Self-Consistent $d_{x^2-y^2}$ Pairing in a Two-Dimensional Hubbard Model

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Results of a conserving fluctuation exchange calculation for the superconducting state of a two-dimensional Hubbard model are presented. Self-consistent solutions for the full momentum- and frequency-dependent gap, renormalization, and frequency shift parameters have been obtained. The resulting frequency- and momentum-dependent gap is found to have $d_{x^2-y^2}$ symmetry. Below T_c, the maximum gap opens rapidly to a low temperature $2\Delta(0)/kT_c$ value of order 10. We find that the effective interaction arising from the exchange of spin and charge fluctuations is stabilized by self-energy feedback effects as the superconducting gap opens.

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For a one-component theory in which the electronic degrees of freedom provide both the pairing interaction and the pair field, it is essential to treat the system self-consistently. In particular, as the superconducting gap develops it can modify the pairing interaction which in turn alters the gap. In the traditional electron-phonon problem, the change in the lattice dynamics produced by the onset of pairing correlations leads to a negligible change in the pairing interaction. However, in a one-component system where the pairing interaction is mediated by the same electrons which are pairing, the interplay between the pairing interaction and the formation of the gap in the quasiparticle spectrum must be taken into account [1]. Here we study this problem for the case of a two-dimensional Hubbard model. Previous calculations for this model have shown that near half filling, strong, nearly antiferromagnetic fluctuations develop as the temperature is lowered [2–4]. At a critical temperature, these fluctuations lead to an instability in the singlet $d_{x^2-y^2}$ pairing channel, and in this Letter we examine what happens below T_c.

The results which will be described are obtained from a conserving fluctuation exchange approximation [5] in which dressed one-electron Green's functions are used to calculate irreducible spin and charge susceptibilities. These susceptibilities are used to construct a Berk-Schrieffer-like [6] interaction describing the exchange of spin and charge fluctuations. This interaction then provides the basis for calculating the one-electron self-energies. The full momentum and Matsubara frequency dependence of these quantities is kept and the entire calculation is iterated to obtain a self-consistent solution.

The Hamiltonian we will study is given by

$$H=-\sum_{\langle ij\rangle s} t_{ij}(c_{is}^{\dagger}c_{js}+c_{js}^{\dagger}c_{is})+\sum_i U n_{i\uparrow}n_{i\downarrow}. \tag{1}$$

Here $c_{is}^{\dagger}$ creates an electron of spin s on site i, U is an on-site Coulomb interaction, and t_{ij} is equal to t for near neighbors on a square lattice and t' for next near neighbors, giving a one-electron band energy $E_p=-2t(\cos p_x+\cos p_y)-4t'\cos p_x\cos p_y$. For the calculations described below we have taken $t'/t=-0.15$, $U/t=4$, and used a chemical potential μ, which gave a band filling $\langle n_{i\uparrow}+n_{i\downarrow}\rangle=0.875$.

In the superconducting state, the diagonal and off-diagonal one-electron Green's functions can be written as [7]

$$G(p,\omega_n)=\frac{i\omega_n Z(p,\omega_n)+[\varepsilon_p+X(p,\omega_n)]}{[i\omega_n Z(p,\omega_n)]^2-[\varepsilon_p+X(p,\omega_n)]^2-\phi^2(p,\omega_n)}, \tag{2}$$

$$F(p,\omega_n)=\frac{\phi(p,\omega_n)}{[i\omega_n Z(p,\omega_n)]^2-[\varepsilon_p+X(p,\omega_n)]^2-\phi^2(p,\omega_n)}, \tag{3}$$

with $\varepsilon_p=E_p-\mu$. The renormalization parameter $Z(p,\omega_n)$, the energy shift $X(p,\omega_n)$, and the gap parameter $\phi(p,\omega_n)$ are determined by a Berk-Schrieffer-like interaction constructed from the irreducible spin and charge susceptibilities

$$\chi_0^{s,c}(q,\omega_m)=-T\sum_{k,n}[G(k+q,\omega_n+\omega_m)G(k,\omega_n) \pm F(k+q,\omega_n+\omega_m)F(k,\omega_n)]. \tag{4}$$

The plus sign is for the spin susceptibility χ_0^s and the minus sign is for the charge susceptibility χ_0^c. The spin and charge fluctuation interactions are given by

$$V_s=\tfrac{3}{2}U^2\frac{\chi_0^s}{1-U\chi_0^s}-\tfrac{1}{2}U^2\chi_0^s \tag{5}$$

and

$$V_c=\tfrac{1}{2}U^2\frac{\chi_0^c}{1+U\chi_0^c}-\tfrac{1}{2}U^2\chi_0^c. \tag{6}$$

The subtracted terms remove a double counting that occurs in second order. In terms of these interactions, the one-electron self-energies are given by

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$$[1-Z(p,\omega_n)]i\omega_n=\frac{T}{N}\sum_{p'n'}\frac{[V_s(p-p',\omega_n-\omega_{n'})+V_c(p-p',\omega_n-\omega_{n'})]i\omega_{n'}Z(p',\omega_{n'})}{[i\omega_{n'}Z(p',\omega_{n'})]^2-[\varepsilon_{p'}+X(p',\omega_{n'})]^2-\phi^2(p',\omega_{n'})}, \tag{7}$$

$$X(p,\omega_n)=\frac{T}{N}\sum_{p'n'}\frac{[V_s(p-p',\omega_n-\omega_{n'})+V_c(p-p',\omega_n-\omega_{n'})][\varepsilon_{p'}+X(p',\omega_{n'})]}{[i\omega_{n'}Z(p',\omega_{n'})]^2-[\varepsilon_{p'}+X(p',\omega_{n'})]^2-\phi^2(p',\omega_{n'})}, \tag{8}$$

$$\phi(p,\omega_n)=\frac{T}{N}\sum_{p'n'}\frac{[V_s(p-p',\omega_n-\omega_{n'})-V_c(p-p',\omega_n-\omega_{n'})+U]\phi(p',\omega_{n'})}{[i\omega_{n'}Z(p',\omega_{n'})]^2-[\varepsilon_{p'}+X(p,\omega_{n'})]^2-\phi^2(p',\omega_{n'})}. \tag{9}$$

The effect of the Coulomb interaction U on $X(p,\omega_n)$ is simply to provide a constant shift which we have absorbed in μ.

These equations are then solved self-consistently on a 128×128 lattice. The convolutions in momentum space are most efficiently carried out with fast Fourier transforms (FFTs) [8]. When expressed in real space, the equations for $\chi_0^{s,c}$ [Eq. (4)], Z, X, and ϕ [Eqs. (7)–(9)] take a very simple form. The value of $\chi_0^{s,c}$, Z, X, or ϕ at lattice point $\mathbf{x}$ only depends on the value of the diagonal or off-diagonal Green's function and the effective interaction at the same lattice point. On the other hand, the equations relating $\chi_0^{s,c}$ to $V_{s,c}$ and Z, X, ϕ, to G and F are simple in momentum space. The fast Fourier transform allows one to go from real to momentum space with a very small overhead in CPU time. One could also treat the convolution in Matsubara frequency space with FFTs. However, at low temperatures, the memory requirements for a frequency cutoff of several times the bandwidth are prohibitive. Instead, we chose to treat the Matsubara frequencies with a spline interpolation procedure, allowing us to keep track of only a subset of the Matsubara frequencies in the range covered, which for the present calculation was 5 times the bandwidth. The details of the method will be presented elsewhere.

As the temperature is lowered, the spin-fluctuation part of the interaction V_s increases, and at a temperature $T_c=0.021t$, we find a pairing instability. Below this instability, we find a self-consistent solution in which $\phi(p,\omega_n)$ is finite. The solid curve in Fig. 1 shows $\Delta(p,\pi T)=\phi(p,\pi T)/Z(p,\pi T)$ at the lowest Matsubara frequency for $T=0.38T_c$ as p moves along the interacting Fermi surface from one antinode at $p=(0.94,0)\pi$ to another at $(0,0.94)\pi$. The dashed curve is proportional to $\cos p_x-\cos p_y$ and the $d_{x^2-y^2}$ symmetry of the gap is clearly evident.

Using Padé approximates we have analytically continued from Matsubara frequencies to real frequencies, obtaining the complex, frequency, momentum, and temperature-dependent gap

$$\Delta(p,\omega)=\frac{\phi(p,i\omega_n\rightarrow\omega+i\delta)}{Z(p,i\omega_n\rightarrow\omega+i\delta)}. \tag{10}$$

For a given momentum, the gap at the gap edge $\Delta_0(p)$ is given by

$$\Delta_0(p)=\mathrm{Re}\Delta(p,\omega=\Delta_0(p)). \tag{11}$$

The temperature dependence of the magnitude of the gap at the antinode is shown as the solid dots in Fig. 2. Here the dashed curve is the weak coupling BCS result. For

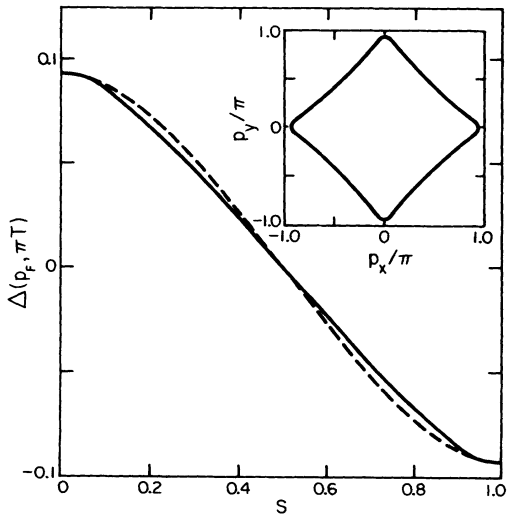

FIG. 1. The solid curve shows the momentum dependence of $\Delta(p_F,\omega_n=\pi t)$ as p_F moves along the interacting Fermi surface shown in the inset. The shape of the noninteracting Fermi surface for the same filling is not very different, with the largest change being near the Van Hove singularity at $(\pi,0)$. All energies are measured in units of t. Here s is parametrized to run along the Fermi surface from one antinode at $(0.94,0)\pi$ to another at $(0,0.94)\pi$. The dashed curve is proportional to $\cos p_x-\cos p_y$.

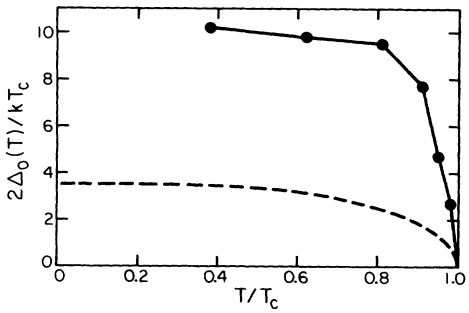

FIG. 2. The temperature dependence of the magnitude of the maximum (antinode) $d_{x^2-y^2}$ gap is shown as the solid dots for a set of temperatures. The dashed curve shows the usual BCS gap. The rapid increase of the $d_{x^2-y^2}$ gap below T_c and its large $2\Delta_0(0)/kT_c$ value are characteristic of a spin fluctuation induced d-wave gap.

conserving approximations of the kind used here, the behavior of the gap near T_c is characterized by the usual mean field exponent.

In order to understand the temperature dependence of the gap shown in Fig. 2, it is necessary to examine the interaction. Just as the coupling parameter λ in the traditional electron-phonon problem characterizes the strength of the interaction, the integral

$$2\int_0^\infty \frac{d\omega}{\pi}\frac{\mathrm{Im}V_s(q,\omega)}{\omega} = \tfrac{3}{2}U^2\frac{\chi_0^s(q,0)}{1-U\chi_0^s(q,0)} - \tfrac{1}{2}U^2\chi_0^s(q,0) \qquad (12)$$

provides a measure of the strength of the spin-fluctuation interaction associated with momentum transfer q. Figure 3 shows a plot of $\chi_0^s(q,0)$ versus q, along the path illustrated in the inset, for various values of the reduced temperature. As expected, the long wavelength spin susceptibility decreases for q values less than the inverse coherence length, reflecting the formation of singlet pairs. Now, if an s-wave gap opened over the entire Fermi surface, the peak in $\chi_0^s(q)$ would also be suppressed. However, for the $d_{x^2-y^2}$ gap found in this calculation, the peak in $\chi_0^s(q)$ at large momentum transfer is essentially unchanged. This behavior is associated with the existence of nodes in the $d_{x^2-y^2}$ gap [9] and the feedback effect of the self-energy. This latter self-energy stabilization is an important example of the feedback that occurs in this strongly correlated one-component system. If $\chi_0^s(q)$ near the peak were to drop, then the interaction V_s would be reduced. This in turn reduces the size of the self-energy leading to an enhancement of $\chi_0^s(q)$. From Fig. 3 we can see how well $\chi_0^s(q)$ is stabilized by the feedback in the large momentum region.

Now, although, as we have seen, the strength of the pairing interaction in the important large momentum transfer region remains essentially constant [10], there is a shift in spectral weight out of the low-frequency region as the gap opens [11]. At T_c, the low-lying spin fluctuations enhance the renormalization factor Z and suppress, via inelastic pair-breaking processes, the gap parameter ϕ. However, as the gap opens and the low-lying interaction spectral weight is reduced, the inelastic pair-breaking processes are suppressed, resulting in an increase in ϕ. In addition, Z is reduced so that $\Delta=\phi/Z$ is increased by both of these effects. The increase of Δ in turn leads to a further suppression of the low-frequency interaction spectral weight, producing a positive feedback. This feedback along with the fact that the interaction strength, Eq. (12), remains essentially constant is responsible for the steep increase of $\Delta_0(T)$ below T_c and the large $2\Delta_0(0)/kT_c$ ratio [12].

In addition to the momentum and temperature dependence of the gap, it is interesting to examine its frequency dependence. From our Padé analysis [13] we find, for p at an antinode on the Fermi surface, the real and imaginary parts of $\Delta(p,\omega)$ shown in Fig. 4(a). The structure at $\omega=2\Delta_0$ reflects structure in the interaction which

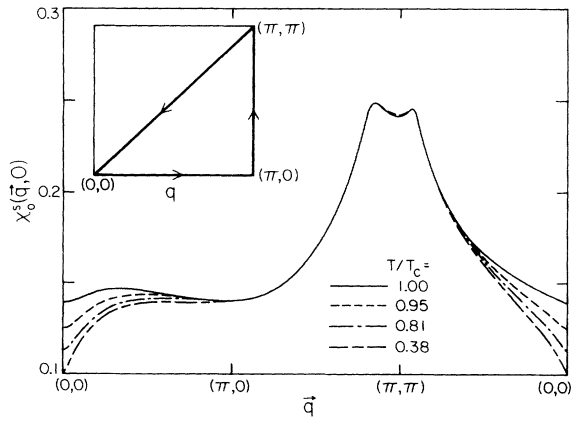

FIG. 3. The irreducible spin susceptibility $\chi_0^s(q)$ for $\omega_m=0$ versus q for various values of T/T_c. The decrease of $\chi_0^s(q)$ for $q\to 0$ reflects the formation of singlet pairs. The stability of $\chi_0^s(q)$ near its peak values is a consequence of the $d_{x^2-y^2}$ nodes and self-energy feedback effects.

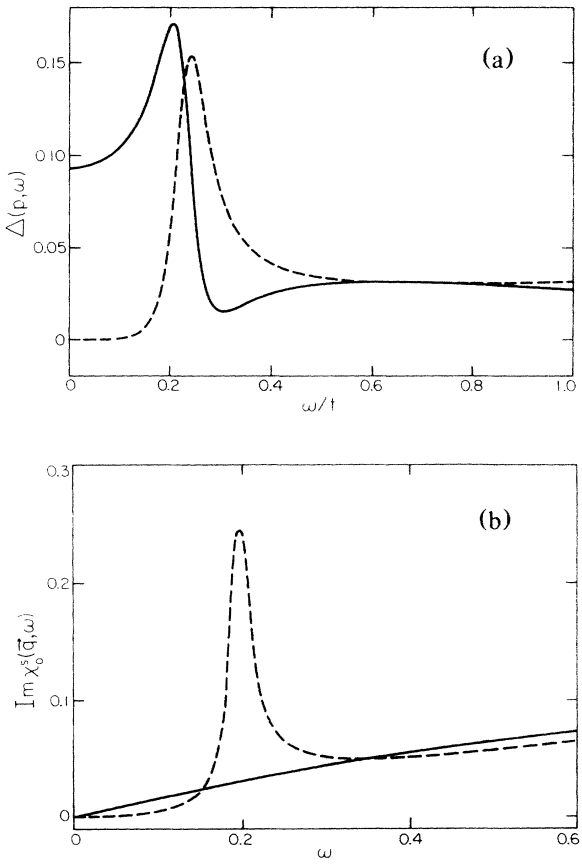

FIG. 4. (a) The real (solid) and imaginary (dashed) parts of $\Delta(p,\omega)$ versus ω for $T/T_c=0.38$ at $p=(0.94,0)\pi$; (b) $\mathrm{Im}\chi_0^s(q,\omega)$ versus ω for $q=(\pi,\pi)$ at $T=T_c$ (solid curve) and $T=0.38T_c$ (dashed curve).

arises from the influence of the gap on the interaction [14]. In Fig. 4(b) we show $\mathrm{Im}\chi_0^\delta(q,\omega)$ versus ω for $q=(\pi,\pi)$ at $T=T_c$ and $T=0.38T_c$. When the $d_{x^2-y^2}$ gap opens, the low-frequency spectral weight decreases as expected and a peak appears near $2\Delta_0$. For a $d_{x^2-y^2}$ gap $\Delta_{p+q}\cong-\Delta_p$ for $q=(\pi,\pi)$ and the coherence factor $(1-\Delta_{p+q}\Delta_p/E_{p+q}E_p)/2$ associated with quasiparticle pair production goes to unity. The peak in $\mathrm{Im}\chi_0^\delta$ marks the onset of pair production and arises from this nonvanishing coherence factor and the overlap of the logarithmic singularities (damped in the dynamic case) at Δ_0 in the single-particle density of states [9].

Thus the interplay between the quasiparticle gap and the interaction in this one-component $d_{x^2-y^2}$ superconductor leads to (1) the stabilization of the strength of the interaction, (2) the rapid onset of the gap below T_c along with a large $2\Delta_0(0)/kT_c$ ratio, and (3) dynamic structure in the frequency dependence of $\Delta(p,\omega)$.

As we have noted, this is a model calculation. We have set the parameters $U/t=4$, $t'/t=-0.15$, and $\langle n\rangle=0.875$ with both the single-layer cuprate $La_{2-x}Sr_xCuO_4$ in mind and to increase T_c in order to have a more numerically accessible T/T_c range. For a bandwidth of 2 eV, the transition temperature $T_c=0.021t$ is of order 60 K. With our choice of parameters, the interaction V_s peaks at the incommensurate momenta $q^*=(\pi,(1-\delta)\pi)$ and $((1-\delta),\pi,\pi)$ with $\delta=0.17$. At T_c, the ratio $V_s(q^*,0)/V_s(0,0)$ is of order 150 and the inverse width of the peak at q^* corresponds to a length of order 10 lattice spacings. As a rough estimate of the compatibility of these parameters with the cuprates, we consider recent neutron scattering data [15] on $La_{1.86}Sr_{0.14}CuO_4$. For this material, measurements of $\chi''(q,\omega)$ give $\delta\simeq0.24$ and a correlation length of order 7 lattice spacings [16]. The low-frequency spectral weight at the peak $\chi''(q^*,\omega)/\omega$ is a factor of 2 smaller than a random phase approximation estimate [17] of $\chi=\chi_0(1-U\chi_0)^{-1}$ using our results [Eq. (4)] for χ_0.

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Note added.—Chien-Hua Pao and N. E. Bickers have carried out conserving fluctuation exchange calculations for the superconducting state of the Hubbard model (Bickers [18]). Lenck, Carbotte, and Dynes [19] have recently solved the Eliashberg equations with a spin-fluctuation interaction based upon a phenomenological form for the spin susceptibility but did not find a superconducting solution when the interaction was self-consistently calculated. We wish to thank N. E. Bickers and J. P. Carbotte for discussing their work with us prior to publication. We also wish to thank S. Quinlan for his insight regarding double counting in the interactions V_s and V_c.

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[12] Chien-Hua Pao and N. E. Bickers [Phys. Rev. B **44**, 10270 (1991)] found that under some circumstances the opening of the $d_{x^2-y^2}$ gap could lead to a weakening of the pairing interaction and, in the absence of dynamic pair breaking, a reduction in the $2\Delta_0(0)/kT_c$ ratio. They also noted that if dynamic inelastic processes were included, $2\Delta_0(0)/kT_c$ could increase over the BCS value.

[13] While numerical Padé continuations are not always reliable, we found that the structure shown in Figs. 4(a) and 4(b) were stable for different Padé orders and believe for this model that they reflect the physical processes described.

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[17] Note, however, that while our calculations for Σ are conserving, one must include vertex corrections in order to maintain a conserving approximation for χ. These vertex corrections will reduce χ.

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