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Superconducting pairing of holes in the antiferromagnetic state of the two-dimensional Hubbard model

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The weak-coupling form of the effective interaction between two holes in the antiferromagnetic state of the two-dimensional Hubbard model near half-filling is derived. It is shown to predict a Cooper instability in the singlet d-wave channel, with binding temperature $T_c > 100$ K. Our results differ from those of the "spin-bag" theory of Schrieffer, Wen, and Zhang.

The two-dimensional Hubbard Hamiltonian

$$H = -t\sum_{\langle ij\rangle\sigma} a_{i\sigma}^{\dagger}a_{j\sigma} + U\sum_{i} n_{i\uparrow}n_{i\downarrow}\,, \tag{1}$$

with nearest-neighbor hopping on a square lattice is presently the object of intensive study, motivated by the hope that this model could capture the essential physics of high-T_c superconductors.[1]

In the limit of a half-filled band the weak-coupling theory (Hartree-Fock, hereafter abbreviated as HF) predicts the occurrence of itinerant antiferromagnetism, i.e., the ground state is a spin-density wave with periodicity commensurate with the lattice spacing.[2]

At present, it is not clear whether high-T_c superconductors are better described by a weak- or by a strong-coupling picture. But, if we adopt the weak coupling point of view seriously, we are then obliged to conclude that a better starting point for an analysis of correlation effects is the antiferromagnetic HF (AFM-HF) state, and not the paramagnetic state.[3]

In this paper, we study the effective interaction between two holes added to the half-filled ground state. The diagrammatic analysis of the scattering amplitudes[4,5] is modified to account for the fact that the zero-order wave functions are Bloch waves in the HF state. Our primary purpose is (i) to derive the weak-coupling form of the effective interaction between two holes in the AFM-HF state near half-filling and (ii) to show that, on the basis of this interaction, the weak-coupling theory unambiguously predicts a Cooper instability in the singlet d-wave channel with binding temperature $T_c > 100$ K for reasonable values of the parameters.

Our results differ from those of the "spin-bag" theory of Schrieffer, Wen, and Zhang,[6] which predicts a nodeless superconducting gap in the AFM state. The reasons for this difference will be discussed in the following.

The AFM-HF ground state at half-filling (noninteracting chemical potential $\mu = 0$) has a completely filled valence band v and an empty conduction band c. The band energies are $E_{v\mathbf{k}} = -E_{\mathbf{k}}$ and $E_{c\mathbf{k}} = +E_{\mathbf{k}}$ where $E_{\mathbf{k}} = (\varepsilon_{\mathbf{k}}^2 + \Delta^2)^{1/2}$ and $\varepsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a)$ (a is the lattice spacing). The antiferromagnetic gap Δ is determined by the usual HF self-consistency condition:

$$U^{-1} = \sum_{\mathbf{k}} E_k^{-1}\,. \tag{2}$$

Here and in the following, the momentum sum is over the reduced Brillouin zone: $-\pi/a \le k_x \le +\pi/a$; $-\pi/a + |k_x| \le k_y \le \pi/a - |k_x|$.

The Bolch wave functions for the two bands are

$$\psi_{v\mathbf{k}\sigma}(\mathbf{l}) = L^{-1/2}(\sigma v_{\mathbf{k}} - u_{\mathbf{k}}e^{i\mathbf{Q}\cdot\mathbf{l}})e^{i\mathbf{k}\cdot\mathbf{l}} \tag{3}$$

and

$$\psi_{c\mathbf{k}\sigma}(\mathbf{l}) = L^{-1/2}(u_{\mathbf{k}} + \sigma v_{\mathbf{k}}e^{i\mathbf{Q}\cdot\mathbf{l}})e^{i\mathbf{k}\cdot\mathbf{l}}\,,$$

where $\sigma = +(-)1$ for spin $\uparrow(\downarrow)$, $\mathbf{Q} = (\pi/a, \pi/a)$ is the nesting wave vector, L is the number of lattice sites, and $u_k^2 = (1 + \varepsilon_k/E_k)/2$, $v_k^2 = 1 - u_k^2$.

Let us introduce two holes with opposite momenta in the valence band and study their effective interaction. With the gap equation (2) to guarantee the vanishing of the first-order self-energy insertions, one can easily verify that the perturbation expansion for the scattering amplitude retains the same form as in a genuine two-band semiconductor. The simplest, nonperturbative form for the effective interaction is given by the sum of the "bubble" and "ladder" diagrams shown in Fig. 1.[4,5] The Green's

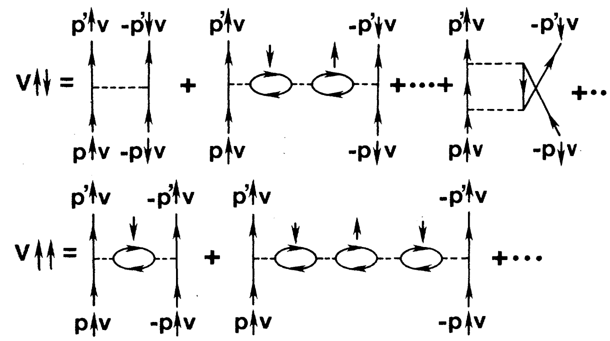

FIG. 1. "Paramagnon-type" diagrams for the effective interaction between valence-band holes in the ↑↓ (singlet + triplet) and ↑↑ (triplet) channels.

function carries a band index $n=c$ or v and the interaction lines represent matrix elements of the Hubbard interaction between the antiferromagnetic wave functions of Eq. (3).

We obtain the following expressions for the effective interaction at half-filling and zero-energy transfer:

$$V_{\uparrow\downarrow}(\mathbf{k},\mathbf{k}')=U\left[\frac{l^2(\mathbf{k},\mathbf{k}')}{1-U^2\chi_\Delta^2(\mathbf{k}-\mathbf{k}')}-\frac{m^2(\mathbf{k},\mathbf{k}')}{1-U^2\chi_\Delta^2(\mathbf{k}-\mathbf{k}'+\mathbf{Q})}\right]+U^2\left[\frac{n^2(\mathbf{k},\mathbf{k}')\tilde{\chi}_\Delta(\mathbf{k}+\mathbf{k}')}{1-U\tilde{\chi}_\Delta(\mathbf{k}+\mathbf{k}')}-\frac{p^2(\mathbf{k},\mathbf{k}')\tilde{\chi}_\Delta(\mathbf{k}+\mathbf{k}'+\mathbf{Q})}{1-U\tilde{\chi}_\Delta(\mathbf{k}+\mathbf{k}'+\mathbf{Q})}\right] \tag{4a}$$

and

$$V_{\uparrow\uparrow}(\mathbf{k},\mathbf{k}')=-U^2\left[\frac{l^2(\mathbf{k},\mathbf{k}')\chi_\Delta(\mathbf{k}-\mathbf{k}')}{1-U^2\chi_\Delta^2(\mathbf{k}-\mathbf{k}')}+\frac{m^2(\mathbf{k},\mathbf{k}')\chi_\Delta(\mathbf{k}-\mathbf{k}'+\mathbf{Q})}{1-U^2\chi_\Delta^2(\mathbf{k}-\mathbf{k}'+\mathbf{Q})}\right], \tag{4b}$$

where

$$\chi_\Delta(\mathbf{q})=2\sum_{\mathbf{k}}\frac{p^2(\mathbf{k},\mathbf{k}+\mathbf{q})}{E_{\mathbf{k}}+E_{\mathbf{k}+\mathbf{q}}} \tag{5}$$

is the longitudinal spin polarizability of the antiferromagnetic state at half-filling and $\tilde{\chi}_\Delta(\mathbf{q})$ is the transverse spin polarizability given by Eq. (5) with the "coherence factor" p replaced by m. The coherence factors are

$$\begin{aligned} l(\mathbf{k},\mathbf{k}')&=u_ku_{k'}+v_kv_{k'}\cong 1\,,\\ m(\mathbf{k},\mathbf{k}')&=u_kv_{k'}+v_ku_{k'}\cong\Delta^2/(\mu^2+\Delta^2)\,,\\ n(\mathbf{k},\mathbf{k}')&=u_ku_{k'}-v_kv_{k'}\cong\mu^2/(\mu^2+\Delta^2)\,,\\ p(\mathbf{k},\mathbf{k}')&=u_kv_{k'}-v_ku_{k'}\cong 0\,, \end{aligned} \tag{6}$$

where the approximate equalities on the right hold when $\mathbf{k}$ and $\mathbf{k}'$ are near the energy line $\varepsilon_{\mathbf{k}}=\mu$. The $\uparrow\downarrow$ interaction contains both the singlet and the triplet scattering amplitudes (parts even and odd in $\mathbf{k}'$, respectively), while in the $\uparrow\uparrow$ interaction only the odd part in $\mathbf{k}'$ is relevant.

We now discuss the physics of the various terms. The second square bracket in Eq. (4a) is the contribution of transverse spin fluctuations and, because of Eq. (6), vanishes in the limit $\mu\to 0$. This means that the spin-wave mode plays essentially no role near half-filling. The expressions $(1-U^2\chi_\Delta^2)^{-1}$ and $U\chi_\Delta(1-U^2\chi_\Delta^2)^{-1}$ in Eqs. (4a) and (4b) can be decomposed as $[(1-U\chi_\Delta)^{-1}\pm(1+U\chi_\Delta)^{-1}]/2$. The first term of the sum is the contribution of longitudinal spin fluctuations, i.e., modulations of the amplitude of the spin-density wave. The second term is the contribution of charge fluctuations. Each contribution appears in two distinct channels, which we denote as the "normal" channel, i.e., the one with momentum transfer $\mathbf{k}-\mathbf{k}'$, and the "umklapp" channel, i.e., the one with momentum transfer $\mathbf{k}-\mathbf{k}'+\mathbf{Q}$.[7] We see that at half-filling the effective interaction between holes of opposite spin is antiperiodic in momentum space, changing sign whenever the nesting wave vector $\mathbf{Q}$ is added. Therefore, any s-wave average of the interaction on the Fermi line vanishes exactly.

Similarly, the p-wave average for parallel spin holes vanishes exactly because the $\uparrow\uparrow$ interaction is periodic with period $\mathbf{Q}$, while the p-wave symmetry factor $g_x(\mathbf{k})=\sin k_xa$ is antiperiodic.[8] Thus, the simplest nonvanishing possibility is given by the symmetry factor $g_{x^2-y^2}(\mathbf{k})=\cos k_xa-\cos k_ya$ which is antiperiodic.

Following a recent treatment by Scalapino, Loh, and Hirsch,[5] we now define the d-wave coupling constant

$$\bar{\lambda}=-\int_{\rm FL}\frac{dk}{|v_k|}\int_{\rm FL}\frac{dk'}{|v_{k'}|(2\pi)^2}g_{x^2-y^2}(\mathbf{k}')V(\mathbf{k}'-\mathbf{k})g_{x^2-y^2}(\mathbf{k})\Big/\int_{\rm FL}\frac{dk}{|v_k|}g^2_{x^2-y^2}(\mathbf{k})\,, \tag{7}$$

where $v_{\mathbf{k}}\equiv\partial E_{\mathbf{k}}/\partial\mathbf{k}$, and $\mathbf{k}$ and $\mathbf{k}'$ are integrated over the Fermi line corresponding to a given band filling set by μ. Just as in Ref. 5 the coupling constant is renormalized by dividing $\bar{\lambda}$ by $1+\lambda_z$ to take into account the wave function and mass renormalizations. The expression for λ_z is similar to Eq. (7) with a symmetry factor $g=1$ and an effective interaction

$$\begin{aligned} V_+(\mathbf{k}-\mathbf{k}')=U^2&\left[l^2(\mathbf{k},\mathbf{k}')\frac{\chi_\Delta(\mathbf{k}-\mathbf{k}')}{1-U^2\chi_\Delta^2(\mathbf{k}-\mathbf{k}')}+m^2(\mathbf{k},\mathbf{k}')\frac{\chi_\Delta(\mathbf{k}-\mathbf{k}'+\mathbf{Q})}{1-U^2\chi_\Delta^2(\mathbf{k}-\mathbf{k}'+\mathbf{Q})}\right]\\ &+U^3\left[n^2(\mathbf{k},\mathbf{k}')\frac{\tilde{\chi}_\Delta^2(\mathbf{k}-\mathbf{k}')}{1-U\tilde{\chi}_\Delta(\mathbf{k}-\mathbf{k}')}+p^2(\mathbf{k},\mathbf{k}')\frac{\tilde{\chi}_\Delta^2(\mathbf{k}-\mathbf{k}'+\mathbf{Q})}{1-U\tilde{\chi}_\Delta(\mathbf{k}-\mathbf{k}'+\mathbf{Q})}\right]. \end{aligned} \tag{8}$$

The effective coupling constant is given by

$$\lambda=\frac{\bar{\lambda}}{1+\lambda_z}\,. \tag{9}$$

Now, although λ and $\bar{\lambda}$ are both divergent (because of the infinite density of states), the ratio $\bar{\lambda}/\lambda_z$ remains finite in the half-filling limit. Furthermore, due to the presence of an extra logarithmic singularity[2] arising from the corners of the Fermi line, we are able to calculate analytically the limit of λ as $\mu\to 0$. We find

$$\lim_{\mu\to 0}\lambda=U\chi_\Delta(\mathbf{Q}) \tag{10}$$

with logarithmic convergence toward the limit. The limiting value of λ as a function of the local magnetic moment $m=(2\Delta/U)\mu_B$ is plotted in Fig. 2. It tends to 1 for small $U(m\to 0)$ and vanishes for large $U(m\to 1)$ as the interband polarizability χ_Δ tends to zero. A crude estimate of the Cooper pair binding temperature is $T_c\simeq\Delta\exp(-1/\lambda)$

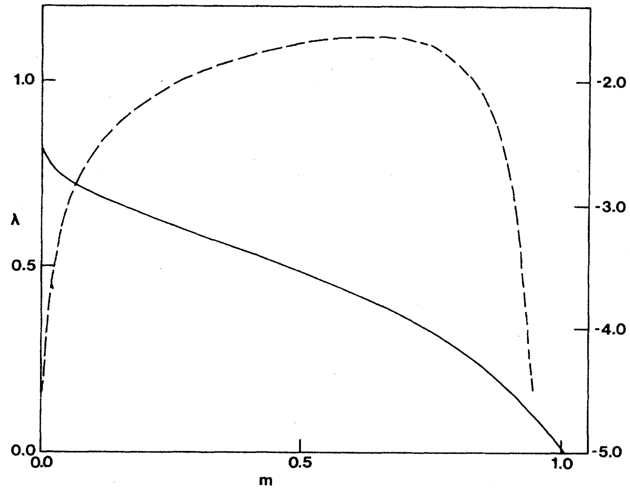

FIG. 2. Effective coupling constant λ and BCS transition temperature $\Delta e^{-1/\lambda}$ as a function of local magnetic moment m (in units of Bohr magneton). m is equal to 0.0, 0.38, 0.69, and 0.93 for $U/t=0$, 2, 4, and 10, respectively.

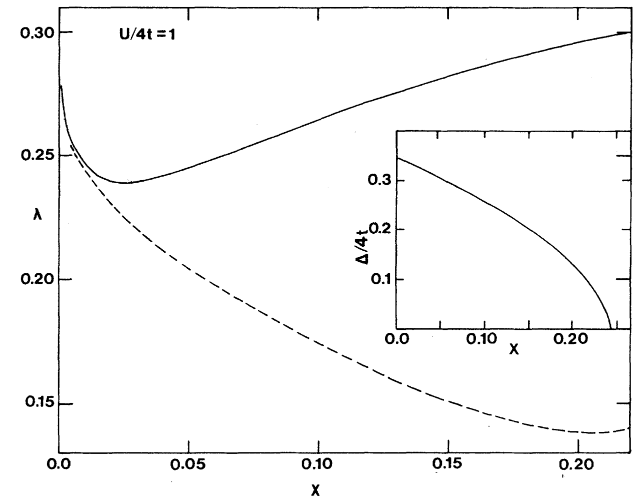

FIG. 3. Effective coupling constant λ as a function of hole concentration. Only interband transitions are included. Dashed line is the result *without* including transverse spin fluctuations. Inset: AFM gap vs hole concentration.

where Δ acts as a high-frequency cutoff for the interaction. (This is substantiated by our calculations of the frequency dependence of the interaction.) The maximum value of $T_c(\sim 0.08t\sim 460$ K for $t=0.5$ eV) is obtained around $U\simeq 3.2t$, $\Delta\simeq t$, and $m=(2\Delta/U)\mu_B\cong 0.6\mu_B$ (see Fig. 2), which is rather close to the experimentally observed value $m\cong 0.5\mu_B^3$.

While the above results predict the existence of a Cooper instability for just two holes in the valence band, it is clear that superconductivity cannot occur at precisely half-filling, since there are no free charge carriers. However, for slightly less than half-filling, whenever a macroscopically large number of holes is present, our results do indicate superconductivity. To substantiate this idea we have calculated numerically the effective coupling constant as a function of hole concentration. The effective interactions and AFM gap are still given by Eqs. (4), (5), and (2), but the momentum sums are now restricted to the occupied states. The integrals in Eq. (7) are performed over the Fermi line corresponding to partial occupation of the valence band. Figure 3 shows λ as a function of hole concentration x at a typical value $U=4t$. At very small values of x, λ extrapolates well to the $x=0$ limit of Fig. 2. In this region λ decreases as a function of x. However, at slightly larger values of x, λ begins to increase due to the switching on of the transverse spin-fluctuation term. This behavior is expected on physical grounds, since spin-wave fluctuations become stronger as the antiferromagnetic gap becomes "softer." (See inset in Fig. 3.) Note that the estimated BCS transition temperature remains quite high ($T_c>100$ K for $t=0.5$ eV) over the whole range of concentrations in which antiferromagnetism is present. The only serious approximation in this calculation was the neglect of intraband transitions within the partly empty valence band. These transitions, if included, would lead to an instability of the AFM state in favor of an incommensurate state which is mathematically difficult to handle. Thus, our point of view has been—as in Ref. 6—to assume that the commensurate state is locked in by some physical mechanism. In this hypothesis, intraband transitions should play essentially no role near half-filling.

Recently, Schrieffer, Wen and Zhang[6] (SWZ) suggested that the exchange of longitudinal spin fluctuations in the AFM background could lead to a *nodeless* superconducting gap. In the present treatment, the "spin-bag" interaction of Ref. 6 is obtained by considering only the umklapp channel in the longitudinal spin-fluctuation term. This part of the interaction is

$$V^{\text{spin bag}}(\mathbf{k}-\mathbf{k}')=-\frac{U}{2}\frac{m^2(\mathbf{k},\mathbf{k}')}{1-U\chi_\Delta(\mathbf{k}-\mathbf{k}'+\mathbf{Q})}\,. \quad (11)$$

In agreement with Ref. 6, it is attractive, independent of spin orientation, and would lead to s-wave pairing. However, our Eq. (4) shows that there is also a "normal" channel contribution which must be treated on equal footing. With both contributions included, the s-wave gap vanishes and a d-wave gap is found instead. Of course this conclusion depends crucially on our Fermi line being assumed close to the large square loop $|k_y|=\pi-|k_x|$. A different form of the hole Fermi line has been recently proposed,[9] which can be mapped into a small circle around one corner of the reduced Brillouin zone. If this were the actual shape of the Fermi line, then only the spin-bag term [Eq. (11)] would dominate and would lead to a nodeless superconducting gap within the circle, in agreement with the original suggestion of SWZ. This possibility has not been considered here.

In summary, the central result of this paper is the derivation of the weak-coupling form of the effective interaction between two holes in the antiferromagnetic state and, particularly, of its antiperiodic momentum dependence which favors d-wave pairing. On this basis we predict (i) coexistence of antiferromagnetism and d-wave superconductivity[10] and (ii) high T_c near half-filling. A preliminary extrapolation of the theory from half-filling indicates that similar features may persist over a wide range of doping concentrations. Thus, the theory does not explain why there is no superconductivity in the oxides for small doping and why antiferromagnetism disappears so rapidly with increasing x. These difficulties are probably related to an insufficient treatment of fluctuations, as they appear also in strong-coupling mean-field theories of the Hubbard model.[11,12]

Note added in proof. After submitting this manuscript we became aware of another paper [Z. Y. Weng, T. K. Lee, and C. S. Ting, Phys. Rev. B **38**, 6561 (1988)] which provides an analysis of the effective interaction between doped holes similar to ours, and reaches similar conclusions about d-wave superconductivity.

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[1]T. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986). For an overview of the recent theoretical literature see *Theories of High-Temperature Superconductivity,* edited by J. Woods Halley (Addison-Wesley, Reading, MA, 1988).

[2]See, for instance, the Hartree-Fock phase diagram calculated by J. E. Hirsch, Phys. Rev. B **31**, 4403 (1985).

[3]Long-range antiferromagnetism with fractional magnetic moment $m \sim 0.5 \mu_B$/Cu *atom* has been observed in La_2CuO_{4-y} by D. Vaknin *et al.* [Phys. Rev. Lett. **58**, 2802 (1987)], and in $YBa_2Cu_3O_{6+x}$ by J. M. Tranquada *et al.* [*ibid.* **60**, 156 (1988)].

[4]G. Vignale and K. S. Singwi, Phys. Rev. B **32**, 2156 (1985).

[5]D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch, Phys. Rev. B. **35**, 6694 (1987).

[6]J. R. Schrieffer, X.-G. Wen, and S.-C. Zhang, Phys. Rev. Lett. **60**, 944 (1988).

[7]This separation into normal and umklapp channels is a special feature of the static interaction at precisely half-filling.

[8]This argument does not apply to the $S_z = 0$ component of the triplet state. However, an explicit calculation with the p-wave average of the $\uparrow\downarrow$ interaction shows that a pairing instability in this channel would have T_c several orders of magnitude lower than the singlet d-wave channel.

[9]J. R. Schrieffer, X.-G. Wen, and S.-C. Zhang (unpublished).

[10]d-wave superconductivity in the presence of strong AF fluctuations has also been predicted by H. J. Schultz, Europhys. Lett. **4**, 609 (1987).

[11]Andrei E. Ruckenstein, Peter J. Hirschfeld, and J. Appel, Phys. Rev. B **36**, 857 (1987); Masahiko Inui, Sebastian Doniach, Peter J. Hirschfeld, and Andrei E. Ruckenstein, Phys. Rev. B **37**, 2320 (1987).

[12]C. Gros, R. Joynt, and T. M. Rice, Z. Phys. B **68**, 425 (1987).