Pairing due to the exchange of magnetic fluctuations in cuprate superconductors

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The possibility for a superconducting instability due to the exchange of magnetic fluctuations is studied by means of low-density expansion. It is shown that if the magnetic fluctuations are centered at $(\pi, \pi)$, they uniquely favor $d_{x^2-y^2}$ superconductivity close to the magnetic instability no matter at which doping concentration this instability occurs. However, if the magnetic fluctuations are centered around the incommensurate $(\pi(1-\delta), \pi)$ point in the Brillouin zone, they tend to suppress any type of superconductivity.

One of the most striking features of high-$T_c$ materials is the proximity of antiferromagnetic and superconducting phases. NMR, neutron, and Raman scattering experiments have established that antiferromagnetic fluctuations are present both in normal and superconducting states of cuprate oxide compounds. Antiferromagnetic fluctuations were shown to account for the number of unusual normal-state properties of these materials, in the first place, for the measured non-Korringa-temperature behavior of the $^{63}$Cu relaxation rate. Less is known about the influence of magnetic fluctuations on the transition into a superconducting state. A conventional paramagnon theory predicts $d$-wave pairing with $\Delta \sim \cos k_x - \cos k_y$ close to the magnetic transition. The same type of instability was also found in a more sophisticated approach with the phenomenological form of the magnetic susceptibility known to fit the NMR data in the normal state. Another currently discussed possibility is a spin-bag mechanism of $s$-wave-like superconductivity due to attractive interaction between the two holes sharing the same region with the reduced antiferromagnetic order.

Two crucial assumptions lie behind these approaches. First, the magnetically ordered state was proposed to be commensurate with the ordering momenta $Q=(\pi, \pi)$, and second, the magnetic transition was predicted to occur near half-filling, and as a consequence, the ordering momenta was supposed to link the particles very near the Fermi surface. For small coupling these assumptions are definitely correct. However, for moderate couplings the momenta of the magnetic instability should not be directly related to the maximum transferred momenta at the Fermi surface. From this point of view, the fact that the antiferromagnetic fluctuations are strong and the static susceptibility is peaked near $(\pi, \pi)$ is crucial for the understanding of the normal-state properties, especially NMR experiments, but is probably less important for the problem of superconductivity since the particles at the Fermi surface probe the susceptibility at smaller momenta, which in the general case lie relatively far from the peak.

On the other hand, recent inelastic-neutron-scattering experiments on La$_{1.9}$Sr$_x$CuO$_4$ (Ref. 3) indicate that for moderate doping concentrations magnetic fluctuations are centered around $(\pi, \pi(1-\delta))$ and $(\pi(1-\delta), \pi)$ rather than near $(\pi, \pi)$; i.e., short-range commensurate magnetic order is substituted by an incommensurate one upon doping. This is qualitatively consistent with the theoretical calculations for the Hubbard model. The values of $\delta$ were reported to increase with the doping concentration: $\delta=0.14$ for $x=0.075$ and $\delta=0.24$ for $x=0.14$. Though the situation with the interpretation of the experimental data is far from being conclusive (the short-range incommensurate ordering seems to be incompatible with the NMR data, especially for the oxygen relaxation in the normal state), it seems interesting to address the question of whether the incommensurate spin fluctuations favor any type of superconducting instability.

In the present paper, I address this issue. I argue that if the magnetic fluctuations are centered at $(\pi, \pi)$, they uniquely favor $d_{x^2-y^2}$ superconductivity close to the magnetic instability no matter at which doping concentration this instability occurs. However, if the magnetic fluctuations are centered around the incommensurate $(\pi(1-\delta), \pi)$ point in the Brillouin zone, they suppress any type of superconductivity, at least if the maximum transferred momentum at the Fermi surface is not very close to the ordering momenta of the magnetic system.

I use a conventional one-band approach and assume that close to magnetic instability the dominant interaction between fermions is the exchange of magnetic fluctuations. In this case the effective interaction between the particles at the Fermi surface is measured by the momentum- and frequency-dependent susceptibility of the magnetic system, $\Gamma(q, \omega) = 3\alpha^2 \chi(q, \omega)$ for even channels and $\Gamma(q, \omega) = -\lambda^2 \chi(q, \omega)$ for odd channels, where $\lambda$ is a coupling constant (in the Hubbard model, $\lambda = U/2$).

For moderate $U$ the magnetic instability occurs relatively far from half-filling. In this case the maximum transferred momenta is definitely smaller than $(\pi, \pi)$. However, the momenta of a magnetic instability can be
either equal or close to \((\pi, \pi)\); in both cases it is located outside the Fermi surface. Close to a transition, the correlation length \(\xi\) is large. Hence the dominant contribution to the pairing interaction comes from those values of \(q\) which deviate from the ordering momenta at distances which are larger than \(\xi^{-1}\). For these \(q\) the susceptibility of a paramagnet nearly coincides with that for the ordered system:

\[
\chi(q) = \frac{1}{2} \frac{1}{J_q - J_Q},
\]

(1)

where \(Q\) is the ordering momenta and \(J_q\) stands for the Fourier component of the exchange integral. The relative difference between the susceptibility of a paramagnet and Eq. (1) scales as \((q\xi)^{-2}\), where \(q\) is measured from \(Q\).

In writing Eq. (1), I neglected the frequency dependence of the susceptibility, which is consistent with a weak-coupling approach presented here.\(^\text{12}\)

The next thing one should do is to find the expressions for \(J_q\) consistent either with \((\pi, \pi)\) or \((\pi(1-\delta), \pi)\) magnetic ordering. For commensurate ordering the simplest possibility is to consider the nearest-neighbor Heisenberg interaction with \(J_q = J (\cos k_x + \cos k_y)\) and \(J_Q = -2J.\)\(^\text{13}\)

The situation with incommensurate ordering is more subtle. Various studies of the Hubbard (or \(t-J\) models\(^\text{5,14}\) predict magnetic incommensurability away from half-filling. The existing scenario of the transition\(^\text{15}\) involves a softening of the collective excitations of holes rather than of spin waves, and the susceptibility in the incommensurate phase is given by a complicated expression which is difficult to analyze. On the other hand, the calculated \(\chi(q)\) fits the general symmetry requirements for a disordered incommensurate antiferromagnet; i.e., it has four equivalent maxima at \((\pi, \pi)\) and \((\pi, \pm Q)\). In view of this, it seems reasonable to model the actual susceptibility in an incommensurate phase by that for a simple magnetic system which has \((\pi, \pi(1-\delta))\) ordering and which susceptibility is given by Eq. (1) for all \(q\) measured as a shift from \(Q\) which are larger than \(\xi^{-1}\). The model of this kind is a well-studied \(J_1-J_2-J_3\) model which involves the interactions between first \((J_1)\), second \((J_2)\), and third \((J_3)\) nearest neighbors.\(^\text{16}\)

Without zero-point fluctuations, the \((Q, \pi)\) phase with varying \(Q = \cos^{-1}((2J_2-J_1)/2J_1)\) is located between three lines in the parametrical space \(2J_2+4J_3 = J_1, 2J_2-4J_3 = J_1, \) and \(2J_3 = J_2\) (Fig. 1). I will use the susceptibility of this model given by Eq. (1) with

\[
J_q = J_1 (\cos k_x + \cos k_y) + 2J_2 \cos k_x \cos k_y
\]

and \(J_Q = -J_1 - (2J_2-J_1)^2/8J_3\) to model the actual interactions governed by the short-range incommensurate \((\pi(1-\delta), \pi)\) magnetic ordering. Note that though the choice of the model is chiefly dictated by the reasons of simplicity, the \(J_2\) and \(J_3\) interactions are generated by the next-to-leading-order terms in the strong-coupling expansion of the Hubbard model.\(^\text{17}\)

A conventional way to study the possibility for a pairing instability is to expand the effective interaction in the eigenfunctions of the corresponding space group of the lattice and to check whether the interaction is attractive at least in a single channel. For the two-dimensional (2D) square lattice, the \(D_4\) space group is known to contain four one-dimensional (singlet) irreducible representations (two for \(s\)-waves, \(A_1\) and \(A_2\), and two for \(d\) waves, \(B_1\) and \(B_2\)) and one two-dimensional representation \((E)\), which corresponds to triplet pairing.\(^\text{18}\)

An arbitrary eigenfunction in each representation then can be written as a product of the corresponding basic eigenfunction \([\cos k_x + \cos k_y\) for \(A_1, \cos k_x - \cos k_y\) for \(B_1, \sin k_x \sin k_y\) for \(B_2, (\cos k_x - \cos k_y) \sin k_x \sin k_y\) for \(A_2,\) and \(A \sin k_x + B \sin k_y\) for \(E)\] and a representative from a complete set of functions which have the whole \(D_4\) symmetry. In the polar coordinates \((|k|, \phi)\), the sequences of eigenfunctions can be rewritten as

\[
A_1: \cos 4n \phi; \quad A_2: \sin 4n \phi; \quad B_1: \cos(4n + 2) \phi; \quad B_2: \sin(4n + 2) \phi; \quad E: A \sin(2n + 1) \phi + B \cos(2n + 1) \phi.
\]

(3)

An obvious advantage of using the eigenfunctions of the space group of the problem is that in solving the gap equation one can decouple between the eigenfunctions from different irreducible representations. However, in the absence of continuous rotational symmetry, the decoupling between different harmonics from the same irreducible representation survives only in the low-density limit, when the characteristic momenta are small and one can neglect the angular dependence of the density of states in the Cooper channel. Otherwise, it is necessary to solve the matrix equation for the gap wave function.
Working along these lines, Monthoux, Balatsky, and Pines' (MBP) solved numerically the reduced integral equation with the phenomenological form of the susceptibility peaked at $(\pi, \pi)$ and found the instability against $d_{x^2-y^2}$ pairing. In what follows I use the alternative approach and study the possibility for a pairing instability in the frameworks of the low-density (i.e., low-$q$) expansion for the effective interaction. In this case the density of states at the Fermi surface is nearly angular independent and the Cooper problem can be solved exactly by perturbative expansion in powers of the Fermi momenta. Indeed, the low-density approach can be well justified only if the magnetic transition occurs far from half-filling.

Obviously, the conventional $s$-wave pairing is suppressed in the low-$q$ approach simply because the interaction given by Eq. (1) is repulsive. The situation with unconventional pairing is, however, more subtle. Indeed, in the leading order in the density, $q^2 \sim \frac{\left[1 + \cos(\phi - \phi')\right]}{8}$, where $\phi$ and $\phi'$ measure a shift from the $x$ axis for incoming and outgoing momenta on a Fermi surface. It then immediately follows from Eq. (3) that one should expand the effective interaction $\Gamma(q) \sim \chi(q)$ at least up to $q^2$, $q^4$, and $q^6$ terms to study the possibility for $p$-wave, $d$-wave (with $B_1$ or $B_2$ symmetry), and unconventional $s$-wave ($A_2$) instabilities, respectively.

The general form of the low-$q$ expansion for the static susceptibility for the 2D square lattice reads

$$\Gamma(q) = A + B(q^2 + (qa)^4(C_1 + C_2 \cos 4\phi) + (qa)^6(D_1 + D_2 \cos 4\phi) + (qa)^8(E_1 + E_2 \cos 4\phi + E_3 \cos 8\phi) + O((qa)^{10}),$$

where $q_x = q \cos \phi$ and $a$ is the lattice constant. For a tight-binding form of the quasiclassical expression, $\varepsilon_n = -2t(\cos k_x a + \cos k_y a) - \mu$, one then obtains for the effective interaction in different channels,

$$\Gamma_E = 2\lambda^2 (ap_F)^2 [B + 4(ap_F)^2C_1] + O(ap_F)^6,$$

$$\Gamma_{B_1} = 6\lambda^2 (ap_F)^4 \left[ (C_1 + 2C_2) \left( 1 + \frac{7(ap_F)^2}{48} \right) + 2(ap_F)^2(3D_1 + 5D_2) + O(ap_F)^4 \right],$$

$$\Gamma_{B_2} = 6\lambda^2 (ap_F)^4 \left[ (C_1 - 2C_2) \left( 1 + \frac{5(ap_F)^2}{48} \right) + 2(ap_F)^2(3D_1 - 5D_2) + O(ap_F)^4 \right],$$

$$\Gamma_{A_2} = 6\lambda^2 (ap_F)^8 [(E_1 - 3E_2) + \cdots],$$

where $(ap_F)^2 = 4 + \mu/t$ is the small parameter in the low-$q$ expansion.

For antiferromagnetic interaction, $p$-wave superconductivity is always suppressed (i.e., $B > 0$), and in what follows I will focus on $d$-wave pairing. For the nearest-neighbor $(\pi, \pi)$ antiferromagnet, the expansion of Eq. (1) up to $q^4$ leads to

$$C_1 = -3C_2 = \frac{1}{8} - \frac{1}{128}.$$  (6a)

It then immediately follows from Eq. (5) that while $d_{xy}$ superconductivity is definitely suppressed ($C_1 - 3C_2 = 2C_2 > 0$), $C_1 + 3C_2 = 0$, and one should pass to the next-order terms in the expansion in $(ap_F)^2$ to check the possibility for $d_{x^2-y^2}$ instability. The expansion up to $q^6$ then yields

$$D_1 = \frac{5}{12} D_2 = \frac{1}{8} - \frac{1}{4608}.$$  (6b)

Hence $3D_1 + 5D_2 < 0$, and it follows from Eq. (5) that the system is unstable against $d_{x^2-y^2}$ pairing no matter where the magnetic instability occurs. The explicit solution of the Cooper problem then yields

$$T_c = \omega_0 \exp \left[ -\frac{1}{g} \right],$$  (7a)

where $\omega_0$ has the order of the spin-wave energy at the maximum transferred momenta on the Fermi surface and

$$g = \frac{1}{8}(3\lambda^2 \chi_0)(ap_F)^6 \frac{128\pi}{128\pi},$$  (7b)

where $\chi_0 = 1/8J$ is the uniform static susceptibility of an antiferromagnet and $(ap_F)^2 = 4 + \mu/t$.

For the incommensurate $(\pi, \pi(1 - \delta))$ spin fluctuations, the calculation of the $d$-wave vertices leads to different results. Now the expansion of Eq. (1) up to $q^4$ gives

$$C_1 = \frac{1}{256 A^2} [4J_1 + 2J_2 + 4J_3]^2 - A(J_1 + 4J_2 + 16J_3)] = \frac{1}{256 A^2} (J_1 + 4J_2 + 16J_3),$$  (8)

where

$$A = \frac{1}{2}J_1 + J_2 + J_3 + \frac{4J_2 - J_1}{16J_3}.$$  (9)

One can immediately make sure that in a whole region of the $(\pi, \pi(1 - \delta))$ phase, both $d$-wave vertices are positive and thus no superconducting instability is expected to occur close to the magnetic transition into the incommensurate state. For completeness, I also investigated the possibility for unconventional $s$-wave instability and found that for the values of $\delta$ related to the experiments the corresponding partial amplitude is positive; that is, unconventional $s$-wave pairing is also suppressed by the incommensurate spin fluctuations.

The suppression of the $d$-wave superconductivity by the $(\pi, \pi(1 - \delta))$ spin fluctuations has a natural physical explanation. Indeed, in the limiting case of $\delta = 1$, the exchange of magnetic fluctuations favors $d_{xy}$ rather than $d_{x^2-y^2}$ superconductivity since the interaction peaked at
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$(\pi,0)$ links two neighboring maxima of the gap wave function with $d_{xy}$ symmetry. The positiveness of the $C_1$ term in Eq. (8) then signifies that, at least at low density of carriers, the two $d$-wave channels cannot be attractive simultaneously. In this case the transition between the $d_{x^2-y^2}$ and $d_{xy}$ superconducting states necessarily occurs in two steps and involves the intermediate normal metallic phase. This is indeed what was found in the calculations. Note that the situation would be completely different if the magnetic fluctuations were centered around the incommensurate point along the diagonal in the Brillouin zone, $(\pi(1-\delta), \pi(1-\delta))$. For $J_1-J_2-J_3$ model, this is the case when the $J_3$ coupling is large. For the incommensurability along the diagonal, the momenta close to the peak in $\chi(q)$ obey $q_x^2 \approx q_y^2$ and thus continue to link the neighboring maxima of the gap wave function with the $d_{x^2-y^2}$ symmetry. Consequently, for a given $\mu$, the critical temperature of the $d_{x^2-y^2}$ instability should grow up rather than fall down with the degree of incommensurability since, when $\delta$ increases, the momenta of the magnetic instability only becomes closer to the characteristic transferred momenta at the Fermi surface.

While the qualitative changes in the $d$-wave vertices with the degree of incommensurability can be predicted on general grounds, one needs more effort to find the precise location of the phase boundaries. In the low-$q$ expansion, the normal state takes up the whole region of the $(\pi, \pi(1-\delta))$ phase. On the other hand, if the magnetic transition occurs very near half-filling, the $d$-wave instability is definitely present in the whole region of the $(\pi, \pi)$ and $(\pi,0)$ states. In this case the small shift from $\delta=0$ or 1 should not change significantly the attractive interaction in the $d_{x^2-y^2}$ or $d_{xy}$ channels, respectively.

To find the location of the superconducting $d_{x^2-y^2}$ phase for various $ap_F$, I have studied how the interactions away from nearest neighbors modify the vertex function in the $d_{x^2-y^2}$ channel inside the region of the $(\pi, \pi)$ phase. For $J_1-J_2-J_3$ model, the stability of the $(\pi, \pi)$ phase is confined to $4J_1+2J_2<J_3$ (Fig. 1). Within this region the susceptibility is peaked at $Q=(\pi, \pi)$ and the low-$q$ expansion of Eq. (1) as in Eq. (2) and $J_Q=-2J_1$ yields, in the leading order in the density,

$$\Gamma_{B_2} = \frac{3a^2}{128J_1^2} \left[ J_2 - 2J_3 + \frac{(J_3+2J_1)^2}{J_1} \right] (ap_F)^4. \quad (9)$$

The transition line $\Gamma_{B_2}=0$ divides the $(\pi, \pi)$ region into normal and superconducting phases. As expected, the superconducting instability becomes stronger when the $J_3$ interaction prevails, while the $J_2$ exchange tends to suppress $d_{x^2-y^2}$ superconductivity. The finite-density corrections lead to the enlargement of the region of the superconducting state, which for finite $ap_F$ should also include the pure Heisenberg model. I expanded $\Gamma(q)$ up to $q^2$ and calculated the boundary line between superconducting and normal phases in the first three orders in $(ap_F)^2$. For $J_3=0$ the critical coupling $J_2$, which destroys $d_{x^2-y^2}$ superconductivity, reads

$$J_2 = \frac{1}{16} \left[ 1 + 0.26 (ap_F)^2 + \cdots \right]. \quad (10a)$$

At the same time, along the boundary line $2J_2+4J_3=J_1$, $d_{x^2-y^2}$ superconductivity survives up to

$$J_2 - \frac{J_1}{8} = 3J_1 \frac{(ap_F)^2}{16} \frac{1}{1 + 8.9 (ap_F)^2}. \quad (10b)$$

The actual boundary of the superconducting phase calculated for $(ap_F)^2=3$, related to the experiments, is given by the solid line in Fig. 1. One can see from the figure that the normal state continues to occupy the whole region of the incommensurate $(\pi, \pi(1-\delta))$ phase even after the finite-density corrections are taken into account. However, the series in $ap_F$ do not converge well, and the continuation of the results of the small-$ap_F$ expansion to $(ap_F)^2=3$ should be taken with caution.

To summarize, in this paper, I addressed the question of whether the exchange of magnetic fluctuations close to the magnetic transition can lead to a superconducting instability. I considered the case when the magnetic instability occurs relatively far from half-filling and found that the fluctuations are centered around $(\pi, \pi)$, they uniquely lead to a transition into the $d$-wave superconducting state with $d_{x^2-y^2}$ symmetry of the gap wave function. However, if the magnetic fluctuations are centered around $(\pi, \pi(1-\delta))$ (this was reported to be the case for Lu2-xSrxCuO4 compounds), they suppress any type of superconductivity, at least if the maximum transferred momenta at the Fermi surface is not very close to the ordering momenta of the magnetic system.

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1S. E. Barrett et al., Phys. Rev. B 41, 6283 (1990), and references therein.


10. D. Pines and D. Thelen (private communication); C. P. Slichter (private communication).
12. In a general case, the use of Eq. (1) for a paramagnet requires symmetrization since incommensurate \((\pi, Q)\) ordering breaks \(Z_2\) symmetry of \(X\rightarrow Y\). However, for \(J_e\) given by Eq. (2), this problem does not arise since \(J_e\) is already symmetric with respect to \(X\rightarrow Y\). This peculiarity of a quasiclassical susceptibility of the \(J_1-J_2-J_3\) model is a reason for a well-studied “order from disorder” phenomenon.
20. The two-step transition between \(d_{x^2-y^2}\) and \(d_{xy}\) states was also found in the 2D Hubbard model at low density of carriers: A. V. Chubukov and J. P. Lu (unpublished).