s pairing as a result of antiferromagnetic fluctuations in a high-T_c superconductor

V. S. Babichenko and Yu. Kagan
Kurchatov Institute Russian Science Center, 123182, Moscow, Russia

(Submitted 20 August 1992)
Pis'ma Zh. Eksp. Teor. Fiz. **56**, No. 6, 305–310 (25 September 1992)

Carrier scattering due to an exchange of antiferromagnetic fluctuations leads to an s pairing if the antiferromagnetic momentum satisfies $k_0 > 2p_F$. The quasicritical nature of the fluctuations gives the effective superconducting coupling constant a value $\lambda \sim 1$.

1. Various properties of high-T_c superconductors—the behavior of the specific heat, the temperature dependence of the penetration depth, the relatively high unsampled current in a ring made of high-T_c (or ordinary) superconductor, the comparatively low sensitivity of T_c to defects, etc.—seem to indicate an s pairing in these systems. On the other hand, recent experiments have revealed that strong antiferromagnetic fluctuations play an important role, for all the high-T_c compounds. In the present letter we show that there is a comparatively general mechanism for the interaction of electrons with antiferromagnetic fluctuations which results in an s pairing with a fairly large coupling constant. A factor of decisive importance here is the predominant phase-space localization of the spectral density of the antiferromagnetic fluctuations in the metallic phase near the vector $\bar{\mathbf{k}}_0$, which is characteristic of an antiferromagnetic order in the CuO_2 plane in the insulating phase. This circumstance has been demonstrated particularly clearly in neutron-scattering experiments (e.g., Refs. 1–3) and through a comparison of measurements of the spin relaxation and the Knight shift at Cu nuclei (e.g., Refs. 4–9). The difference between the spin relaxation at Cu and that at O^{17} has constituted independent evidence regarding the nature of the distribution of the spectral density of antiferromagnetic fluctuations.[9,10]

Let us assume that the carrier density in the metallic phase is low and that the condition $2p_F \ll k_0$ holds. In this case, the scattering of electrons by each other through the exchange of a single spin excitation moves the electron (or hole) far away from the Fermi surface. As a result, the contribution of this process to the effective seed vertex in the Cooper channel is suppressed. This vertex is then determined by the exchange of at least two spin excitations. As we will see below, the results are an attraction in the singlet channel and an s pairing occur as a result. In the case of a large Fermi surface, the vectors $\bar{\mathbf{k}}_0$ may link discrete points on the surface, and the scattering of electrons in the Cooper channel accompanied by a transition between narrow regions near these points will be determined by the exchange of a single-spin excitation. Elsewhere on the Fermi surface, on the other hand, the scattering will again be determined by the exchange of two-spin excitations. The general solution of the problem in this case again leads to a singlet pairing with a complex angular dependence of the superconducting gap. An important point, however, is that the s component of the order parameter is nonzero and thereby guarantees that there is only a limited sensitivity to nonmagnetic impurities.

To make the discussion as clear as possible, we restrict the analysis to the case of a small Fermi surface.

We assume below that a strong Hubbard repulsion is operating at the Cooper ions. As a result, the half-filled band splits into two subbands, and an insulating antiferromagnetic state arises. The free carriers are formed either in the oxygen subband (in which case the carriers are holes) or in the upper Hubbard subband (electrons). We assume that when the doping level is comparatively low, the lower filled subband retains its individuality, and the carriers interact with a spin liquid having strong antiferromagnetic fluctuations. This model has been used widely (see, for example, Ref. 11–13).

In the formal analysis, we take the approach that the antiferromagnetic fluctuations in phase regions near $\bar{\mathbf{k}}_0$ are of a quasicritical nature. The disruption of the long-range order even at a very low carrier density, combined with the condition $T_c \ll \omega_0$ (ω_0 is a characteristic energy of the antiferromagnetic interaction), makes this assertion almost obvious, at least if the carrier density is limited.

An analysis of antiferromagnetic fluctuations and of the interaction with them in this model is quite different from an analysis of these fluctuations in a single-band model with a weak Hubbard interaction and an approximately half-filled band. This model apparently always leads to a depairing (see Refs. 4–16 and also an earlier paper[17]).

When the static dielectric constant of the medium is large ($\epsilon_0 \approx 30$ in La_2CuO_4; Ref. 18), the direct Coulomb interaction is greatly suppressed, or it may even promote pairing.

2. Let us consider a two-band model with a Hamiltonian representing an exchange interaction between the carriers and the spin subsystem in the 2D case. We write

$$H_{\rm int}=I^2\int d^2\mathbf{r}\Psi^+(r)\bar{\sigma}\Psi(r)\bar{S}(r),$$
$$\bar{\mathbf{S}}(r)=a^2\sum_n \bar{S}_n\,\delta(\bar{\mathbf{r}}-\bar{\mathbf{R}}_n). \qquad (1)$$

Here $\bar{\mathbf{S}}_n$ is the spin operator at site R_n, and the operator $\Psi^+\bar{\sigma}\Psi$ represents the spin

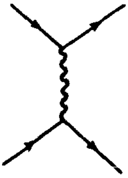

FIG. 1.

density of the holes (or electrons) in the second band. The seed electron–electron interaction is the exchange of a spin excitation (a paramagnon; Fig. 1). Under the assumption that the spin liquid is isotropic, this vertex can be written

$$\gamma_{\alpha\beta\gamma\delta}=I^2 D(\bar{\mathbf{k}},\omega)(\bar{\sigma}_{\alpha\gamma}\bar{\sigma}_{\beta\delta}), \tag{2}$$

where $D(\bar{\mathbf{k}},t)=-\frac{1}{3}\langle T_t\bar{\mathbf{S}}(\bar{\mathbf{k}},t)\bar{\mathbf{S}}(-\bar{\mathbf{k}},0)\rangle$.

We assume that the propagator $D(k,\omega)$ is localized in phase space primarily in a small momentum region around the antiferromagnetic vector $\bar{\mathbf{k}}_0$. For a carrier density for which the condition $2p_F\ll k_0$ holds, the vertex (Fig. 1) is therefore suppressed in the Cooper channel, and the effective interaction begins in second order in the paramagnetic interaction. The diagrams in Figs. 2a and 2b dominate the situation. The other second-order diagrams can be ignored for the same reason that the diagram in Fig. 1 can be. The analytic expressions for the diagrams in Figs. 2a and 2b can be written

$$\Gamma^{(-,+)}_{\alpha\beta\gamma\delta}=\{3\delta_{\alpha\gamma}\delta_{\beta\delta}\mp 2(\bar{\sigma}_{\alpha\gamma}\bar{\sigma}_{\beta\delta})\}I_{-,+}, \tag{3}$$

where

$$\begin{aligned} I_-&=-I^4T\sum_\omega\int d^2\mathbf{k}/(2\pi)^2D(k)D(p-p'-k)G(p-k)G(k-p),\\ I_+&=-I^4T\sum_\omega\int d^2\mathbf{k}/(2\pi)^2D(k)D(p-p'-k)G(p-k)G(-p'-k). \end{aligned} \tag{4}$$

The minus sign in (3) corresponds to Fig. 2a, and the plus sign to Fig. 2b. It is easy to show that we have

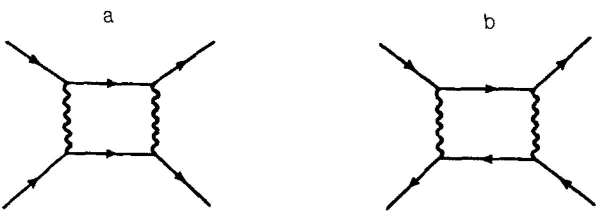

FIG. 2.

$$I_-+I_+=-I^4\frac{T}{2}\sum_\omega \int d^2\mathbf{k}/(2\pi)^2 D(k)\,D(p-p'-k)F^*(p,p',k)F(p,p',k),$$

$$I_-+I_+=-I^4\frac{T}{2}\sum_\omega \int d^2\,\mathbf{k}/(2\pi)^2 D(k)\,D(p-p'-k)\Phi^*(p,p',k)\Phi(p,p',k), \tag{5}$$

where $F(p,p',k)=G(k-p)+G(-p'-k)$ and $\Phi(p,p',k)=G(k-p)-G(-p'-k)$. In the temperature technique, $D(\bar{\mathbf{k}},\omega)$ is a function of constant sign, so the relations $I_-+I_+<0$ and $I_--I_+<0$ hold for any p and p'. The effective seed vertices in the singlet and triplet channels are, respectively,

$$\Gamma_s=3(I_-+I_+)+6(I_--I_+), \tag{6}$$

$$\Gamma_t=3(I_-+I_+)-2(I_--I_+).$$

It can be seen from these expressions that the relations $\Gamma_s<0$ and $|\Gamma_s|>|\Gamma_t|$ hold. The effective vertex Γ_s thus corresponds to an attraction, and since it is of constant sign, there is an s pairing. We should stress that this assertion is of fairly general applicability.

3. To determine Γ_s, we use the relations $|\bar{\mathbf{k}}_0|\gg|\bar{\mathbf{p}}|\sim|\bar{\mathbf{p}}'|\sim p_F$ and $E_0=k_0^2/2m^*\gg\omega_0$. Since the range of the integration in the integrals in (4) and (5) is concentrated near $\bar{\mathbf{k}}\sim\bar{\mathbf{k}}_0$, the Green's function in these expressions can be replaced by $G\approx-1/E_0$. Using the known representation for the spin susceptibility in the critical region,[19]

$$\chi^R(\bar{\mathbf{k}},\omega)=A\sum_{k_0}\frac{1}{(\mathbf{k}-\mathbf{k}_0)^2+\kappa^2-i\Omega/\Gamma}\quad(\kappa\ll|\bar{\mathbf{k}}_0|), \tag{7}$$

we can determine the retarded Green's function $D^R(k,\omega)$ for the spin components and also the causal Green's function $D(k,\omega)$ in (5). Expressions (5) and (6) can be evaluated directly. Determining the scattering averaged over angles, $\bar{\Gamma}=\frac{1}{2}\pi\int_0^{2\pi}d\varphi\Gamma_s(\varphi)$, where $\varphi=\bar{\mathbf{p}}\,\hat{}\,\bar{\mathbf{p}}'$, we find the following expression for the dimensionless coupling constant in the case $T\ll\omega_0$:

$$\lambda_s=\Gamma_s\rho(\epsilon_F)\approx-\frac{6A}{\pi^3}\frac{I^4a^2m^*\Omega}{E_0^2(\kappa a)^2}\ln\frac{k_0}{(\kappa,p)}. \tag{8}$$

Here we have allowed for the presence of four equivalent vectors k_0, and we have used the value of the density of states in the 2D case, $\rho(\epsilon_F)=m^*/2\pi$. The parameter $\Omega=\Gamma\kappa^2$ characterizes the actual frequency interval of the quasicritical antiferromagnetic fluctuations.

It was recently found[8] on the basis of a change in the NQR in the compound $La_{2-x}Sr_xCuO_4$ that the behavior of Ω as a function of x and T can be described by the simple expression $(x<0.15)$

$$\Omega(x,T)\approx\theta(x)+T,\quad T>T_c, \tag{9}$$

where $\theta(x)$ increases linearly with x. The structure of expression (9) reflects the presence of two mechanisms for the disruption of the antiferromagnetic order: an interaction with carriers and a nonzero temperature. An important point is that we have $\theta(x) > T_c$; at $T \sim T_c$ the ratio $\Omega/(\kappa a)^2$ thus depends only weakly on x, since we have $\kappa \propto x^{1/2}$ (Ref. 1).

We find the quantity A in (7) and (8) from the sum rule

$$\int d^2\mathbf{k} d\omega/(2\pi)^3 K(\bar{\mathbf{k}},\omega) = \frac{1}{3} s(s+1), \tag{10}$$

$$K(\bar{\mathbf{k}},\omega) = \frac{1}{3}\langle S_{\bar{\mathbf{k}},\omega} S_{-\bar{\mathbf{k}},-\omega}\rangle = 2\mathrm{Im}\chi(\bar{\mathbf{k}},\omega)\left\{1-\exp\left(-\frac{\omega}{T}\right)\right\}^{-1}.$$

Experimental NMR and NQR results (e.g., Refs. 4–8) can be used to show that the contribution from the region far from all k_0's in (10) is small.[9] Substituting (7) into (10), we then find $A \sim \pi/2\omega_0$. We can now estimate λ_s for $La_{2-x}Sr_xCuO_4$, using the values found for $\theta(x)$ (Ref. 8) and $\kappa^{-1} \sim 3.8x^{-1/2}$ Å (Ref. 1), and also noting that m^* is several times m_0 according to most measurements. It is easy to show that we have $\lambda_s \sim 1$. This s-pairing mechanism thus leads to a comparatively strong interaction.

From the Bardeen–Cooper–Schrieffer theory we find the approximation $T_c(x) \sim \Omega(x)\exp\{-1/\lambda_s\}$. Interestingly, as x decreases, the logarithmic increase in λ_s strengthens the tendency toward the onset of a dependence $T_c \propto \Omega \propto \theta(x)$. However, this is the correlation which has been found[8] for lanthanum systems. As x increases, λ_s decreases, since the role of the noncritical part of the interaction increases in relative importance. The latter increases the role of single-magnon scattering, which results in a repulsion. As a result, the increase in T_c with increasing x should give way to a decrease.

In the estimates above we restricted the analysis to only two-paramagnon processes for the effective seed vertex in the Cooper channel. This approach is valid if $\Gamma\rho(\epsilon_F) \ll 1$. We furthermore assumed that the approximation of a self-consistent field is valid for the spin subsystem. This assumption is equivalent to the assumption that it is valid to split the four-spin correlator into a product of binary correlators: $\langle SSSS\rangle = \langle SS\rangle\langle SS\rangle$. We believe that the results found here will not be changed in a qualitative way by a more rigorous analysis.

4. As we have already mentioned, the role played by the direct Coulomb interaction changes sharply if the value of ϵ_0 of the medium is large. In this case the first-order vertex is suppressed in the Cooper channel. Accordingly, we need to retain terms of at least second order in the effective vertex. These terms are sharply strengthened, by a factor of $\epsilon_0/\epsilon_\infty \gg 1$, in comparison with the first-order terms. The reason is that the interaction goes into vertices of order higher than the first at frequencies $\omega \gg \omega_c$, where ω_c is a characteristic frequency of the dispersion of the dielectric constant. A direct calculation leads to the following expression for the effective vertex in the Cooper channel:

$$\Gamma_c - V_c(0) - V_c(\infty) + \frac{V_c(\infty)+\gamma_c}{1+\{V_c+\gamma_c\}\rho(\epsilon_F)\ln(\epsilon_F/\omega_c)}, \tag{11}$$

where $V_c(0)$ and $V_c(\infty)$ are the Coulomb interaction screened by ϵ_0 and ϵ_∞, respectively, and γ_c is a vertex which is irreducible in the Cooper channel. A result analogous to (11) is known in the theory of the superconductivity of doped polar semiconductors.[20] It follows from (11) that in this case the Coulomb interaction either strengthens the pairing or plays a negative role, in a very weakened form.

[1] R. J. Birgeneau and G. Shirane, in *Physical Properties of High-Temperature Superconductors* (ed. D. M. Ginzberg), World Scientific, Singapore, 1990.
[2] J. M. Tranguada, W. J. L. Buyers, H. Chou, T. E. Mason, M. Sato, S. Samoto, and G. Shirane, Phys. Rev. Lett. **64**, 800 (1990).
[3] G. Shirane, R. J. Birgeneau, Y. Endoh, P. Gehring, and K. Yamada, Phys. Rev. Lett. **63**, 330 (1989).
[4] T. Imai, T. Shimizu, Y. Yasuoka, Y. Ueda, and H. Kosuge, J. Phys. Soc. Jpn. **57**, 2280 (1988).
[5] R. E. Walstedt, W. W. Warren, R. F. Bell, G. F. Brennert, G. P. Espinosa, R. J. Cava, L. F. Schneemeyer, and J. V. Waszczak, Phys. Rev. B **38**, 9299 (1989).
[6] C. H. Pennington, D. J. Durand, C. P. Slichter, J. P. Rice, E. D. Bukowski, and D. M. Ginsberg, Phys. Rev. B **39**, 2902 (1989).
[7] T. Imai, J. Phys. Soc. Jpn. **59**, 2508 (1990).
[8] Sh. Ohsugi, Y. Kitaoka, K. Ishida, and K. Asayama, J. Phys. Soc. Jpn. **60**, 2351 (1991).
[9] M. Monien and D. Pines, Phys. Rev. B **41**, 6297 (1990).
[10] N. Bulut, D. Hone, D. J. Scalapino, and N. E. Birckers, Phys. Rev. B **41**, 1797 (1990).
[11] C. Castellani, C. Di Castro, and M. Grilly, Physica C **153–155**, 1659 (1988).
[12] N. Andrei and P. Coleman, Phys. Rev. Lett. **62**, 959 (1989).
[13] A. Ramsak and P. Prelovsek, Phys. Rev. B **37**, 2239 (1989).
[14] I. R. Schrieffer, X. G. Wen, and S. C. Zhang, Phys. Rev. B **39**, 11663 (1989).
[15] A. Kampf and I. R. Schrieffer, Phys. Rev. B **41**, 6399 (1990).
[16] A. N. Kozlov, Sverkhprovodimost' (KIAE) **2**(6), 64 (1989) [Superconductivity **2**(6), 75 (1989)].
[17] D. J. Scalapino, E. Loh, and I. E. Hirsch, Phys. Rev. B **34**, 8190 (1986).
[18] C. Y. Chen, R. I. Birgeneau, and M. A. Kastner, Preprint MIT, 1990.
[19] A. Z. Patashinskiĭ and V. L. Pokrovskiĭ, *Fluctuation Theory of Phase Transitions*, Nauka, 1982.
[20] V. L. Gurevich, A. I. Larkin, and Yu. A. Firsov, Fiz. Tverd. Tela (Leningrad) **4**, 185 (1962) [Sov. Phys. Solid State **4**, 131 (1962)].

Translated by D. Parsons