Spin-Bag Mechanism of High-Temperature Superconductivity

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A new approach to the theory of high-temperature superconductivity is proposed, based on the two-dimensional antiferromagnetic spin correlations observed in these materials over distances large compared to the lattice spacing. The spin ordering produces an electronic pseudogap Δ_{SDW} which is locally suppressed by the addition of a hole. This suppression forms a bag inside which the hole is self-consistently trapped. Two holes are attracted by sharing a common bag. The resulting pairing interaction $V_{k-k'}$ leads to a superconducting energy gap Δ_{SC} which is nodeless over the Fermi surface, where $\Delta_{SC} \simeq \Delta_{SDW} \exp(-t/\alpha U)$, with α of order unity.

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In the high-temperature oxide superconductors[1] $La_{2-x}(Sr,Ba)_xCuO_{4-y}$ (denoted by 214) and $YBa_2Cu_3O_{7-y}$ (123) strong antiferromagnetic spin order[2-4] has been observed in neutron-scattering experiments in the region of the phase diagram near to those exhibiting superconductivity. The ordered moment per site corresponds to approximately one-half of an electron spin per Cu site.

Since these materials are highly anisotropic, being based on a CuO layered structure, the effective exchange interaction $J_\perp$ between spins in different layers is weak compared to $J_\parallel$ between spins in a given plane. As a consequence, two-dimensional spin ordering is observed above the Néel temperature T_N with a spin-correlation length L of order 200 Å for La_2CuO_{4-y}.[3]

Doping of the 214 material with Sr or Ba decreases T_N, with T_N vanishing for $x \simeq 3\%$. While superconductivity occurs for $x \gtrsim 5\%$, it has been difficult to grow single crystals in this regime which are sufficiently large to observe strong in-plane spin order directly by neutron scattering. Nevertheless, it is reasonable to assume that two-dimensional spin order exists over distances L large compared to the size of the CuO unit cell in these superconducting materials as in the more weakly doped normal materials.

In the treatment of the influence of spin correlations on superconductivity in oxide superconductors, there are two limiting points of view, (1) $U \gg W$ and (2) $U \lesssim W$, where U is the effective Hubbard on-site interelectronic Coulomb repulsion and W is the valence-band width. Band-structure calculations show that the valence band arises from the antibonding combination of Cu $d_{x^2-y^2}$ and O $p\sigma$ orbitals, with W of order 2 eV. In undoped La_2CuO_4, there is one valence electron per Cu atom on average. At present, experiments cannot unambiguously determine which of these limits is closer to the actual physical situation.

For large U the valence electrons are Mott-Hubbard condensed,[5] corresponding to one electron localized on each Cu site (or more precisely localized in the relevant valence-band Wannier function). To lowest order in t/U, where $t = W/8$ is the hopping interaction, there is an antiferromagnetic exchange interaction J of order $-t^2/U$, which produces spin ordering. We note that the Mott-Hubbard state is insulating not because of the spin order but because of the strong on-site correlations. On p-type doping, such as by Sr or Ba in the 214 material, the holes are mobile and lead to nonzero conductivity under suitable circumstances. In the resonating-valence-bond approach, it is assumed that the spin $\frac{1}{2}$ and charge $(+e)$ of each hole are separated and become independent excitations, just like a hole in polyacetylene which splits into a spinless positively charged soliton and a spin-$\frac{1}{2}$ neutral soliton. The spinless charge objects of the resonating-valence-bond approach are presumed to be condensed in three dimensions, in the presence of interplanar hopping by boson pairs.

In the second point of view, U is assumed to be sufficiently small that the Mott-Hubbard condensation does not occur, although strong interelectronic correlations of a quite different type are present. In this limit, Bloch states form a convenient basis set to describe the problem. The Fermi surface for the half-filled band in a nearest-neighbor tight-binding model is shown in Fig. 1, illustrating the Fermi-surface nesting with wave vector $\mathbf{Q} = (\pi/a, \pi/b)$. Because of this nesting, a spin-density wave (SDW) occurs, whose period is commensurate (2:1) with that of the crystal lattice. This spin-density wave causes an energy gap $2\Delta_{SDW}$ at the Fermi surface for the undoped material, leading to an insulator. Residual two-dimensional finite-range spin order leads to a pseudogap, i.e., one which is spatially and temporally slowly varying.

An essential point is that the period of the SDW remains commensurate with the lattice period for a finite range of doping x about $x = 0$, including doping beyond $T_N = 0$. This condition ensures that doping adds holes to an essentially rigid band structure as opposed to shifting the gap edge to track the Fermi level, removing the possibility of adding holes below the gap edge. This latter

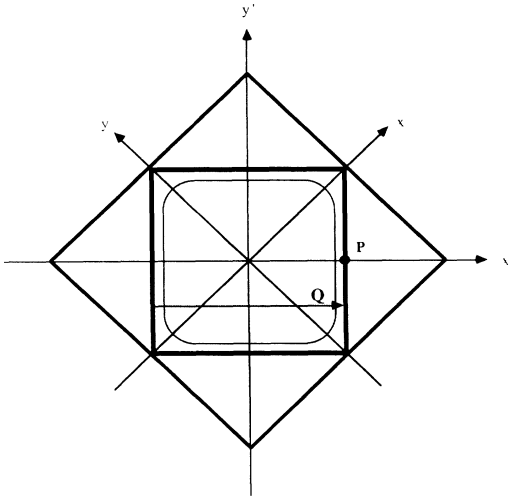

FIG. 1. The large square represents the first Brillouin zone; the small square represents the Fermi surface at half-filling, which is also taken to be the reduced Brillouin zone for the Bloch states in the SDW background. Near half filling, the shaded region is occupied by the electrons. Q is the nesting vector.

possibility occurs for an incommensurate SDW. In particular, the commensurate nature of the SDW leads to the Hall coefficient being positive for the doped 214 material with the Hall coefficient being proportional to $1/x$, as is observed experimentally.

In this paper we propose a new approach to high-temperature oxide superconductivity based on the following picture. Other approaches to the superconductivity based on antiparamagnon exchange may be found in the literature.[6] Let $\mathbf{m}(\mathbf{x}_n)=\mathbf{S}(\mathbf{x}_n)\cos\mathbf{Q}\cdot\mathbf{x}_n$ be the staggered-spin order parameter. Within a given domain, $\mathbf{m}(\mathbf{x}_n)$ is essentially uniform but it changes on the scale of the length L measured in neutron scattering. Consider the addition of a hole to the system in a spatially localized wave packet, with the size l and shape to be determined variationally. Initially we assume that $l<L$, so that the local band structure prior to insertion of the hole can be considered to be that for a uniform order parameter.

There are two qualitative effects of the hole on the spin order. First, the spin of the hole couples to the spin density of the antiferromagnetic background through an exchange interaction. While this effect appears to be analogous to the conventional spin-polaron effect in which an electron is coupled to an array of localized Heisenberg spins, the spin polaron has a ferromagnetic core while the spin bag has reduced antiferromagnetic order inside. The problem is closely related to the polaron in dimerized polyacetylene.[7]

Second, the added hole locally depletes the electronic charge density, pulling the Fermi surface further from the nesting surface, and thereby reducing the order parameter $\mathbf{m}(\mathbf{x}_n)$.[8] Since the local value of the energy gap Δ_{SDW} is proportional to $\mathbf{m}(\mathbf{x}_n)$, it follows that the hole depresses the gap in its vicinity, lowering the energy of the hole in this region. Thus, within a given domain, a hole produces an effective potential well or bag in its vicinity in which the hole is self-consistently trapped. Of course the hole and its surrounding bag move through the crystal and act as a fermionic quasiparticle, having charge $+e$ and spin $\frac{1}{2}$. As we show below, the spin effect also leads to the local suppression of Δ_{SDW} and reinforces the charge effect.

It is reasonable when two such quasiparticles interact that the effective potential arising from the shared bag will be attractive and have a range of order the bag size l. This attraction is opposed by the Coulomb repulsion. We find that the net effective interaction is attractive leading to a pair condensation because the short-range nature of the Coulomb potential permits the holes to avoid the electrostatic repulsion yet remain within the bag.

To make an estimate of the bag size, shape, and energy, we consider a simple model analogous to that used in QCD bag models.[9] For simplicity we assume that the SDW gap parameter is equal to a constant value Δ_B inside the bag and is Δ_{SDW} outside. Consider a hole near the gap edge at point p in Fig. 1. In this vicinity, the hole energy is essentially independent of $p_{y'}$ since the constant-energy contours are nearly parallel to the nesting surface. Therefore, one can form wave packets in $p_{y'}$ about the point p with little cost of energy. The same is true about p_z since the interplanar hopping is weak. Thus, kinetic-energy effects are important only for hole localization along x'. The other terms in the energy shrink the bag size along y' and z to approximately the unit-cell dimensions, thereby leading to a cigar-shaped bag oriented along the local velocity direction, x' in this case. Thus, bags corresponding to perpendicular sheets of the Fermi surface are oriented in perpendicular directions.

A second term is the energy increase due to the decreased magnitude of the exchange energy inside the bag. In addition, the energy of the hole at the gap edge is reduced inside the bag. These three terms lead to the total bag energy

$$E(l,\Delta_B)=E_{\mathrm{loc}}(l)+(a/2W)(\Delta_B-\Delta_{\mathrm{SDW}})^2 l/a+(\Delta_B-\Delta_{\mathrm{SDW}}),$$

where $\Delta_B\geq 0$ and a is of order unity. The localization energy is given by

$$E_{\mathrm{loc}}=\begin{cases}1/2m_h l^2, & l>\xi_{\mathrm{SDW}}\equiv v_F/\pi\Delta_{\mathrm{SDW}},\\ v_F/l, & l<\xi_{\mathrm{SDW}},\end{cases}$$

and $m_h = \Delta_{SDW}/v_F^2$. Minimizing with respect to the bag size l and the gap Δ_B one finds that l is of order of the coherence length ξ_{SDW} and the hole occupies an effective well whose depth $\Delta_{SDW} - \Delta_B$ is a fraction of the SDW gap Δ_{SDW}.

We note that the effect of the hole charge on the bag parameters is to decrease the tendency to antiferromagnetic ordering, further decreasing Δ_B.

When two holes are in the same region, they share each other's bag potential, leading to an attractive potential whose range along x' is l and along y' or z is roughly the cell dimension. The depth of the potential is of order $\Delta_{SDW} - \Delta_B$. The pairing potential $V_{kk'}$ corresponding to this potential is anisotropic in momentum space, having a peak when $q_{x'}=0$ and range $1/l$ for $q_{x'}$ nonzero, while $V_{kk'}$ drops slowly as a function of $q_{y'}$ and $q_{z'}$. Below we show how these results can be made more quantitative by diagram methods.

The kinetic term of the Hubbard Hamiltonian leads to a simple band structure

$$\epsilon_p = -2t(\cos p_x + \cos p_y). \tag{1}$$

The mean-field spin density

$$\mathbf{m}(\mathbf{x}_n) = \mathbf{S}\cos(\mathbf{Q}\cdot\mathbf{x}_n) \tag{2}$$

couples the electronic states on opposite sides of the Fermi surface and opens an SDW gap. Without loss of generality we assume that the spin-density wave is polarized in the z direction, i.e., $S^z = S$, $S^x = S^y = 0$, and the resulting SDW gap is constant, $\Delta_{SDW} = US$. The electronic eigenstates in the presence (due to the momentum independence of the Hubbard interaction) of the SDW background are obtained by a standard canonical transformation

$$\begin{aligned}
\gamma_{k,\uparrow,c} &= u_k c_{k\uparrow} + v_k c_{k+Q,\uparrow},\\
\gamma_{k,\downarrow,c} &= u_k c_{k\downarrow} - v_k c_{k+Q,\downarrow},\\
\gamma_{k,\uparrow,v} &= v_k c_{k\uparrow} - u_k c_{k+Q,\uparrow},\\
\gamma_{k,\downarrow,v} &= -v_k c_{k\downarrow} - u_k c_{k+Q,\downarrow},
\end{aligned} \tag{3}$$

where the subscripts v and c denote the valence and conducting bands below and above the SDW gap. k extends over half of the original Brillouin zone; our choice is illustrated in Fig. 1. u_k and v_k are given by

$$\begin{aligned}
u_k &= +[\tfrac{1}{2}(1+\epsilon_k/E_k)]^{1/2},\\
v_k &= +[\tfrac{1}{2}(1-\epsilon_k/E_k)]^{1/2},\\
E_k &= +(\epsilon_k^2 + \Delta_{SDW}^2)^{1/2}.
\end{aligned} \tag{4}$$

In this SDW state, there are collective excitation modes about the mean-field order parameter **S**, namely the amplitude fluctuation $\delta S^z(x)$ and the orientation fluctuation $\delta S^{\pm}(x)$. The doped electrons (or holes) interact with each other through exchange of these fluctuations. Expressed in terms of the original fermion operators the interaction of a pair of electrons having momentum k, $-k$ through exchange of an amplitude fluctuation is of the form

$$H = -\tfrac{1}{2}\sum_{k,k'}\sum_{\substack{\alpha\alpha'\\ \beta\beta'}} V_z(k-k')\sigma^z_{\alpha'\alpha}\sigma^z_{\beta'\beta} c^{\dagger}_{k'+Q,\alpha'} c^{\dagger}_{-k'+Q,\beta'} c_{-k,\beta} c_{k,\alpha}, \tag{5}$$

where $V_z(k-k')$ is given by

$$V_z(q) = +U/[1 - U\chi^{zz}_{\Delta}(q+Q)] \tag{6}$$

within the random-phase approximation and $\chi^{zz}_{\Delta}(k)$ is the static susceptibility in the SDW background. As a pairing interaction of the original fermions, this potential is effective at large momentum transfer Q and is attractive for parallel spin and repulsive for antiparallel spin.[6] However, it is crucial to observe that, as discussed above, the pairing interaction occurs between the Bloch states in the presence of the SDW. These states are linear combinations of the original states; the interference effects change the pairing potential dramatically. Making the canonical transformation (3) in (5), we find the pairing interaction between two doped holes to be

$$H = -\tfrac{1}{2}{\sum_{kk'}}'\sum_{\substack{\alpha\alpha'\\ \beta\beta'}} V_z(k-k') m^2(k,k') \delta_{\alpha\alpha'}\delta_{\beta\beta'} \gamma^{\dagger}_{k',\alpha'} \gamma^{\dagger}_{-k',\beta'} \gamma_{-k,\beta}\gamma_{k,\alpha}, \tag{7}$$

where k and k' are summed over the reduced Brillouin zone. We have assumed that the holes are near the top of the valence band. $m(k,k')$ is the coherence factor defined by

$$m(k,k') = u_k v_{k'} + v_k u_{k'}. \tag{8}$$

The pairing potential is attractive independent of spin orientations and has a natural physical interpretation in terms of the bag picture discussed above. A doped hole, independent of its spin, always disturbs the medium by reducing the SDW amplitude thereby lowering its self-energy, and the region of the medium with reduced SDW amplitude always attracts a second electron since the SDW energy gap is smaller in this region. Besides the amplitude fluctuations, doped holes can also interact by exchanging orientation fluctuations; however, these interactions are accompanied by the coherence factor

$$p(k,k') = u_k v_{k'} - v_k u_{k'} \tag{9}$$

which is small at the top of the valence band, where $u_k^2 \approx v_k^2 \approx \frac{1}{2}$. For this reason, they are neglected from our considerations.

In order to estimate the superconducting gap, we evaluate the pairing potential $V_z(q)$ in Eq. (6), where $\chi_\Delta^{zz}(q)$ is given by

$$\chi_\Delta^{zz}(q) = \frac{1}{N_0}\sum_k \frac{E_k E_{k+q} - \epsilon_k \epsilon_{k+q} - \Delta_{SDW}^2}{2E_k E_{k+q}(E_k + E_{k+q})}.$$

Δ_{SDW} is determined by the requirement that the orientation fluctuation (spin-wave modes) of the SDW be gapless at $q = Q$. Near half-filling, the spectrum (1) has a quasi one-dimensional structure, i.e., large portions of the Fermi surface are parallel to each other (Fig. 1). Because of this quasi one-dimensional property, $\chi_\Delta^{zz}(q)$ has a logarithmic divergence near a set of nesting vectors Q' given by

$$\mathbf{Q}' = Q\hat{\mathbf{x}}' + q_{y'}\hat{\mathbf{y}}',$$

where $q_{y'}$ is arbitrary. As a consequence of the logarithmic divergence, the pairing potential $V_2(q)$ is strongly enhanced along the line $q_{x'} = 0$. The width of potential with respect to $q_{x'}$ is of order $1/\xi_{SDW}$ (Fig. 2). Since the pairing potential between holes is essentially a constant when the holes are scattered along the Fermi surface in the y' direction, the solution of the superconducting gap equation

$$\Delta_{SCk} = \sum_{k'} V_z(k-k')m^2(k,k')\frac{\Delta_{SCk'}}{\tilde{E}_{k'}}\tanh\frac{\beta\tilde{E}_{k'}}{2}$$

is relatively straightforward. Since the potential is attractive for all momenta, it follows that Δ_{SCk} is nodeless. $\tilde{E}_k$ in the above equation is given by

$$\tilde{E}_k = [(E_k - \mu)^2 + \Delta_{SCk}^2]^{1/2}.$$

The frequency cutoff ω_0, familiar from the conventional phonon interaction, is replaced here by the momentum cutoff normal to the Fermi surface, provided by the product $V_z m^2$. One finds $\omega_0 \sim \Delta_{SDW}$ and

$$\Delta_{SC}(0) \sim \Delta_{SDW}\exp[-1/N(E_{k_F})U^*],$$

where the density of states $N(E)$ is given by

$$N(E) = \frac{\sqrt{2}}{4\pi W}\frac{|E|}{(E^2 - \Delta_{SDW}^2)^{1/2}}$$

and $U^* = V_z m^2 \sim U$ is the strength of the pairing potential near the Fermi surface. The above calculation was carried out in a static SDW backward. However, in analogy with the damping of phonons in conventional superconductors, broadening of spin fluctuations due to domain motion is not expected to alter T_c significantly.

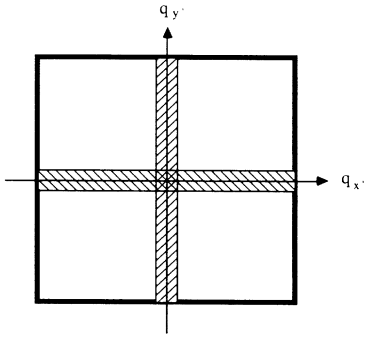

FIG. 2. The potential $V_z(q_{x'}, q_{y'})$ is significantly enhanced in the shaded stripes with a width of order of $1/\xi_{SDW}$.

In conclusion, we have shown how two-dimensional antiferromagnetic spin order over large domains leads to a (pseudo) gap whose value is strongly reduced in the presence of a hole. The resulting bag provides a strong attraction to a second hole over a distance ξ_{SDW} which appears to be sufficiently large enough to lead to high-temperature superconductivity.

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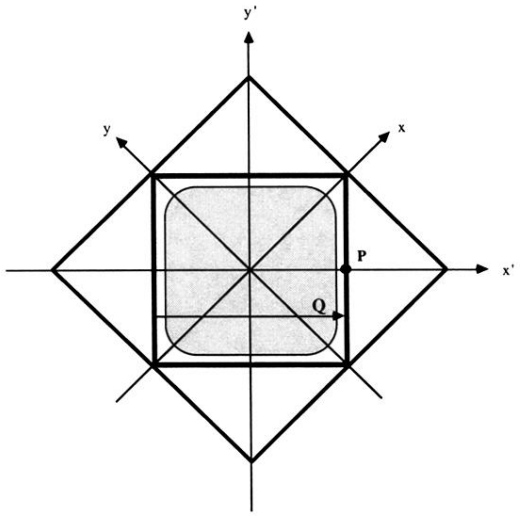

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