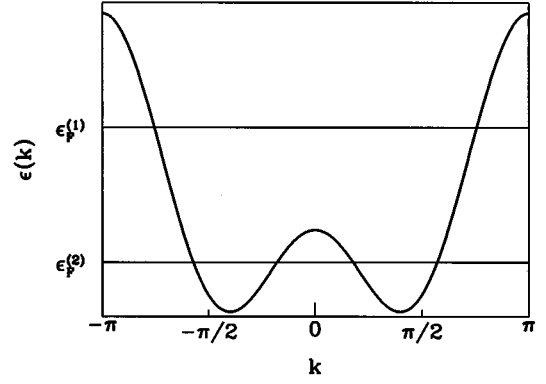


FIG. 2. Energy dispersion relation of the t - t' - U model for $t' > t/4$. Also drawn are the chemical potentials corresponding to two different fillings: $\epsilon_F^{(1)}$ refers to the case when only one band is involved at low energy while $\epsilon_F^{(2)}$ refers to the case when two bands are involved.

fectively a one-band model, for which the previous conclusions for the case $t' < t/4$ apply.

(2) If, on the contrary, the chemical potential is smaller than $\epsilon(0)$, there are four Fermi points ($\pm k_{F1}$ and $\pm k_{F2}$); thus, the model at low energy behaves as a two-band model. At half filling this implies the following.

(1) If $t' < t/2$, there are only two Fermi points $\pm k_F = \pm \pi/2$. There is therefore a simple umklapp scattering since $4k_F = 2\pi$, exactly like in the standard Hubbard model.

(2) If $t' > t/2$, there are four Fermi points (see Fig. 2) satisfying the relation $2k_{F2} - 2k_{F1} = \pi$. In this case, as we are going to discuss in the following section, there is only a higher-order umklapp scattering which involves four-electron scattering at the Fermi surface, since $4k_{F2} - 4k_{F1} = 2\pi$.

If $U \neq 0$ and one is interested in the low-energy behavior, a standard approach for a 1D system is to linearize the band around the Fermi points: $\epsilon(k) = \pm v_F(k \mp k_F)$ [see Fig. 3(a)] if there are only two Fermi points, while $\epsilon_1(k) = \mp v_{F1}(k \mp k_{F1})$ and $\epsilon_2(k) = \pm v_{F2}(k \mp k_{F2})$ if four Fermi points are involved [see Fig. 3(b)]. The linearization is

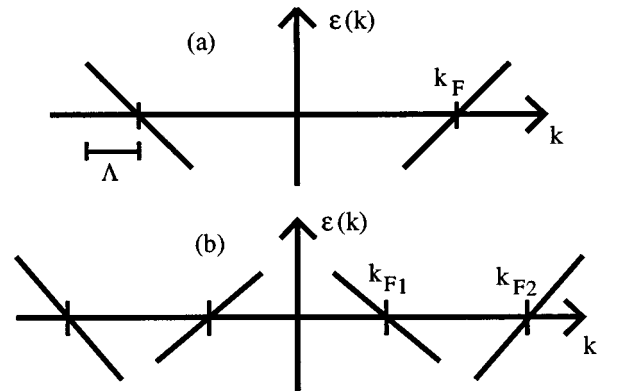


FIG. 3. The effective low-energy models: (a) simple one-band model and (b) two-band model.

assumed to be valid only within some cutoff range of width Λ . The interaction U causes scattering among these Fermi points. These scattering processes are relevant since they generate in perturbation theory logarithmic singularities (the usual Cooper's singularity in the particle-particle channel and additional singularities in the particle-hole channels due to the nesting property of a 1D Fermi surface). A standard way to cope with such a logarithmic singularities is the weak-coupling renormalization group (RG), which, along with the bosonization technique, is a very powerful tool in 1D. Although our analysis will make use of these techniques, we are not going to introduce them since there exists a wide number of articles where they have been intensively discussed.¹⁸⁻²⁰ For the two-band model, in particular, I will closely follow the analysis of Ref.4. In this reference a two-band model resulting from a two-coupled-chain model was analyzed both via bosonization and the RG. The only difference with Ref.4 is that the inner bands [which are $\epsilon_1(k)$ in the present case and the antibonding band with transverse momentum $k_\perp = \pi$ in the two-chain model] have opposite slopes in the two cases. The correct mapping between the two models is therefore⁴

$$\pm k_{F1} \mapsto \mp k_F^\pi,$$

$$\pm k_{F2} \mapsto \pm k_F^0.$$

On provision that the previous mapping is performed, the perturbation expansion of the $t-t'-U$ two-band model and of the two-chain Hubbard model is exactly the same at low energy (apart from an important difference at half filling; see next section). Therefore we can simply borrow all the results which have been obtained for the two-chain models and use them for the present case. This is what we are going to do in the following sections.²¹

Already at this stage it is apparent that the behavior of the two-chain models is similar to that of a single-chain $t-t'-U$ model and that the feature which makes the two class of models equivalent is the presence of four Fermi points in some parameter range.

III. MODEL AT HALF FILLING

If the density corresponds to one electron per site, two cases occur, as previously discussed.

A. $t' < t/2$

If $t' < t/2$, the low-energy model is a one-band model with Fermi momenta $\pm \pi/2$. There is a relevant umklapp process which makes the system an insulator. However, the spin excitations are gapless and, as a consequence, the spin correlations have a power-law decay at large distance. The model, for what it concerns the spin degrees of freedom, behaves exactly like a Heisenberg model.^{17,12}

B. $t' > t/2$

If $t' > t/2$, the effective model is a two-band model. It is therefore worthwhile to start with a broad outline of the behavior of such a two-band model in 1D.

Without umklapp terms, two different phases exist depending on the ratio of the Fermi velocities, v_{F1}/v_{F2} , and U/t . If $t' \simeq t/2$, the Fermi velocity of the inner band $v_{F1} \ll v_{F2}$. In this case the RG predicts^{4,2} that the model is a metal with four gapless excitations (two spin and two charge sound modes). The properties of the ground state can be inferred from the correlation functions which have the slowest decay at large distances. In this case these correlation functions describe spin and charge density waves at the incommensurate momenta $2k_{F2}$ and $2k_{F1}$. By increasing t' also v_{F1}/v_{F2} increases and at a critical t'_c a transition to a different phase occurs.^{4,2,22} In this new phase the model has a gap for the spin excitations and a single gapless charge mode which corresponds to the ordinary zero sound.^{4,2,7} There are two competing correlation functions which have the slowest asymptotic decay. One is, in two-chain language, the $4k_F$ charge density wave.^{6,2,7} In the language appropriate to the $t-t'-U$ model this function translates into the dimer wave (DW) correlation function which decays at large distances like

$$\begin{aligned} \chi_{\text{DW}}(x) &= \langle O_{\text{DW}}(x) O_{\text{DW}}(0) \rangle \sim \frac{\cos[2(k_{F2} - k_{F1})x]}{x^{2K}} \\ &= \frac{\cos(\pi x)}{x^{2K}}, \end{aligned} \quad (4)$$

the last equivalence being true only at half filling and

$$O_{\text{DW}}(x) = S^+(x)S^-(x+a) - S^+(x-a)S^-(x) \quad (5)$$

being the dimer order parameter,¹⁵ with a the lattice constant.

The other competing correlation function is what in two-chain language has been identified as a kind of d -wave superconducting correlation function (SC).⁴ In the $t-t'-U$ model,

$$\chi_{\text{SC}}(x) = \langle \Delta(x) \Delta^\dagger(0) \rangle \sim \frac{1}{x^{1/2K}}, \quad (6)$$

where

$$\Delta(x) = \sum_{p=\pm} \psi_{pk_{F1}\uparrow}(x) \psi_{-pk_{F1}\downarrow}(x) - \psi_{pk_{F2}\uparrow}(x) \psi_{-pk_{F2}\downarrow}(x). \quad (7)$$

The Fermi operators ψ 's in Eq. (7) are defined around each Fermi point, i.e.,

$$\psi_{pk_{Fi}\sigma}(x) \sim e^{ipk_{Fi}x} \sum_{|k| < \Lambda} e^{ikx} c_{pk_{Fi}+k,\sigma},$$

where $i=1,2$. Notice that the existence of a spin gap already signals some kind of electron pairing. Due to the repulsive nature of the interaction, the pair wave function should have a minimum whenever the two electrons approach each other. This is accomplished by the minus sign in the expression of the pair operator $\Delta(x)$, Eq. (7), which in turns shows the importance of having more than two Fermi points at our disposal. However, the existence of electron pairs does not

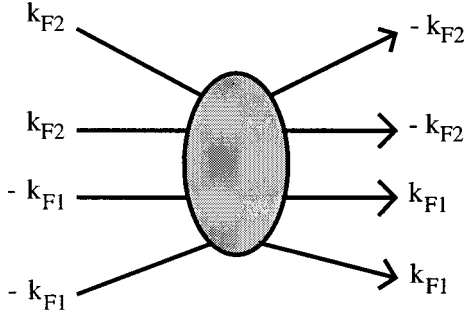


FIG. 4. The relevant umklapp scattering when the Fermi surface is made by four Fermi points.

necessarily imply dominant superconductivity. This depends upon the pair-pair interaction which in turn determines the value of the parameter K .

From Eqs. (4)–(6), we see in fact that if $K > 1/2$ the pairing fluctuations indeed dominate over the DW fluctuations, while the opposite occurs if $K < 1/2$. According to bosonization,^{19,12} K is related to the charge compressibility. In particular,

$$\frac{1}{K} = \frac{4L}{\pi v_\rho} \frac{\partial^2 E}{\partial N^2}, \quad (8)$$

where L is the length of the chain, E the ground-state energy, N the electron number, and v_ρ the velocity of the charge zero sound. The latter can be determined numerically by calculating the energy gap between the ground state (for closed shells at total momentum $P=0$) and the first excited state at total momentum $P=2\pi/L$:

$$E(P=2\pi/L) - E(P=0) = \frac{2\pi}{L} v_\rho.$$

The larger the electron-electron repulsion, the smaller the compressibility and consequently K , and the more unlikely is the dominance of superconductivity.

Since we are at half filling, we have also to take into account umklapp scattering. In this case there is only one higher-order umklapp process, which involves a four-electron scattering at the Fermi surface (see Fig. 4). From dimensional analysis it turns out that this umklapp process is

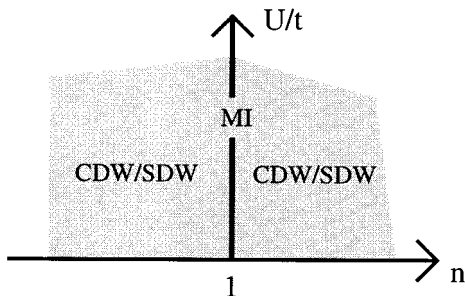


FIG. 5. Phase diagram of the t - t' - U model for $t' < t/4$ as a function of U/t and of the density n .

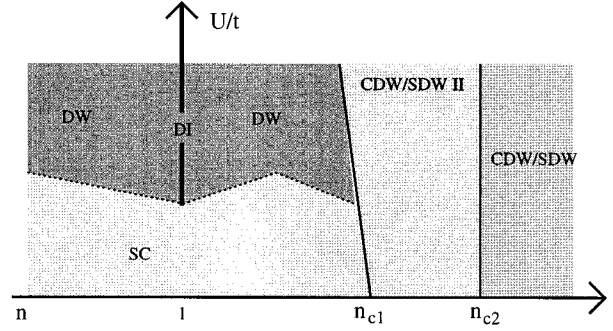


FIG. 6. Qualitative phase diagram of the t - t' - U model for t' sufficiently larger than $t/2$ as a function of U/t and of the density n .

relevant if $K < 1/2$. In this case the zero-sound mode acquires a gap and the model becomes insulating.

Having discussed the possible phases of the t - t' - U model when the Fermi surface has two branches, let us study in detail their occurrence at half filling.

If $t' > t'_c$ and $K < 1/2$, the umklapp process is relevant and therefore the model is insulating with a gap in the whole excitation spectrum and a finite average value of the dimer order parameter, Eq. (5):

$$\langle O_{\text{DW}}(x) \rangle = (-1)^x \times \text{const.}$$

This insulating phase certainly occurs for $U \gg (t, t')$ when the mapping to the spin model (1) is justified. On the other hand, for very small U , the parameter K can be evaluated by perturbation theory and it turns out to be close to 1, modulo corrections of order U . Therefore, provided perturbation theory is valid, $K > 1/2$ for $U \ll t$, which implies that the umklapp scattering is irrelevant and the model is metallic with the dominant superconducting fluctuations, Eq. (6). Consequently we expect a transition at a finite $U = U_c$ from a metal with superconducting correlations *directly* to an insulator with a dimer order. In Fig. 6, below, we have drawn a qualitative phase diagram for $t' > t'_c > t/2$. At half filling, $n=1$ in the figure, there is a critical U which separates the insulating regime (the bold line in the figure which we label DI, meaning a dimer insulator) at larger U from the metal with superconducting fluctuations at smaller U (which we label SC).

If $t/2 < t' < t'_c$ we still expect a metal-to-insulator transition at a finite U , but this time the metal has no spin gap and shows dominant density wave fluctuations. The properties of the insulating phase into which the above metal transforms at large U cannot be simply deduced by means of the RG, whose validity is doubtful at finite U . However, we tend to believe²³ that this insulator should have the same properties of the dimer insulator which occurs for $t' > t'_c$.

Notice that the behavior of the t - t' - U model at half filling is different from the behavior of the two-chain models also at half filling. There, the umklapp term is a two-electron scattering process and is relevant for any $K < 1$, which implies that the model is an insulator for any $U \neq 0$.² [This coincidence, which might well be accidental, is quite surprising,

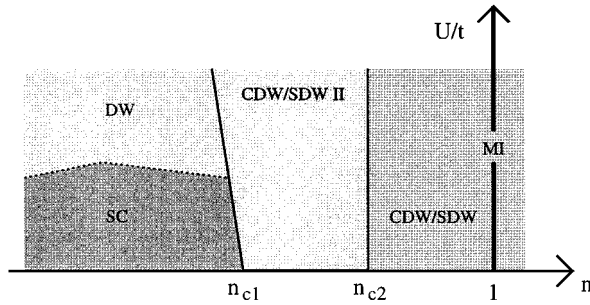


FIG. 7. Qualitative phase diagram of the t - t' - U model for $t/4 < t' < t/2$ as a function of U/t and of the density n .

since our prediction is based simply on *band-structure arguments* (modification of the Fermi surface). In fact, one would rather believe that band structure details are irrelevant for electron systems in the strong correlation limit where the interaction is much larger than the bandwidth, which is the case of the model (1).]

To conclude this section, we like to point out that, according to our analysis, the transition at large U between the insulating phase with power-law decay of the spin correlations and the dimer insulator with a spin gap is predicted to occur at $t' \approx t/2$ or, in terms of the exchange couplings, at $J' \approx J/4$. This is exactly the value found by numerical investigation of the spin model (1) in Ref.16.

IV. MODEL AWAY FROM HALF FILLING

We have seen that already at half filling the t - t' - U model shows the unusual property of a transition at a critical U from a metal with superconducting fluctuations to an insulator, when $t' > t/2$. Away from half filling the behavior is even more interesting, for smaller and larger t' . Let us consider in detail the various possible scenarios.

A. $t' < t/4$

In this case the model is for any filling always an effective one-band model, where nothing special occurs. Whether we dope with holes or electrons, as soon as we move away from half-filling the charge gap closes and the system becomes a metal with gapless spin and charge sound modes. The dominant fluctuations are both spin and charge density wave (SDW and CDW) fluctuations at momentum $2k_F$. In Fig. 5 we have drawn the phase diagram for this case as a function of U/t and of the density n . The bold line at density $n=1$, labeled MI, identifies the magnetic insulator with power-law decay of the spin correlations, while the rest of the phase diagram has been labeled with SDW/CDW, implying it is a metal with dominant density wave fluctuations. These labels will be used with the same meaning also in the following cases.

B. $t' > t/2$

Here, it makes a difference whether we dope with holes or electrons (the model is not particle-hole symmetric). In Fig. 6 we have drawn a qualitative phase diagram for $t' > t'_c > t/2$.

For hole doping ($n < 1$), the effective low-energy model involves always two bands. Therefore we predict that for any hole doping the spin gap will survive. As concerns the charge gap, it will immediately disappear as soon as we move away from half filling. Therefore, as U increases, we expect a crossover from a metal with dominant superconducting fluctuations [see Eq. (6)], which we still label in Fig. 6 as SC since it is continuously connected to the analogous state at $n=1$, to a metal with dominant dimer wave fluctuations [see Eq. (4)], which is labeled by DW.

At this point, it is worthwhile to discuss briefly the properties of the weakly doped dimer insulator. If we approach half filling with $U > U_c$ then, according to the theory of the incommensurate-to-commensurate transitions in 1D,²⁴ K tends asymptotically to the value $1/4$ and, exactly at half filling, it jumps abruptly to zero. With the asymptotic value $K=1/4$ valid at low doping, the dimer wave correlation function, Eq. (4), decays like $\chi_{\text{DW}} \sim (-1)^x/\sqrt{x}$, while the superconducting correlation, Eq. (6), decays quadratically $\chi_{\text{SC}} \sim 1/x^2$. Notice that these power-law decays are typical of the Green functions and of the density-density correlation functions, respectively, of a hard-core Bose gas. The situation is opposite for the metallic phase at $U \ll t$. In this case, provided perturbation theory is valid, $K \approx 1$ and the behaviors of the two correlation functions are exchanged: $\chi_{\text{SC}} \sim 1/\sqrt{x}$ while $\chi_{\text{DW}} \sim (-1)^x/x^2$.

In the case of electron doping the situation is in general different but for low doping where all is the same except the chemical potential which moves up instead of down (see Fig. 2). At the same time the Fermi velocities v_{F1} and v_{F2} of the two linear bands get more and more different (actually $v_{F1} \rightarrow 0$). As we said in the previous section, at a critical value of v_{F2}/v_{F1} or equivalently, a critical density n_{c1} in Fig. 6, the RG predicts a transition to another phase where also the spin gap closes (see, e.g., Appendix B in Ref. 4). In this phase the model is a metal with four gapless sound modes (two spin and two charge modes). The dominant fluctuations describe charge and spin density waves. We have labeled this phase in Fig. 6 as SDW/CDW II, implying that the number of gapless excitations is twice that of the phase SDW/CDW.

Finally, at a second critical doping n_{c2} , the topology of the Fermi surface changes from a four-point to a two-point Fermi surface. At the transition the density of states of the inner band diverges due to a van Hove singularity. For this reason we are not able to predict what happens exactly at the transition. According to Balents and Fisher,² the van Hove singularity induces again a spin gap and therefore they expect the properties of the model to be similar to those at low doping. On the other hand, if we assume that the RG equations of Ref.4 can be extended up to a very large v_{F2}/v_{F1} (where their validity is not fully guaranteed), we would rather expect that for $v_{F2}/v_{F1} \gg 1$ the two linear bands effectively decouple. In this case the transition would be a standard metal-to-metal transition with a topological modification of the Fermi surface. The van Hove singularity related to the low (hole) doping of the inner band is not expected to play any fundamental role, similarly to what happens to any one-band model close to filling zero or one. Although we

have no rigorous proof, we tend to believe that nothing special occurs at the transition (the latter scenario), rather than in the scenario proposed in Ref. 2. Coming back to the phase diagram, in the region where only two Fermi points are involved the model should be metallic with still dominant density wave fluctuations (see Fig. 6) and only two gapless modes (therefore this phase is labeled SDW/CDW).

In Fig. 6 we have assumed that the critical density n_{c1} decreases by increasing U . This is true for very small U where perturbation theory is valid. For finite U , unfortunately, we have no reliable method to evaluate n_{c1} . It might well be that $n_{c1} \rightarrow n_{c2}$ at $U \gg (t, t')$, which would be more consistent with the proposed transition upon increasing U at half filling and for $t' \approx t/2$ from the phase CDW/SDW II to the dimer insulator DI. The uncertainty about the precise behavior of n_{c1} as a function of U is also the reason why we have preferred not to draw even a qualitative phase diagram for t' close to $t/2$.

C. $t/4 < t' < t/2$

This case is in our opinion the most interesting one for its surprising similarities with the behavior of high- T_c compounds. We said in the previous section that at half filling the model is an insulator (MI in Fig. 7 at $n=1$) with power-law decaying spin correlations. If we dope with electrons ($n > 1$), the charge gap suddenly closes and the model turns into a metal with dominant spin and charge density wave fluctuations, for arbitrary doping (SDW/CDW in Fig. 7).

If we dope with holes ($n < 1$), at low doping the Fermi surface still consists of two points, and therefore the properties are similar to what we just described for electron doping; i.e., the phase is a SDW/CDW. However, as the chemical potential moves down (see Fig. 2), the same situation encountered earlier reappears, now in reverse. At a lower critical doping (n_{c2} , in analogy with the previous case) there will be a topological modification of the Fermi surface from a two-point to a four-point surface. The model turns from a one-band to a two-band model. Until the Fermi velocities remain quite different ($v_{F2}/v_{F1} \gg 1$) the system is a metal with four gapless modes (two charge and two spin modes) and dominant density wave fluctuations (phase SDW/CDW II in Fig. 7). At a critical value of v_{F2}/v_{F1} or, equivalently, a critical doping n_{c1} , a spin gap opens and only one charge mode (the ordinary zero sound) remains gapless. The dominant fluctuations are dimer waves, Eq. (5), or pairing fluctuations, Eq. (7). The one which dominates depends on the value of the parameter K , Eq. (8), which in turns depends on U . As we said before, if $K < 1/2$, the dimer fluctuations win (DW phase in Fig. 7), while for $K > 1/2$ superconductivity is more relevant (SC phase in Fig. 7). As in the previous case, we cannot establish the precise behavior at large U of the critical line between the CDW/SDW II phase and the SC or DW phase. Therefore the shape of the phase diagram drawn in Fig. 7 has not to be taken too literally close to that critical line.

Notice that the appearance of the spin gap upon hole doping the magnetic insulator indicates that in this model the holes *increase* the spin frustration. In the large U limit, one

can map the t - t' - U model onto a generalized t - J model with the Hamiltonian

$$\begin{aligned} \hat{H} = & -t \sum_{\sigma=\uparrow,\downarrow} \sum_{i=1}^L (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{H.c.}) \\ & + t' \sum_{\sigma=\uparrow,\downarrow} \sum_{i=1}^L (c_{i\sigma}^\dagger c_{i+2\sigma} + \text{H.c.}) + J \sum_{i=1}^L \vec{S}_i \cdot \vec{S}_{i+1} \\ & + J' \sum_{i=1}^L \vec{S}_i \cdot \vec{S}_{i+2}, \end{aligned}$$

defined in the reduced Hilbert space where double occupancies are forbidden. This model with $t'=0$ has been numerically investigated by Ogata, Luchini, and Rice.²⁵ They find that the hole doping effectively reduces the frustration due to J' . Since we instead find an increase of frustration, we have to conclude that this is mainly a consequence of the next-to-nearest-neighbor hopping t' .²⁶

V. CONCLUSIONS

In this paper we have studied the phase diagram of a one-dimensional t - t' - U model where, in addition to the on-site repulsion U and nearest-neighbor hopping t , we have included a next-to-nearest-neighbor hopping t' . Although very simple, this single-chain model has the interesting property to be at half filling and large U either an insulator with gapless spin excitations or a dimerized insulator with a spin gap.¹⁵ The transition between the two insulators should occur, according to our analysis, at $t' \approx t/2$. This model is therefore particularly suited to study the occurrence of superconductivity upon doping an insulator which has a charge gap and a spin gap. In fact, recent theoretical and numerical investigations of two-coupled-chain models,^{3,8} suggest that the presence of a spin gap in the insulating phase of two chains at half filling may lead to superconductivity upon doping and for not too large a repulsion. We have shown that precisely this behavior is realized here. Moreover, the weak-coupling analysis seems to suggest that the key feature which is responsible for the spin gap and possibly for the superconductivity is the topology of the Fermi surface in both models, which in the interesting parameter range has two branches, i.e., four Fermi points.

The present t - t' - U model has additional properties which make this model interesting in its own right. In particular at half filling and for t' sufficiently larger than $t/2$, we predict a *direct* transition at a critical U_c from a metal with dominant superconducting fluctuations at $U < U_c$ to a dimerized insulator at $U > U_c$.

Interestingly, for $t/4 < t' < t/2$ the phase diagram for hole doping shows some similarities with the phase diagram of high- T_c compounds (see Fig. 7). At half filling we have a magnetic insulator with power-law decay of the spin corre-

lations. For low doping we move to a metal with dominant spin and charge density wave fluctuations. Above a critical doping, a spin gap opens and the model has either dominant superconductivity or dimer waves depending upon the strength of the on-site repulsion.

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