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d-wave pairing near a spin-density-wave instability

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We investigate the three-dimensional Hubbard model and show that paramagnon exchange near a spin-density-wave instability gives rise to a strong singlet d-wave pairing interaction. For a cubic band the singlet ($d_{x^2-y^2}$ and $d_{3z^2-r^2}$) channels are enhanced while the singlet (d_{xy},d_{xz},d_{yz}) and triplet p-wave channels are suppressed. A unique feature of this pairing mechanism is its sensitivity to band structure and band filling.

Pairing interactions for continuum fermion systems with short-range repulsive interactions have been modeled in terms of paramagnon exchange.[1-3] Here the bare single-particle energies are described in terms of an effective mass, and the Fermi surface is spherical. As the strength of the short-range interaction U increases, ferromagnetic correlations are energetically favored, and s-wave pairing is suppressed while p-wave pairing is enhanced. If the magnetic instability occurs at a finite wave vector, it was recently found that both triplet and singlet pairing are suppressed by backscattering.[4] However, in a fermion lattice system the band structure and band filling enter in an essential manner, and it is possible to choose a pair wave function which avoids backward scattering. Monte Carlo simulations of the Hubbard model on a lattice and a strong-coupling expansion have suggested pairing in an even-parity anisotropic state.[5] The purpose of this Rapid Communication is to show, within a paramagnon model on a lattice, that a short-ranged electron-electron repulsion can give rise to even-parity anisotropic pairing near a spin-density-wave (SDW) instability. Emergy has suggested[6] that this type of mechanism may be responsible for pairing in the Bechgaard salts, and recent experiments[7] on UPt_3 suggest a close relationship between SDW Fermi-surface instabilities and superconductivity. As we will show, in a Hubbard model on a cubic lattice a singlet d-wave pairing interaction dominates over a wide range of band filling, and the triplet interaction is significant only at very low band filling.[8]

In the Hubbard model, dimensionless coupling constants characterizing the paramagnon mediated pairing interaction in the singlet and triplet channels are obtained from Fermi-surface averages of the zero-frequency singlet

$$V_s=\frac{U^2\chi_0(\mathbf{p}'+\mathbf{p})}{1-U\chi_0(\mathbf{p}'+\mathbf{p})}+\frac{U^3\chi_0^2(\mathbf{p}'-\mathbf{p})}{1-U^2\chi_0^2(\mathbf{p}'-\mathbf{p})}\ , \tag{1}$$

and triplet interactions

$$V_t=-\frac{U^2\chi_0(\mathbf{p}'-\mathbf{p})}{1-U^2\chi_0^2(\mathbf{p}'-\mathbf{p})} \tag{2}$$

illustrated in Fig. 1. Here $\chi_0(q)$ is the wave-vector dependent susceptibility of the noninteracting band electrons

$$\chi_0(q)=\sum_k\frac{f(\epsilon_{k+q})-f(\epsilon_k)}{\epsilon_k-\epsilon_{k+q}}\ , \tag{3}$$

with $\epsilon_k=-2t(\cos k_x+\cos k_y+\cos k_z)-\mu$ for a cubic lattice. The first term in V_s arises from the particle-hole t matrix, while the second term corresponds to the even bubble screening of the interaction.[9] The triplet interaction V_t in the $s=\pm1$ channels arises from the odd bubble screening of the interaction or equivalently in the $s=0$ channel as the difference between the interactions in Eq. (1).

For a continuum system, one projects the $l=0,2,\ldots$ parts of V_s and the $l=1,3,\ldots$ parts of V_t to obtain the paramagnon coupling constants for $s,d,\ldots$ and $p,f,\ldots$ pairing, respectively. In this case, as is well known, the ferromagnetic nature of the paramagnons favors triplet p-wave pairing. This is also appropriate for a lattice with a small number of electrons in which the Fermi surface is well separated from the Brillouin-zone boundaries and an isotropic effective-mass approximation can be used. However, as more electrons are added to the band and the Fermi surface moves near, or intersects the Brillouin zone, the single-particle energy-band structure modifies the interaction.

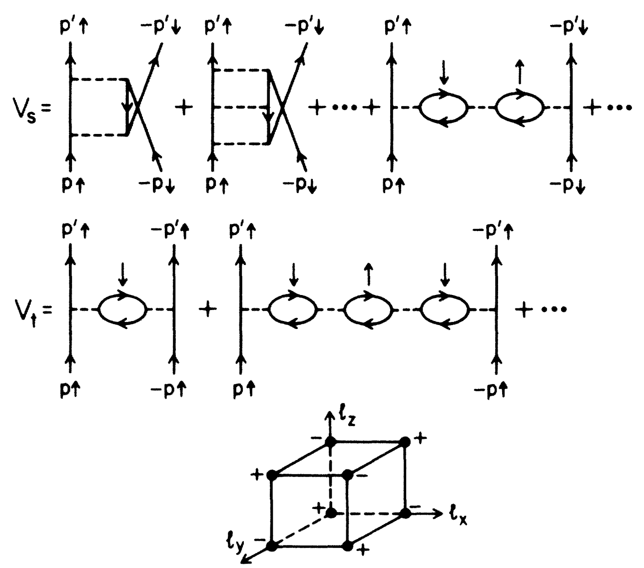

FIG. 1. The paramagnon contributions to the singlet and triplet pairing channels for a Hubbard model. The inset shows the sign of the effective real-space pairing potential for pairs separated by $\mathbf{l}$ sites on the lattice for $\mu=0$.

Figures 2(a)–2(c) show $\chi_0(q)$ plotted along the [1,1,1], [1,1,0], and [1,0,0] directions for different values of μ at a temperature $\beta=4$. Here we measure energies in units where the one-electron transfer integral $t=1$ (e.g., the bandwidth is 12). For $\mu=0$, the Fermi surface has perfect nesting and exhibits an antiferromagnetic peak at $\mathbf{q}=(\pi,\pi,\pi)$, which diverges logarithmically as the temperature goes to zero. As μ decreases, this peak becomes finite and shifts to a value of $\mathbf{q}^*$, corresponding to the momentum spanning the Fermi surface in the [1,1,1] direction. In this case, as U is increased for a fixed filling, the paramagnon interaction diverges at the spin-density-wave instability, where $U\chi_0(q^*)=1$. Finally, for sufficiently small values of μ, the antiferromagnetic peak disappears and $\chi_0(q)$ approaches the usual free-electron (Lindhard) behavior. It is in this latter range of fillings that the paramagnon correlations are ferromagnetic and their exchange can give rise to p wave pairing.

For a general filling it is useful to project out s-, p-, and d-wave coupling constants using simple functions defined on the Fermi surface which are appropriate to a cubic lattice. Thus, for the singlet channel, we define

$$\bar{\lambda}_a=-\int\frac{d^2p'}{|v_{p'}|}\int\frac{d^2p}{|v_p|}g_a(p')V_s(p',p)g_a(p)\Big/\int\frac{d^2p}{|v_p|}g_a^2(p)\ . \tag{4}$$

Here p' and p are integrated over the Fermi surface corresponding to a given band filling set by μ. We have followed the standard practice of putting a minus sign in Eq. (4) so that *positive* values of the couplings will correspond to an attractive pairing interaction. For the singlet channel, we consider s and d waves. Clearly, for the usual s wave with $g_0(p)=1$, the direct Coulomb repulsion will strongly suppress pairing. However, an extended s wave can be constructed which has the form

$$g_{s^*}(p)=A+(\cos p_x+\cos p_y+\cos p_z)\ . \tag{5}$$

If $A=-\mu/2$, the direct Coulomb interaction will not couple to g_{s^*}. For d-wave pairing we use the $d_{x^2-y^2}$ and d_{xy} wave functions

$$g_{x^2-y^2}=\cos p_x-\cos p_y,\quad g_{xy}=\sin p_x\sin p_y\ . \tag{6}$$

The other Γ_{3g} channel $g_{3z^2-r^2}=2\cos p_z-\cos p_x-\cos p_y$ has the same coupling as $g_{x^2-y^2}$, while the other Γ_{5g} channels $\sin p_x\sin p_z$ and $\sin p_y\sin p_z$ have the same coupling as g_{xy}. For the triplet channel, V_s in Eq. (4) is replaced by V_t and, for example, the p_x-wave function is

$$g_x=\sin p_x\ . \tag{7}$$

Just as in the usual electron-phonon theory, the coupling constants are renormalized. We have estimated this by dividing $\bar{\lambda}_a$ by $1+\lambda_z$ to take into account the wave function and effective-mass renormalizations. Here λ_z is given by

$$\lambda_z=\int\frac{d^2p'}{|v_{p'}|}\int\frac{d^2p}{|v_p|}\left[\frac{U^3\chi_0^2(p-p')}{1-U\chi_0(p-p')}+\frac{U^2\chi_0(p-p')}{1-U^2\chi_0^2(p-p')}\right]\Big/\int\frac{d^2p}{|v_p|}\ . \tag{8}$$

Thus the effective coupling constant for a-wave pairing is

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

Figure 3 shows the effective coupling λ for the different pairing configurations versus μ for $U=4$. In this case, the paramagnon propagator exhibits a spin-density-wave instability when μ exceeds -0.8. For μ values just below this, the paramagnon interaction strongly favors singlet $d_{x^2-y^2}$ (or $d_{3z^2-r^2}$) pairing. The extended s-wave coupling, denoted by s^* is also attractive near the SDW instability, but it is significantly weaker than the $d_{x^2-y^2}$ coupling. In this region, the d_{xy} and p_x couplings are repulsive. As μ decreases, moving away from the SDW insta-

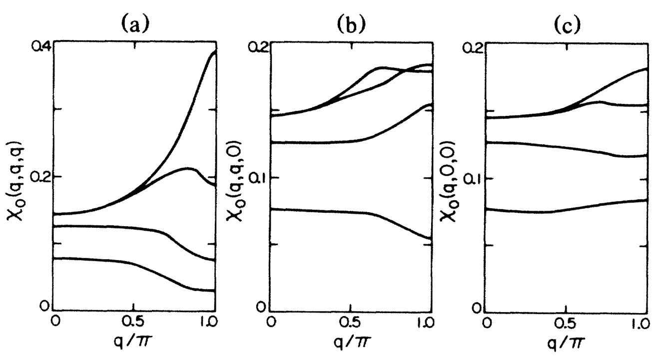

FIG. 2. The susceptibility $\chi_0(q_x,q_y,q_z)$ for a simple cubic band with different fillings plotted along (a) [1,1,1], (b) [1,1,0], and (c) [1,0,0]. The curves on each figure, top to bottom, correspond to $\mu=0$, -1, -2, and -3, respectively.

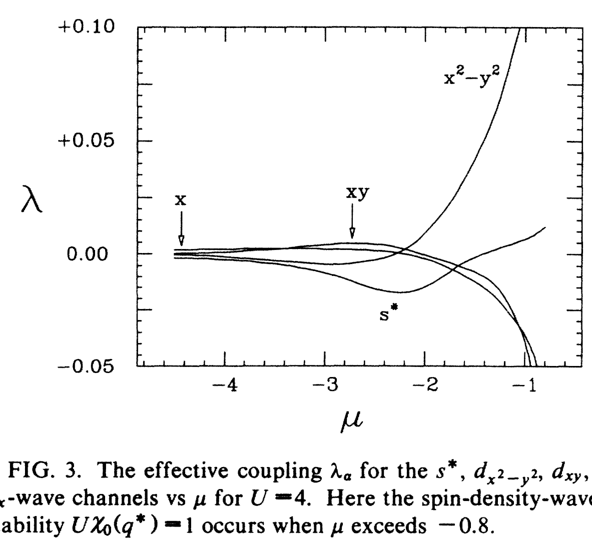

FIG. 3. The effective coupling λ_a for the s^*, $d_{x^2-y^2}$, d_{xy}, and p_x-wave channels vs μ for $U=4$. Here the spin-density-wave instability $U\chi_0(q^*)=1$ occurs when μ exceeds -0.8.

bility, the s^* and $d_{x^2-y^2}$ couplings decrease, becoming repulsive, while the d_{xy} and p_x couplings become attractive. For μ slightly below -2.0, there is a crossover from $d_{x^2-y^2}$ to d_{xy} pairing. At lower fillings where the paramagnon is ferromagnetic, the p-wave channel denoted by x in Fig. 3 is favored. However, in this low filling region with $U=4$, the system is far away from the ferromagnetic instability, so that the p-wave attraction is extremely weak.

Although the interactions given by Eqs. (1) and (2) have $\omega=0$, they arise in the Eliashberg[10] formalism from integrations over ω-dependent spectral weights divided by an energy denominator ω. Their simple real, $\omega=0$, form is just a consequence of the Kramer-Kronig relation. It is useful to keep this in mind, since for values of μ below the SDW instability the interaction $V_s(p',p)$, Eq. (1), is positive definite. However, its Fourier transform can oscillate and the electrons making up a pair can arrange their space-time correlations to fit into the attractive regions.[11] To see this in more detail, consider the pairing interaction for $\mu=0$. From Fig. 2, it is clear that χ_0 peaks at the corners of the Brillouin zone. Dynamic correlations enhance and narrow these peaks in the pairing potentials Eqs. (1) and (2). The Fourier transform of V_s leads to a real-space pairing potential. For μ near 0, this real space pairing potential is approximately given by

$$\frac{3}{2}\frac{U^2\chi_0^*}{1-U\chi_0^*}e^{-(l^2/l_0^2)}[\cos(\pi l_x+\pi l_y+\pi l_z)+\cos(\pi l_x-\pi l_y-\pi l_z)+\cos(\pi l_x+\pi l_y-\pi l_z)+\cos(\pi l_x-\pi l_y+\pi l_z)] \ , \tag{10}$$

where $l_0^2 \sim (1-U\chi_0^*)^{-1}$ with $\chi_0^*=\chi_0(\pi,\pi,\pi)$. The staggered structure of this potential is illustrated in the inset of Fig. 1. It is repulsive for zero pair separation $\mathbf{l}=0$, attractive for a near-neighbor separation, repulsive for a next-near-neighbor separation, etc. It is clearly attractive for $(d_{x^2-y^2},d_{3z^2-r^2})$ pairing, less so for s^* pairing, and repulsive for (d_{xy},d_{yz},d_{xz}) pairing.

Now, just as for ^{3}He, the simple paramagnon theory cannot provide definitive results. Rather it suggests possible phenomenological relations. In particular, the occurrence of a strongly enhanced singlet d-wave coupling mediated by spin fluctuations near an SDW instability provides a framework for thinking about some of the heavy-fermion superconductors such as UPt_3 and the Bechgaard salts ditetramethyltetraselenafulvalene$X$. The strong interplay of band structure, band filling, and many-body effects appears in a natural manner reflecting the role of Fermi surface nesting on the pairing interactions. The effect of pressure can clearly alter the one-electron transfer matrix elements which directly affect the band structure and this nesting. Once the band structure and μ are fixed, one coupling constant U determines both the SDW and pairing responses. This unified theory should provide important constraints for the competition and possible coexistence of the SDW and pairing phases.[12]

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