Strong-Coupling Field Theory and Soliton Doping in a One-Dimensional Copper-Oxide Model

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(Received 8 March 1990)

A field theory for the strong-coupling limit of a one-dimensional copper-oxide model is obtained from a weak-coupling point of view. Complementary aspects of strong correlations and band motion are incorporated in a natural way. Doping induces soliton or antisoliton charge excitations into a state with explicitly broken chiral symmetry. The solitons or antisolitons have divergent superconductive pairing correlation functions and various properties reminiscent of doped holes or electrons in high-temperature superconductors.

PACS numbers: 72.15.Nj, 71.10.+x, 74.70.Vy

It has been clear for some time that an improved understanding of many-body theory in two dimensions is necessary for the development of a microscopic theory of high-temperature superconductors.[1] This conclusion is reinforced by an increasing body of data for the normal state,[2] showing some features that are more easily understood from a weak-coupling point of view, despite ample evidence of strong correlations (for a review, see Lee[3]). It is natural, therefore, to see how this problem is resolved in one dimension, where the many-body theory is well understood.[4,5] A number of papers[6] have been concerned with one-dimensional analogs of models related to high-temperature superconductors. The purpose of this paper is to obtain a suitable field theory for the strong-coupling limit of a one-dimensional copper-oxide model, starting from a weak-coupling point of view, and to explore the properties of doped holes and electrons. The theory is very general and applies to a wide variety of initial Hamiltonians. But it is convenient to work explicitly with a two-band model,[7,8] incorporating both copper and oxygen sites. Hole doping may involve both bands but electron doping has essentially the same physics[9] as a single-band Hubbard model.[10] Therefore it is possible to study one- and two-band models on the same footing and to explore their differences, which have been the subject of some debate.[11,12]

The physical picture emerges as follows. In undoped materials (analogous to La_2CuO_4 and $YBa_2Cu_3O_6$) there is an explicitly broken chiral symmetry associated with the charge-density-wave (CDW) degrees of freedom, together with algebraic spin-density-wave (SDW) correlations. Doping induces (sine-Gordon) soliton or antisoliton CDW excitations, and a "*Fermi surface*" following a modified form of Luttinger's theorem (Lee[3]). Superconductive pairing-correlation functions for solitons or antisolitons may diverge at low temperatures even if the initial Hamiltonian has purely repulsive interactions. The "*superconductivity*" disappears at sufficiently high doping when the solitons overlap and cease to have a distinct identity. The soliton picture suggests explanations for various properties of high-temperature superconductors, such as the change in sign of the Hall coefficient on doping,[2] the increased room-temperature conductivity of highly doped, nonsuperconducting samples,[2] and the different temperature dependences of the spin-relaxation rates of copper and oxygen nuclei.[13] One- and two-band models differ in the number of spin degrees of freedom.

The Hamiltonian is assumed to be

$$H=\sum_{n,\sigma}\{-ta^{\dagger}_{n\sigma}a_{n+1,\sigma}+\text{H.c.}+\tfrac{1}{2}\epsilon(-1)^n\rho_{n\sigma}+\tfrac{1}{2}U_n\rho_{n\sigma}\rho_{n,-\sigma}+V\rho_{n\sigma}\rho_{n+1,\sigma}\}, \quad (1)$$

where $a^{\dagger}_{n\sigma}$ and $\rho_{n\sigma}\equiv a^{\dagger}_{n\sigma}a_{n\sigma}$ are, respectively, the creation and number operators for a hole with spin σ at site n. This is a one-dimensional version of a model proposed[7,8] for the copper-oxide planes of high-temperature superconductors if $U_n=U_d$ at odd sites (copper) and $U_n=U_p$ at even sites (oxygen). There are N_h holes and N_s sites with $2N_h/N_s=1+\delta$, where δ is the dopant concentration and $\delta>0$ for hole doping, $\delta<0$ for electron doping. Because of the ϵ term in Eq. (1), there is a gap in the spectrum at $k=\pm\pi/2d$, where d is the Cu-O lattice spacing. The lower band has more copper character and the upper one more oxygen, depending on the value of ϵ. To start out, the solution of the problem in the continuum and strong-coupling limits will be described. In each case, the CDW part of the Hamiltonian will be written in terms of spinless fermions which are CDW excitations *not* electrons. Following Eq. (6), a discussion of the physical consequences will be given.

The procedure for taking the continuum limit of one-dimensional models is well known.[4,5] In that limit, there is separation of spin and charge in the sense that the Hamiltonian may be written as a sum of SDW and CDW parts, H_s and H_c, respectively, and the correlation functions *in space and time* are products of SDW and CDW factors. The Hamiltonian H_s is parametrized by (g_1,θ_s) and H_c by (g_3,θ_c), where g_1,g_3 are backward- and umklapp-scattering coupling constants, respectively, and θ_s,θ_c are functions of g_1,g_3 and forward-scattering coupling constants. For free fermions with spin, $g_1=g_3=0$ and $\theta_s=\theta_c=1$. Explicit expressions for these variables may be obtained by taking the naive continuum

limit,[4,5] but this is inaccurate for strong coupling: A better procedure is to use numerical methods, general arguments, or known properties of the original system to identify the exact values. The formulation is quite general: All singular-scattering processes near the Fermi surface are taken into account, and the asymptotic behavior of any system is governed by symmetry, the number of degrees of freedom, and the values of (g_1,θ_s) and (g_3,θ_c), regardless of the details of the interactions in the original Hamiltonian. (It is assumed that the interactions have finite range.) The correlation functions are power laws in the temperature T or frequency ω, with critical exponents that are functions of θ_c and θ_s.

There are separate renormalization-group equations for H_s and H_c with lines of fixed points $g_1=0$ and $g_3=0$ parametrized by θ_s and θ_c, respectively.[4,5] For the repulsive spin-rotation-invariant interactions of interest here, (g_1,θ_s) scale to the fixed point (0,1) at which both are marginal variables. Thus the renormalization group is sufficient to obtain the asymptotic SDW behavior. However, in the same region of coupling, the fixed line $g_3=0$ is unstable, and it is necessary to specify H_c. There are several different representations, but the most useful one for present purposes is in terms of spinless fermions:

$$H_c=\int dx\left[iv\left(\psi_1^\dagger\frac{\partial\psi_1}{\partial x}-\psi_2^\dagger\frac{\partial\psi_2}{\partial x}\right)+\bar{g}_3(\psi_2^\dagger\psi_1+\psi_1^\dagger\psi_2)+g\rho_1\rho_2\right], \tag{2}$$

where $\psi_1(x)$ and $\psi_2(x)$ are annihilation operators for right-going and left-going fermions, $\rho_i(x)\equiv\psi_i^\dagger(x)\psi_i(x)$, v is the Fermi velocity, $\bar{g}_3\equiv k_F g_3/\pi^2$, and k_F is the Fermi wave vector of the original holes. The spinless fermions have Fermi wave vector $k_F'=2k_F-\pi/2d$ (a Galilean transformation has been used to shift momenta by $\pm\pi/2d$ in order to incorporate the momentum taken up by the lattice). A detailed derivation of Eq. (2) is given in Ref. 4. The essential steps are (a) introduce a boson representation of the original fermions, (b) combine the bosons into SDW and CDW fields in order to separate the Hamiltonian into H_s and H_c, (c) use a boson representation of the spinless-fermion operators $\psi_i(x)$ to obtain Eq. (2). The boson form of H_c is a sine-Gordon Hamiltonian, with the cosine term proportional to $\bar{g}_3$. In the fermionic form of H_c, given in Eq. (2), the $\psi_i^\dagger(x)$ are soliton rather than electron creation operators. In other words they create clumps of charge of finite extent. Evidently, H_c could be parametrized by $\bar{g}_3/v$ and g/v, but it is more useful to work with the explicit expression[4]

$$\frac{g}{v}=2\pi\left(\frac{1-4\theta_c^2}{1+4\theta_c^2}\right) \tag{3}$$

for g/v in terms of θ_c which characterizes the critical exponents. Note that the free-fermion point ($g=0$) for H_c corresponds to $\theta_c=\frac{1}{2}$.

This general theory will form the basis for the discussion of doping into a half-filled band ($k_F'=0$, $g_3\neq0$) as a strong-coupling theory. The essential point is that step (c) in the derivation is a quantum dual transformation relating weak-coupling variables (the bosons of the sine-Gordon theory) to strong-coupling variables (the spinless fermions). But that step would be unnecessary if g_3 were zero since H_c in Eq. (2) would be a Luttinger model corresponding to free bosons.[4,5]

The identification of H_c as a strong-coupling Hamiltonian may be demonstrated explicitly in the limit $U_p,U_d\rightarrow\infty$ for which the spatial motion is governed by the Hamiltonian

$$H_\infty=\sum_n[-t(c_{n+1}^\dagger c_n+c_n^\dagger c_{n+1})+\tfrac{1}{2}\epsilon(-1)^n c_n^\dagger c_n+V\rho_n\rho_{n+1}], \tag{4}$$

where $c_n^\dagger$ creates a *spinless* fermion at site n and $\rho_n\equiv c_n^\dagger c_n$. Here, the exclusion principle enforces the constraint that no site is doubly occupied and gives a Fermi wave vector $2k_F$. Such a representation of the spatial motion may be obtained by generalizing arguments previously used for the single-band Hubbard model.[14] Taking the (naive) continuum limit of H_∞ in the usual way[4,5] gives H_c with $v=2td\sin2k_Fd$, $\bar{g}_3=\epsilon/2$, and $g=4k_FV/\pi$. Note that the $c_n^\dagger$ refer to CDW excitations and not electrons. Also, the continuum limit of H_∞ is a special case of H_c: In general, the parameters of the fixed-point Hamiltonian are not so simply related to those of the original Hamiltonian. The spin degrees of freedom are equivalent because (i) when $U_p,U_d\rightarrow\infty$ the spin part of the wave function is an eigenstate of the Heisenberg chain, and (ii) the renormalization-group equations for the Heisenberg-Ising model[15,16] have the same structure as for H_s—two variables, both of which are marginal at the spin-rotation-invariant fixed point. Here, (i) was obtained by Ogata and Shiba[17] for the single-band model $U_p=U_d$, $\epsilon=V=0$ by taking the limit of the exact Bethe-ansatz solution. But it may also be proved for the more general model by using second-order perturbation theory in t: The spin degeneracy is resolved by superexchange and pair hopping when two holes are on neighboring sites.

The relationship to the $U_p,U_d\rightarrow\infty$ limit may also be illustrated by comparing correlation functions. For $k_F'=0$, the charge degrees of freedom are frozen and both the Heisenberg model[18] and the electron gas[4,5] have spin-spin correlation functions varying as x^{-1} for large x, with logarithmic corrections.[15] Furthermore, it is a general consequence of the weak-coupling theory[4,5] that the momentum distribution of the original fermions is given by

$$n(k)=\tfrac{1}{2}-\text{const}\times|k\mp k_F|^\alpha\,\text{sgn}(\pm k-k_F) \tag{5}$$

near to the Fermi points $k = \pm k_F$, where

$$\alpha = \tfrac{1}{4}(\theta_s + \theta_s^{-1} + \theta_c + \theta_c^{-1}) - 1 . \quad (6)$$

Since $\theta_s = 1$, it follows quite generally that $\alpha = \frac{1}{8}$ at the free-fermion point $\theta_c = \frac{1}{2}$. From Eqs. (2)–(4), it can be seen that the $U \to \infty$ limit of the single-band Hubbard model is such a point and indeed the value $\alpha = \frac{1}{8}$ has been obtained from the Bethe-ansatz solution by Haldane[3] (analytically) and Ogata and Shiba[17] (numerically). Other critical exponents may be obtained from Tables 2 and 3 of Ref. 4. Note that a form of Luttinger's theorem is satisfied in the sense that the location of the singularity in $n(k)$ is determined by the position of the Fermi surface for the noninteracting holes.

The continuum and large-U_p, U_d theories are complementary. The former is a general fixed-point theory for a wide variety of initial Hamiltonians, including those with extended Coulomb interactions. Correlation functions are easily evaluated, and the crossover from weak to strong coupling is clear. On the other hand, the large-U_p, U_d theory is easier to derive and gives a lattice theory which is useful when the shape of the energy spectrum or the number of degrees of freedom is important. However, in order to realize all of the intermediate-coupling physics, it would be necessary to generalize the U_p, $U_d \to \infty$ model to allow $V < 0$ since the corresponding coupling constant g in Eq. (3) is negative when $\theta_c > \frac{1}{2}$. Note that the t-J model, or the large-U limit of the *single-band* Hubbard model (H_∞ with $\epsilon = 0 = V$), does not give a faithful realization of the continuum Hamiltonians H_c and H_s. In particular, the chiral-symmetry-breaking term (ϵ) and the (possibly attractive) direct interaction (V) are missing. The consequences will be made clear in the ensuing discussion.

When $V = 0$ and there is one hole per unit cell, H_∞ describes noninteracting fermions with a gap for excitations above the ground state. The gap is a consequence of umklapp scattering (the ϵ term of H_∞) which drives an excess of holes on copper sites. Hole or electron doping produces holes in the oxygen band[7] or holons,[10,18] respectively. In the continuum language, H_c describes free massive fermions—the solitons of the sine-Gordon theory.[4] The mass is a consequence of the explicitly broken chiral symmetry (the $\bar{g}_3$ term of H_c). Doping produces soliton or antisoliton CDW excitations. In either case, current is a flow of defects and the carrier concentration n_c is equal to the dopant concentration δ. In this sense, the CDW degrees of freedom are electron-hole (i.e., soliton-antisoliton) symmetric in the two-band model. The spins will be considered later.

The soliton pairing correlation function, generated by the operator $\psi_1^\dagger \psi_2^\dagger$, may be evaluated by standard techniques.[4,5] For attractive interactions ($\theta_c > \frac{1}{2}$ or $V < 0$) it diverges as a power of the inverse temperature T^{-1} as $T \to 0$. This is the one-dimensional analog of pairing of holons[19] except that the attractive interaction is a property of the renormalized Hamiltonian H_c and does not require extrinsic processes such as tunneling between chains.[19] The soliton pairing operator $\psi_1^\dagger \psi_2^\dagger$ couples to a gauge field in exactly the same way as $\psi_{1\uparrow}^\dagger \psi_{2\downarrow}^\dagger$ (singlet pairing of holes). This result follows from the boson representation[4,5] in which both operators involve the exponential of $\int_{-\infty}^{x} dx' \hat{\Pi}(x')$, where $\hat{\Pi}(x)$ is the momentum conjugate to the Bose field $\phi(x)$ which, in turn, is related to the charge density $\rho(x) = \pi^{-1/2} \partial\phi/\partial x$. In the presence of an electromagnetic field, $\hat{\Pi}$ becomes $\hat{\Pi} - eA_1/\pi^{1/2}$ where A_1 is the space component of the vector potential.[20] Thus the soliton pairs have charge $2e$, and a Ginzburg-Landau theory of an ordered state would be very similar to that of a conventional superconductor. However, it has not yet been shown that such an ordered state would exist in a full three-dimensional theory.

The solitons have a finite size determined by the value of ϵ or $\bar{g}_3$. Then the entire picture breaks down when the density of solitons is too high since the size of the solitons exceeds their average separation and the solitons are not well defined. In that case, the behavior of the system is the same as if $\bar{g}_3 = 0$: When $\theta_c > \frac{1}{2}$, the concept of soliton pairing has no meaning, and all of the holes participate in the flow of current ($n_c = 1 + \delta$). However, at elevated temperatures, the system may have a higher conductivity than in the "*soliton*" region because the carrier concentration is higher. This behavior is reminsicent of the properties of high-temperature superconductors.[2,21] Moreover, the spectrum of H_∞ has inflections above and below the Fermi level for a half-filled band, a signature of the solitons' or antisolitons' losing their identity. This is what is needed to give a change in sign of the Hall coefficient as superconductivity disappears at high doping levels.[2] The soliton picture also suggests an explanation of the difference between the spin-relaxation rates measured on copper and oxygen nuclei.[13] There are two contributions, one from the *commensurate* SDW regions, the other a Korringa relaxation from the solitons. Oxygen nuclei do not see the former because it is suppressed by a form factor which vanishes at the SDW wave vector;[13] thus they should only show the Korringa relaxation, as observed.[13] On the other hand, the oxygen nuclei would be affected if the doping simply produced an incommensurate SDW. Of course, a proper discussion of the experiments requires a consideration of the two-dimensional version of the model[7,8] for which the relationship between the charge and spin degrees of freedom is not so simple as in one dimension.

The spin degrees of freedom do not appear to be involved in the properties of the solitons but, in fact, they play a role in the global renormalization from H to H_c. From the strong-coupling point of view, the effective interaction g in H_c is kinetic in origin. In the $U_p, U_d \to \infty$ limit, the zero-point kinetic energy is very high. This is a collective effect—the high Fermi energy is a consequence of the exclusion principle for *spinless* fermions.

When U_p, U_d are finite, the zero-point energy is lowered because excursions onto already occupied sites are allowed. The attractive interaction is a consequence of the fact that the zero-point energy is lowered even further when two holes are close together.

Finally, the difference between electron and hole doping is in the number of spin degrees of freedom. This is clear from the large-U_p, U_d limit for which the number of spins in the Heisenberg wave function is $(1+\delta)N_s/2$. In a single-band model for *hole* doping[10,11] the number of spins is $(1-\delta)N_s/2$ with $\delta > 0$. The number of spin degrees of freedom is not reduced by the formation of singlets involving copper and oxygen spins as suggested by Zhang and Rice.[11]

I thank S. Kivelson for constructive comments. This work was supported by the Division of Materials Sciences, Office of Basic Energy Sciences, U.S. Department of Energy under Contract No. DE-AC02-76CH00016.

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