PHYSICAL REVIEW B VOLUME 41, NUMBER 1 1 JANUARY 1990

BCS versus Josephson pair hopping between the CuO_2 layers in high-T_c superconductors

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(Received 13 September 1989)

We start with the two-dimensional (2D) scattering matrix for two electrons of opposite spin and momentum, accounting for the fluctuating pair correlations in a single CuO_2 layer, and consider the interlayer pair hopping by (a) BCS scattering out of the layer and (b) Josephson tunneling between layers. The experimental 3D transition temperature T_c is found as a function of the interlayer BCS coupling parameter and the Josephson-tunneling matrix element. We discuss the relative importance of both of these transfer mechanisms for the Y and Tl compounds.

In the theory of high-T_c superconductors the question arises as to how the quasiparticle pairs move, from a CuO_2 layer, across the interlayer spacing of $d \sim 4$ Å in $YBa_2Cu_3O_7$ and $d \sim 11.5$ Å in $Tl_2Ba_2CaCu_2O_8$ or $Bi_2(Sr,Ca)_3Cu_2O_8$ to a neighbor layer. Independent of the symmetry of the pair states and the exact nature of the pairing mechanism within a layer, there is the basic problem of how the interlayer pair hopping gives rise to the observed superconductivity. In a purely two-dimensional (2D) system, superconductivity is suppressed by fluctuations at any finite temperature.[1] Hence, no matter how strong an interaction mediates the pairing *in* the layer, the perpendicular coupling determines the experimental transition temperature T_c. This coupling plays a crucial role in the resonating-valence-band theory[2] where holon pairs hop between the layers and also in the conventional theory where Cooper pairs traverse the interlayer distance either by virtue of a BCS pairing interaction or by Josephson tunneling.[3-6] Dzyaloshinski and Kats[7] have found that real one-electron transitions can also limit the fluctuations within a layer and yield an upper bound for T_c of the order of the bandwidth for these transitions. The actual value of T_c will be determined, however, by the coherent pair transitions of the incipient superconducting state.

We address the problem of interlayer hopping first by considering the 2D system corresponding to a single CuO_2 layer and then, by switching on the interlayer transfer of pairs, we get the 3D transition. We consider here the *Gaussian* thermodynamic fluctuations of the order parameter corresponding to the fluctuation in the Cooper-pair formation outside of the critical region, i.e., for $\ln(T/T_c) \gtrsim \eta_c$. In our case reasonable values of η_c are of order 10^{-2}.[8] Hence, critical fluctuations are absent outside of ~ 1 K around T_c. Just above the transition, the resonant scattering between two electrons that tend to form a pair of momentum $\mathbf{p}$ and energy $i\mu_m = i2\pi mkT$ manifests itself by the particular form of the particle-particle t matrix obtained by Patton[9] for a dirty 2D superconductor,

$$t_{\parallel}^{-1}(\mathbf{p},i\mu_m) = N_{\parallel}(0)a^2\left[\eta + \frac{\pi|i\mu_m|}{8kT} + \xi_{\parallel}^2(0)p^2\right], \quad (1)$$

where

$$\eta = \ln\frac{T}{T_c^{\mathrm{MF}}} + \frac{7\zeta(3)}{8}\eta_c \ln\left[\frac{\pi^2}{8\eta} - 1\right], \quad (2)$$

and

$$\eta_c = \frac{a^2}{4\pi^3 N_{\parallel}(0)\xi_{\parallel}^2(0)kT} = \frac{0.607\times 10^4}{(m_{\parallel}^*/m_0)T_c^{\mathrm{MF}}\xi_{\parallel}^2(0)}. \quad (3)$$

Here T_c^{MF} is the mean field T_c in K, $N_{\parallel}(0) = m_{\parallel}a^2/2\pi h^2$ is the 2D density of states (energy per spin), a = lattice constant, and $\xi_{\parallel}(0) = (\xi_0 l)^{1/2}$ is the coherence length in Å of a dirty superconductor with mean free path l; ξ_0 is the BCS coherence length. The width of the critical region η_c is given by Ginsberg's criterion that the condensation energy within a coherence area $\xi_{\parallel}^2(0)$ is of order unity. The function $\eta(T)$ determines the pole of the t matrix for an incipient Cooper pair of zero momentum and energy; η decreases linearly with $T - T_c^{\mathrm{MF}}$ for $\eta > \eta_c$ and exponentially for $\eta < \eta_c$, without ever going to zero when $T > 0$. When interlayer coupling is switched on, η goes to zero at a finite temperature T_c determined by both the intralayer and interlayer coupling constants.

We now determine the ratio T_c/T_c^{MF} for BCS and Josephson-pair hopping between two neighbor layers. The assumption of the dirty limit is not strictly valid; in fact, $l \sim \xi_0$. However, this assumption does not significantly alter the conclusions for a pure superconductor with such a small coherence length ξ_0.

(a) *BCS interlayer coupling.* The coupled t-matrix equations for scattering in the layer, $t_{\parallel}^{\mathrm{BCS}}$, and out of the layer, $t_{\perp}^{\mathrm{BCS}}$, are shown in Fig. 1. Here $k = [\mathbf{k}, i\omega_n = i\pi(2n+1)kT]$ labels a 2D Green's function *in* the layer and $q = (\mathbf{q}, i\nu_n)$ labels a 3D Green's function *out of* the layer. The BCS pairing interactions are $V_{\parallel}$ and $V_{\perp}$, respectively. Two neighbor layers are coupled via a process in which a pair is scattered out of a layer, receiving a perpendicular momentum component, followed by a similar process that scatters the pair "back" into a neighbor layer. This procedure for determining T_c requires that $|V_{\perp}|$ be sufficiently small compared with $V_{\parallel}$; otherwise we would have essentially 3D superconductivity. The solution of the

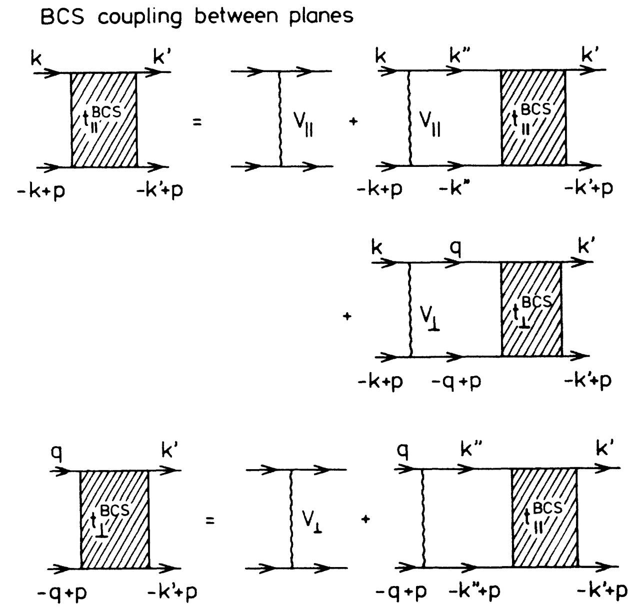

FIG. 1. BCS coupling: Diagram representation of the coupled t-matrix equations for $t_{\parallel}^{\rm BCS}$ (in-plane scattering) and $t_{\perp}^{\rm BCS}$ (out-of-plane scattering); $V_{\parallel}$ and $V_{\perp}$ are the BCS pairing interactions.

equations of Fig. 1 is

$$t_{\parallel}^{\rm BCS}(\mathbf{p},i\mu_m)=[V_{\parallel}^{-1}-I_{\parallel}(1+\alpha I_{\perp})](1+\alpha I_{\perp})^{-1}, \quad (4)$$

where the perpendicular coupling parameter is $\alpha = N_{\perp}(0)V_{\perp}^2/V_{\parallel}$, and

$$I_j = t_j(\mathbf{p},i\mu_m) - \frac{1}{V_j}, \quad (5)$$

with $j=\parallel$ or $\perp$. $t_{\parallel}$ is given by Eq. (1), $t_{\perp}$ is the standard t matrix in 3D (Ref. 10) and $N_{\perp}(0)$ is the density of states per spin for the narrow Bloch band out of the plane. T_c is determined by the pole of $t_{\parallel}^{\rm BCS}$ for $\mathbf{p}=0$ and $i\mu_m=0$. We obtain

$$\eta(T)=\frac{(\alpha/\lambda_{\parallel})\ln(1.14\hbar\omega_{\perp}/kT)}{1+\alpha\ln(1.14\hbar\omega_{\perp}/kT)}. \quad (6)$$

Using the parameter values given in Tables I and II, we plot in Fig. 2 T_c vs $\lambda_{\perp}/\lambda_{\parallel}$ for different values of the parameter η_c. Here $\lambda_{\parallel}=N_{\parallel}(0)V_{\parallel}$ and $\lambda_{\perp}=N_{\perp}(0)V_{\perp}$. Note that 3D superconductivity is also possible when $V_{\perp}$ is repulsive, if $V_{\parallel}$ is attractive and sufficiently large.

(b) *Josephson coupling.* When the distance between the CuO_2 layers is sufficiently large and the bandwidth is small, then pair hopping due to Josephson tunneling becomes a possible interlayer transfer mechanism. At any instant of time in a single layer above T_c, a fluctuating superconducting state can exist which foreshadows the true equilibrium pairing state. Ferrel[11] points out that the instantaneous Cooper-pair field can give rise to incipient Josephson tunneling processes above T_c. For our case this implies that Josephson-pair hopping between the neighboring CuO_2 layers can occur due to pair fluctuations in both of these layers. We thus have the coupled t-matrix equations for two neighbor layers a and b, shown in Fig. 3. For the two identical layers the BCS interactions $V_a=V_b$ and the t matrices $t_a^J=t_b^J=t^J$ are identical. Hence, we have a single equation,

$$t^J(\mathbf{p},i\mu_m)^{-1}=V_{\parallel}^{-1}-I_{\parallel}(1+|\Delta E|/V_{\parallel}), \quad (7)$$

where $I_{\parallel}$ is given by Eq. (5) and the temperature-dependent Josephson coupling energy is given by second-

TABLE I. Values of η_c, Eq. (3), for $T_c^{\rm MF}=93$ K and for two different experimental values of $\xi_{\parallel}(0)$ (Ref. 8). The lower mass ratio $m_{\parallel}/m_0$ is about the band-structure mass ratio and the larger value corresponds to a polaron mass lying between the values of 4.1 and 9 derived from the specific-heat jump at T_c and the Drude analysis of the infrared conductivity, correspondingly (Refs. 13 and 14).

$m_{\parallel}/m_0$	$\xi_{\parallel}(0)$ (Å)	η_c
2.3	16	0.11
2.3	37	0.021
6	16	0.043
6	37	0.0080

TABLE II. BCS parameter for the T_c equation, Eq. (7).

$\lambda_{\parallel}=0.399$, $\hbar\omega_{\parallel}/k=10^3$ K	$T_c^{\rm MF}=93$ K
$\lambda_{\perp}/\lambda_{\parallel}=10^{-5}-1$	
$\omega_{\perp}/\omega_{\parallel}=N_{\parallel}(0)/N_{\perp}(0)=0.2;1$	

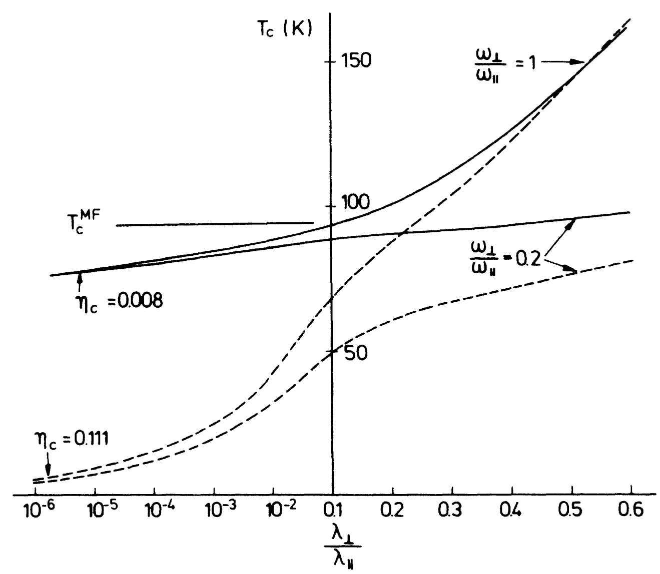

FIG. 2. Transition temperature T_c vs the out-of-plane BCS pairing parameter $\lambda_{\perp}/\lambda_{\parallel}$ where the in-plane coupling constant $\lambda_{\parallel}=0.399$ determines the mean-field transition temperature, $T_c^{\rm MF}=(1.14\hbar\omega_{\parallel}/k)\exp(-1/\lambda_{\parallel})=93$ K. The cutoff frequency, $\omega_{\parallel}=1000$ K.

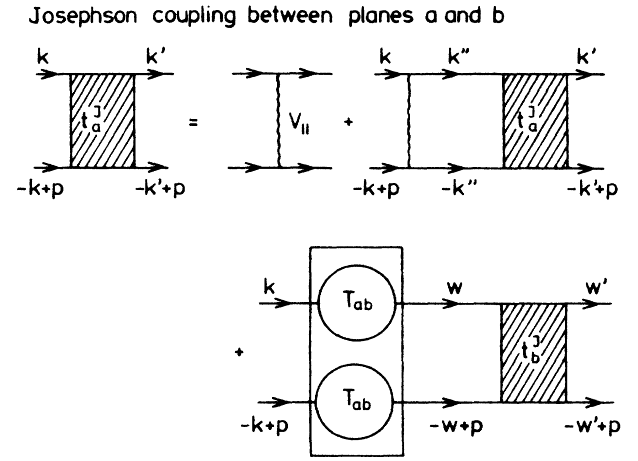

FIG. 3. Josephson coupling: Diagram representation of the coupled t-matrix equations for the two neighbor layers a and b; T_{ab} is the single-particle tunneling matrix element.

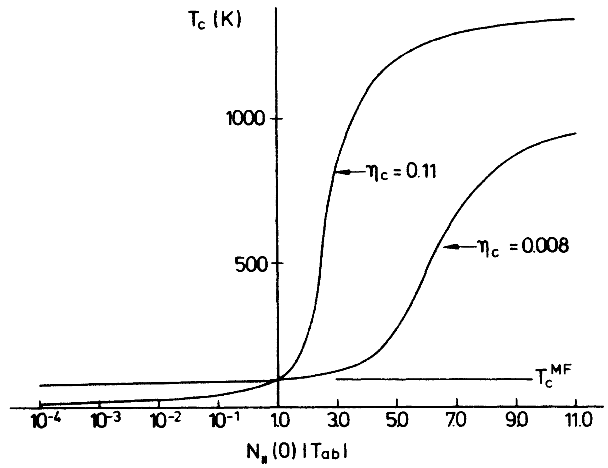

FIG. 4. Transition temperature T_c vs the Josephson coupling parameter, $N_{\parallel}(0)\,|T_{ab}|$; $T_c^{\rm MF}=93$ K.

order perturbation theory,

$$\Delta E = -\pi^2\Delta(N_{\parallel}(0)\,|T_{ab}|)^2\tanh(\Delta/2kT)\cos(\phi_a-\phi_b)\,, \tag{8}$$

cf. Anderson,[12] $|T_{ab}|$ is the exponentially small tunnel matrix element between the layers a and b, averaged over all Fermi-surface momenta **k** and **w** in the layers a and b, respectively. The effective gap Δ is given by[9]

$$\begin{aligned}\Delta^2 &= kT\sum_p t_{\parallel}(\mathbf{p},0)\,,\\ \Delta^2 &= kTa^2\int_0^{\xi_{\parallel}^{-1}(T)}\frac{p\,dp}{2\pi}\\ &\quad\times\frac{1}{N_{\parallel}(0)[\ln(T/T_c)+\xi_{\parallel}^2(0)p^2]}\,,\\ \Delta^2 &= (\pi kT)^2\eta_c\ln 2\,.\end{aligned} \tag{9}$$

The temperature T_c is determined by the pole of $t_{\parallel}^J(0,0)$. We obtain

$$\eta(T) = [\lambda_J(T)/\lambda_{\parallel}^2][1+\lambda_J(T)/\lambda_{\parallel}]^{-1}\,, \tag{10}$$

where $\lambda_J = N_{\parallel}(0)\,|\Delta E|$. Using the band mass $m_{\parallel}/m_0 = 2.3$,[13] rather than the polaron mass[14] for the pair-hopping process, we get the results shown in Fig. 4 for T_c versus the tunneling strength, $N_{\parallel}(0)\,|T_{ab}|$. The η_c values are given in Table I. For strong Josephson coupling, $\lambda_J \gg \lambda_{\parallel}$, T_c saturates at a maximum value determined by the intralayer pairing constant, $\eta(T_c^{\rm max}) = 1/\lambda_{\parallel}$. We note that a *repulsive* interaction in the layer cannot lead to 3D superconductivity no matter how large the Josephson coupling may be.

In comparing the BCS and Josephson cases, we see that in either case switching on a *small* interlayer coupling between the fluctuating pair fields in the 2D systems can lead to the observed superconductivity. How large an interlayer coupling is required to yield the observed T_c, $\lambda_{\perp}$ or λ_J, depends primarily on the size of the critical region, η_c. The smaller η_c is, i.e., the *weaker* the fluctuation effects in a single layer, the *smaller* the coupling parameters $\lambda_{\perp}$ or λ_J are that produce the observed T_c's. In both cases, T_c can be larger or smaller than the mean-field temperature $T_c^{\rm MF}$. The critical region of $YBa_2Cu_3O_7$ is discussed by Kapitulnik *et al.*[8] Recent experimental results[15] on the temperature dependence of the in-plane paraconductivity of a single crystal of $YBa_2Cu_3O_{7-x}$ give a T_c value that lies 5.6 K above $T_c^{\rm MF} = 87.4$ K, when the measured conductivity is fitted to the 2D Aslamasov-Larkin model. For a BCS interlayer coupling, this requires $\lambda_{\perp}/\lambda_{\parallel} \sim 0.1-0.2$, for $\eta_c = 0.0080$ and $\omega_{\perp}/\omega_{\parallel} = 1.0$ (Fig. 2). The cutoff frequency for the perpendicular pairing interaction weakens the dependence of T_c on $\lambda_{\perp}$ for $\omega_{\perp} \ll \omega_{\parallel}$. This inequality implies a smaller cutoff frequency for the BCS scattering out of the plane, consistent with a narrow band for the z direction.

For a typical Josephson junction with an oxide barrier, the hopping parameter $N_{\parallel}(0)\,|T_{ab}|$ is related to the normal-state resistance $R_N(\Omega)$ by the relation $N_{\parallel}(0)^2\,|T_{ab}|^2 = 327/R_N$. The equivalent resistivity is $\rho_J = 100\ \Omega\,\rm cm$ for a barrier of thickness 20 Å with a cross section S^2 that, for a standard junction, is given by $R_N \times S^2 = 2\times10^{-5}\ \Omega\,\rm cm^2$. On the other hand, the c-axis resistivities directly above T_c have the experimental values $\rho_{\perp} = 0.0175\ \Omega\,\rm cm$ for $YBa_2Cu_3O_{7-x}$ and $\rho_{\perp} = 10\ \Omega\,\rm cm$ for $BiSr_{2.2}Ca_{0.8}Cu_2O_8$.[16] This large value of $\rho_{\perp}$ indicates that Josephson coupling may play an important role in the Bi and Tl systems, at least for the pair hopping across the two Tl-O layers that intercalate the large distance of 11.5 Å between two CuO_2 planes. Whether Josephson-pair hopping of BCS scattering causes the coupling between the "closer" layers which are 3–4 Å apart in the Y, Tl, and Bi compounds is not so clear. The small coherence length in the c direction $\xi_{\perp}(0)$ is comparable with d.[15,17] The yttrium ions between two neighboring CuO_2 layers can be replaced with magnetic ions without a large pair-breaking effect on T_c.[18] This experimental result is not compatible with Josephson tunneling for the following reason: Magnetic impurities in the "barrier" lead to a reduction of the tunnel current by diminishing the spinconserving matrix elements, T_{ab}. Probably more important, the magnetic dipole fields of the $4f$ moments affect the tunnel process by destroying the phase coherence, $\cos(\phi_a - \phi_b)$, which we have set equal to one. Hence the small reduction of T_c in the presence of the $4f$ moments makes Josephson tunneling an unlikely transfer process. On the other hand, the pair-breaking effect of the magnetic ions on the BCS state is governed by the exchange interaction between the $4f$ moments and the conduction electrons. This interaction is weak, as is seen from the low Curie temperature $T_c \sim 0.3$ K, at which the Yb ions undergo magnetic ordering in $YbBa_2Cu_3O_{7-x}$.[19] A BCS pairing interaction between layers is thus compatible with experiment. However, for the *distant* CuO_2 layers in $TlBa_2CaCu_2O_8$, Josephson tunneling is suggested by the large values of both $\rho_\perp$ and $\rho_\perp/\rho_\parallel \sim 10^5$. This can be tested experimentally if magnetic impurities can be introduced into the Tl-O layers of such compounds. The T_c reduction is expected to be larger than that observed for the $Y_{1-y}R_yBa_2Cu_3O_{7-x}$ compounds (R represents the rare-earth element).

In conclusion, we find that the transition temperature T_c that stabilizes the 2D Cooper-pair fluctuations in a CuO_2 layer requires either a weak BCS scattering out of the plane, $\lambda_\perp/\lambda_\parallel \sim 0.1$–$0.3$, or a small Josephson tunneling parameter between the layers, $N_\parallel(0)|T_{ab}| \sim 1$. The results are shown in Figs. 2 and 4 for parameter values we believe are relevant. Depending on the parameters, 2D fluctuations and 3D coupling can *raise* a low 2D T_c^{MF} (as may be expected for usual phonon pairing) or *reduce* a high 2D T_c^{MF} (electronic pairing mechanisms) to yield the observed T_c. The latter case may apply to the precursor effect in the T dependence of the NMR relaxation rate observed[20] in $YBa_2Cu_3O_{6.7}$, $T_c = 60$ K. This experiment suggests the onset of fluctuating spin pairing in the individual layers far above the observed 3D T_c.

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