Mechanism for disruption of antiferromagnetism in the two-band Hubbard model

D. O. Livdan, M. A. Strzhemechnyĭ, O. I. Tokar', and D. V. Fil'
Monokristallreaktiv Scientific-Industrial Association

(Submitted 16 March 1990)
Pis'ma Zh. Eksp. Teor. Fiz. **51**, No. 9, 461–464 (10 May 1990)

In the two-band Hubbard model of a Cu–O plane of a high-T_c superconductor, a hole at oxygen induces an *RVB* polaron in the Cu subsystem. The reason is that a Cu–O Rice singlet cannot exist against the background of an antiferromagnetism of Cu spins; an *RVB* ordering of these spins is necessary.

A fundamental question for reaching an understanding of the nature of high-T_c superconductivity is the mechanism for the disruption of antiferromagnetism (AF) at a low doping level and the accompanying insulator–metal transition. If the vacancies in the CuO_2 planes of a high-T_c superconductor are at oxygen, this system can be described by the two-band Hubbard model, in which the antiferromagnetism is disrupted as a result of a spin–spin exchange interaction between p and d electrons. Such an interaction may lead[1] to a large-radius spin disorder and to a disruption of antiferromagnetism. To take that approach, however, is to leave unanswered the question of whether this system can go into a conducting state. The possible formation of polarons was also discussed in Ref. 2, where it was shown that a ferromagnetic state is not favored. In the present letter we propose the following mechanism for the disruption of the antiferromagnetic order: An *RVB* polaron arises against the antiferromagnetic background. This polaron is induced by an oxygen hole, which requires an *RVB* neighborhood if it is to form a paired state—a Rice singlet[3]—with neighboring Cu spins. We show that the corresponding parameter of the Cu–O pairing is nonzero in the case of an *RVB* neighborhood, while it is identically zero in the case of an antiferromagnetic order of copper spins. At low concentrations, an oxygen hole is localized in an *RVB* polaron, and there is no conductivity. At a higher doping level, as the radii of the *RVB* polarons overlap, the entire system of copper spins goes into an *RVB* state, and we are dealing with a system of interacting quasiparticles: quasispinons and charge carriers. A spinon superconductivity mechanism operates here.[4]

We start from the Hamiltonian of the two-band Hubbard model:

$$H=\epsilon_p \sum_{j\sigma} n^p_{j\sigma} + \epsilon_d \sum_{i\sigma} n^d_{i\sigma} + U_p \sum_j n^p_{j\downarrow} n^p_{j\uparrow} + U_d \sum_i n^d_{i\downarrow} n^d_{i\uparrow} + H_{p-d}, \qquad (1)$$

where $H_{p-d} = t\sum_{\langle ij\rangle\sigma}(d^+_{i\sigma}c_{j\sigma} + \text{H.a.})$. Here $n^{p(d)}_{i\sigma} = c^+_{i\sigma}c_{i\sigma}(d^+_{i\sigma}d_{i\sigma})$, where $c^+(d^+)$ are the operators which create a hole at an O(Cu) site. A second-order perturbation theory in H_{p-d} leads to a Hamiltonian which provides (in particular) a Cu–O exchange and an O–O tunneling. This Hamiltonian can be written[5]

$$H^{(2)} = \frac{t^2}{\epsilon}\sum_{\langle jij'\rangle\sigma} c^+_{j\sigma}c_{j'\sigma} - \frac{t^2}{\epsilon}\sum_{\langle ij\rangle\sigma} n^d_{i\sigma}(1-n^p_{j\sigma})$$

$$-\left(\frac{4t^2}{U_p+\epsilon} + \frac{4t^2}{U_d-\epsilon}\right)\sum_{\langle ij\rangle} B^+_{ji}B_{ij} - \frac{4t^2}{\epsilon}\sum_{\langle jij'\rangle} B^+_{ji}B_{ij'}, \qquad (2)$$

where the operator $B^+_{ji} = (1/\sqrt{2})(c^+_{j\uparrow}d^+_{i\downarrow} - c^+_{j\downarrow}d^+_{i\uparrow})$ creates a Cu–O singlet, and $\epsilon = \epsilon_p - \epsilon_d$. The operators d and c in (2) are to be understood as multiplied by corresponding projection operators which take into account that there are no states with two holes at a site.

In fourth order in H_{p-d} we have Cu–Cu exchange:

$$H^{(4)} = J\sum_{\langle ii'\rangle} \mathbf{S}_i\mathbf{S}_{i'}, \qquad (3)$$

where $S_i = 0.5 d^+_i \hat{\sigma} d_i$ and $J = 4t^4/\epsilon^2 U_d$.

As was shown in Ref. 3, the ground state of a Cu–O cell with a vacancy is a Rice singlet. The appearance of a Rice singlet can be described in the mean-field approximation by a nonzero expectation value $\langle B_{ij}\rangle$. An expectation value of this type also arises in a Cu–O plane, so we will examine the critical parameters for Cu–O pairing in the case in which the Cu subsystem contains an *RVB* order[6] and an antiferromagnetic order, which are described in the mean-field approximation by

$$\Delta_{RVB} = \langle d_{i\uparrow}d_{j\downarrow} - d_{i\downarrow}d_{j\uparrow}\rangle \qquad (4)$$

$$\Delta_{\text{AF}} = \langle S_{iz}\exp(i\mathbf{QR}_i)\rangle.$$

Diagonalizing in the standard way the effective Hamiltonians which result from (2) and (3) in the approximation of the corresponding mean field, we find a system of self-consistency equations for the order parameters and the chemical potentials of the copper and oxygen subsystems.

In the case $\Delta_{RVB} = \Delta_{\text{AF}} = 0$ we are dealing with a "pure" Cu–O pairing. The equation for the transition temperature T_c,

$$1 = \frac{J_1}{4} \sum_{\mathbf{k}} \frac{\tau^2(\mathbf{k}/2)}{\xi_{\mathbf{k}}} \tanh\left(\frac{\xi_{\mathbf{k}}}{2T_c}\right) , \tag{5}$$

along with the equation for the chemical potential of the oxygen vacancies,

$$\delta = 2 \sum_{\mathbf{k}} (\exp(\xi_{\mathbf{k}}/T_c) + 1)^{-1} , \tag{6}$$

(where $\xi_{\mathbf{k}} = 0.25\, J_1 \tau^2(\mathbf{k}/2) - \mu_p$; $\tau(\mathbf{k}) = 2[\cos(k_x a) + \cos(k_y a)]$; $J_1 = 4t^2/\epsilon$), yields an essentially linear dependence $T_c(\delta) \approx J_1\delta/4$. In the case of a long-range antiferromagnetic order, Eq. (5) becomes

$$1 = \frac{J_1}{8} \sum_{\mathbf{k}} \tau^2(\mathbf{k}/2) \left[\frac{\tanh\frac{\xi_{\mathbf{k}}}{2T_c} - \tanh\frac{S}{2T_c}}{\xi_{\mathbf{k}} - S} + \frac{\tanh\frac{\xi_{\mathbf{k}}}{2T_c} + \tanh\frac{S}{2T_c}}{\xi_{\mathbf{k}} + S} \right] \tag{7}$$

($S = J\Delta_{\mathrm{AF}}$). The solution of Eq. (7), $T_c(S)$, is shown in Fig. 1. We see that the antiferromagnetism which occurs in a high T_c superconductor (in which the condition $J \gg J_1\delta$ definitely holds) destroys a Rice singlet.

In the case $\Delta_{RVB} \neq 0$ (in the absence of antiferromagnetism) Eq. (5) becomes

$$1 = \frac{J_1}{4} \sum_{\mathbf{k}} \left[\frac{\tau^2(\mathbf{k})}{\xi_{\mathbf{k}}} \tanh\left(\frac{\xi_{\mathbf{k}}}{2T_c}\right) + \frac{\tau^2(\mathbf{k}) R_{\mathbf{k}}^2}{2\xi_{\mathbf{k}}(\xi_{\mathbf{k}}^2 - R_{\mathbf{k}}^2)} \tanh\left(\frac{\xi_{\mathbf{k}}}{2T_c}\right) - \frac{\tau^2(\mathbf{k}) R_{\mathbf{k}}}{\xi_{\mathbf{k}}^2 - R_{\mathbf{k}}^2} \tanh\left(\frac{R_{\mathbf{k}}}{2T_c}\right) - \frac{\tau^2(\mathbf{k}) R_{\mathbf{k}}^2}{2\xi_{\mathbf{k}}(\xi_{\mathbf{k}}^2 - R_{\mathbf{k}}^2)} \right] \tag{8}$$

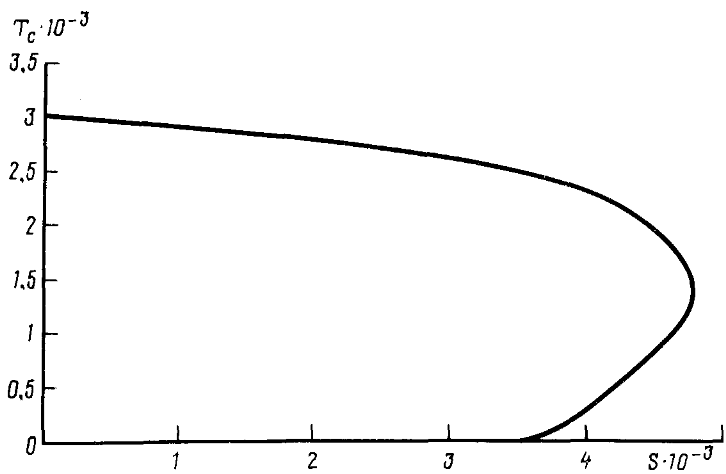

FIG. 1. T_c versus the antiferromagnetism order parameter ($J_1 = 1$) with $\delta = 0.01$.

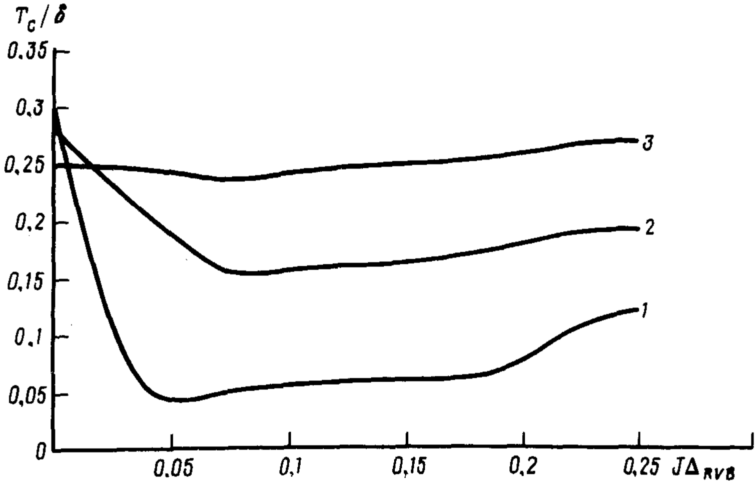

FIG. 2. T_c versus the RVB order parameter ($J_1 = 1$). *1*—$\delta = 0.01$; *2*—$\delta = 0.05$; *3*—$\delta = 0.2$.

[where $R_k = J\Delta_{RVB}\tau(\mathbf{k})$]. A solution of Eq. (8) as a function of Δ_{RVB} and δ is shown in Fig. 2.

On the other hand, an analysis of the equation for Δ_{RVB} shows that in the region $\delta < (J/J_1)^{1/2}$ the Cu–O pairing has no substantial effect on the RVBs, while at $\delta > (J/J_1)^{1/2}$ the RVB state is disrupted by Cu–O pairing. In other words, under the condition $\delta > (J/J_1)^{1/2}$, RVB and Cu–O pairing coexist.

An oxygen vacancy, as it tends to form a Rice singlet (in a Cu neighborhood), thus forms an RVB state in the nearest neighborhood, i.e., an RVB polaron. Its radius is found by minimizing the energy $E_{\text{pol}} = -J_1(1 - R^{-2}) + \Delta E_M R^2$, where the first term is the benefit resulting from the delocalization of the Rice singlet within the RVB polaron (cf. Ref. 7), and the second term is the RVB-order penalty which is paid in comparison with antiferromagnetism ($\Delta E_M = E_{AF} - E_{RVB} \ll J$). As a result, we find $R_{\text{pol}} = (J_1/\Delta E_M)^{1/4}$ (in units of a). Correspondingly, AF–RVB and insulator–metal transitions occur at a concentration $\delta_0 = (\Delta E_M/J_1)^{1/2}$, while at $\delta > \delta_0$ the RVB and Cu–O pairing and a spinon mechanism for superconductivity coexist.[4] As the doping level is increased further, at $\delta_k \sim (J/J_1)^{1/2}$, the RVB order is disrupted as a result of the suppression of the RVBs by Cu–O pairing, and the superconductivity disappears.

We wish to thank L. A. Maksimov and L. I. Glazman for a useful discussion of these results.

[1]L. I. Glazman and A. S. Ioselevich, Pis'ma Zh. Eksp. Teor. Fiz. **49**, 503 (1989) [JETP Lett. **49**, 579 (1989)].
[2]A. F. Barabanov *et al.*, Zh. Eksp. Teor. Fiz. **96**, 665 (1989) [Sov. Phys. JETP **69**, 371 (1989)].
[3]F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).
[4]D. O. Livdan *et al.*, Physica C **161**, 517 (1989).
[5]J. Zaanen and A. M. Oles, Phys. Rev. B **37**, 9423 (1988).
[6]G. Baskaran *et al.*, Solid State Commun. **63**, 973 (1987).
[7]A. F. Andreev, Pis'ma Zh. Eksp. Teor. Fiz. **24**, 608 (1976) [JETP Lett. **24**, 564 (1976)].

Translated by Dave Parsons