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LETTER TO THE EDITOR

Enhanced pairing interaction in a two-band model

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Abstract. The Kondo picture for the electron–electron attraction due to transfer of pairs of electrons between two bands is investigated. This interaction may reduce the Coulomb repulsion considerably, leading to enhancement of the superconducting transition temperature and a substantial weakening of the isotope effect. The special screening effect is large when the empty band is narrow and the energy gap between the two bands is small. Possible relevance to the superconducting oxides is suggested.

The high superconducting transition temperature oxides [1] present a most interesting challenge to theorists. At this point a solution to the problem remains elusive despite numerous interesting suggestions for novel mechanisms. The new superconductors appear experimentally to have a BCS-type gap [2]; the superconducting unit appears to be a two-electron pair, from both the flux quantum and the AC Josephson effect [3]. Thus a BCS-type approach seems to be a reasonable starting point. Since conduction takes place in the O 2p bands, as was first argued by Emery [4] and subsequently confirmed experimentally [5], and a transition metal band is expected to be not too far off, one is led very naturally to a two-band model. (We use, for convenience, the term 'electron', while the charge carriers are usually holes in the present oxide superconductors). Also, while coupling to phonons is probably very important, one should like to have an electronic mechanism that would effectively screen the strong Coulomb repulsion and would have the potential to be specific and to choose a limited class of materials. Here we present evidence that the two-band mechanism, first proposed by Suhl and coworkers [6] and Kondo [7], and later investigated by several others [8–10], may well be the relevant one. We show that in favourable cases the strong intraband Coulomb repulsion becomes renormalised into a quantity less than or of the order of the, much smaller, band-structure gap. We demonstrate that with the above reduction of the Coulomb pseudopotential, a strong but reasonably-sized coupling to optical phonons may be sufficient to account for the observed T_cs of the new superconductors. Strong coupling to oxygen vibrations was argued by Eliashberg [11] to follow naturally from the association of the conduction band with the oxygens.

An important issue [12] of principle is the validity of a quasiparticle picture in the normal state of the conductors. We point out in this connection the recent determination of the quasiparticles' lifetime τ_p by Aronov *et al* [13]. They find $\hbar/\tau_p$ of the same order

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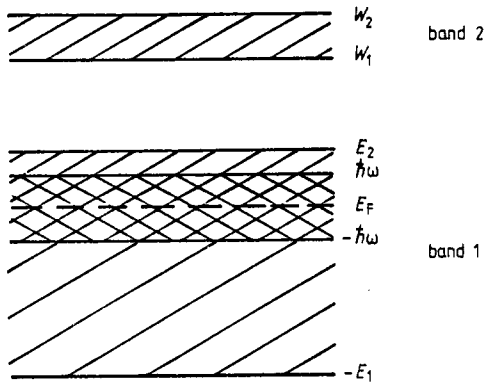

Figure 1. Schematic description of the band structure. Energies are measured from the Fermi level. An attractive electron–electron mechanism (e.g. via phonons) acts in the hatched region.

of magnitude, but *not* larger than the quasiparticles' energy. Thus, the Landau picture is on the verge of its validity but might still be used for qualitative considerations.

The process we focus upon is the transfer of a pair of electrons, by the interband Coulomb interaction, from band 1 to band 2 and *vice versa*. It give rise to an effective attraction, which is second-order in the interband vertex. This attraction acts as to reduce the single-band Coulomb repulsion considerably. The process was proposed by Kondo [7] as an explanation for the superconducting properties of transition metals. Here we extend Kondo's model to include Coulomb repulsion in both bands with parameters qualitatively appropriate to the superconducting oxides, and argue that this mechanism may well be the relevant one for the new superconductors.

We consider the schematic band-structure depicted in figure 1. The Fermi level lies within band 1. This band is in the energy range $\{-E_1, E_2\}$ (energies are measured from the Fermi energy). The second band is above the first one, in the energy range $\{W_1, W_2\}$ such that the lower band-edge is much larger than the thermal energy. The second band may be, for example, the empty (full, in the case of holes) part of the Cu-band (or even localised Cu Wannier states), or a split-off oxygen band. The final identification of the relevant bands must await a complete band-structure determination.

A simple BCS-type consideration based on Kondo's work [7] (see below) yields that the total repulsion between the electrons takes the form

$$V_{\text{tot}} = \Gamma_1' - \Gamma_4'^2 a/(1 + \Gamma_2' a). \tag{1}$$

Here Γ_1' is the modified [14] repulsive Coulomb interaction in band 1

$$\Gamma_1' = \Gamma_1/\{1 + N_1\Gamma_1 \ln[(E_1E_2)^{1/2}/\hbar\omega]\}$$

where Γ_1 is the screened Coulomb vertex of the first band, N_1 is the density of states of that band (assumed for simplicity to be constant) and $\hbar\omega$ is the energy shell in which some attraction mechanism (e.g. due to exchange of optical phonons) between the electrons operates (see figure 1). The first term in (1) gives the usual BCS-type form of the modified Coulomb repulsion in a single-band picture [14]. The second term leads to a further reduction of the repulsive interaction. Here

$$\Gamma_4' = \Gamma_4/\{1 + N_1\Gamma_1 \ln[(E_1E_2)^{1/2}/\hbar\omega]\} \tag{2}$$

where Γ_4 is the interband Coulomb vertex, and

$$\Gamma_2' = \Gamma_2 - \Gamma_4\Gamma_4' N_1 \ln[(E_1E_2)^{1/2}/\hbar\omega] \tag{3}$$

Γ_2 being the screened intraband Coulomb vertex of band 2. Finally, the quantity a in (1)

depends on the second band parameters. Assuming again a constant density of states, N_2, $a = (N_2/2)\ln(W_2/W_1)$. One notes that the interband repulsion (Γ_4) acts so as to reduce the repulsion within both band 2 (equation (3)) and band 1 (equation (1)), the magnitude of the reduction being determined by band-structure parameters.

The interesting situation arises when the two bands are separated by a gap which is not too large and band 2 is narrow. Let us denote the attractive interaction operating in band 1 in the energy range $\{-\hbar\omega, \hbar\omega\}$ by λ. Then $\lambda - \Gamma_1'$ is the effective attractive coupling of band 1 in the absence of coupling to band 2, and $\Gamma_4'^2 a/(1 + \Gamma_2' a)$ is an aditional attraction, brought about by the presence of the second band. When this band is narrow, a is of the order of $1/W_1$, i.e., of the order of the inverse energy gap between the two bands (the density of states N_2 being of the order of the inverse band width). The additional attraction will then be of the order $\Gamma_4'^2/E_{\text{gap}}$ (for $\Gamma_2' < E_{\text{gap}}$) or $\Gamma_4'^2/\Gamma_2'$ (for $\Gamma_2' > E_{\text{gap}}$). We further note that when all three Coulomb vertices are of the same order of magnitude ($\Gamma_1 \simeq \Gamma_2 \simeq \Gamma_4$) the total repulsion becomes

$$V_{\text{tot}} = \Gamma_1'/(1 + \Gamma_2' a) \sim E_{\text{gap}}\Gamma_1'/\Gamma_2' \sim E_{\text{gap}} \tag{4}$$

(for $\Gamma_2' > E_{\text{gap}}$), i.e., considerably smaller than the single-band repulsion. Essentially, the mechanism renormalises the large intraband Coulomb repulsion into the, much smaller, band-structure gap.

A case which may be of relevance to oxide superconductors is when the screening reduces Γ_1 much more than Γ_2, but Γ_4 stays relatively large [9, 15] so tht there is a considerable cancellation of $\Gamma_1'\Gamma_2' - \Gamma_4'^2$. In this case $V_{\text{tot}} = \Gamma_1'/(1 + \Gamma_2' a) \simeq E_{\text{gap}}(\Gamma_1'/\Gamma_2') \ll E_{\text{gap}}$, i.e., an extremely effective reduction of the Coulomb repulsion. A full random-phase-approximation treatment of the two-band screening [8, 9, 15] for the case where band 2 is empty shows that Γ_1 has ordinary metallic screening, Γ_2 has a much weaker screening and the 'screening' of Γ_4 is independent of the above and does not necessarily reduce the bare value.

These considerations affect the isotope effect remarkably. As was pointed out by Kondo [7], when the interband interaction is appreciable, the isotope effect is far less effective than in the simple BCS picture in which the attractive coupling does not depend upon ω. Writing

$$k_B T_c = 1.14\hbar\omega \exp[-1/N_1(\lambda - V_{\text{tot}})] \tag{5}$$

the isotope effect can be expressed in the form

$$\Delta T_c/T_c = (\Delta\omega/\omega)\{1 - \omega(\partial/\partial\omega)[1/N_1(\lambda - V_{\text{tot}})]\}. \tag{6}$$

A complete isotope effect is obtained when the second term in the square brackets disappears. In the present case this factor becomes $[V_{\text{tot}}/(\lambda - V_{\text{tot}})]^2$. When all three Coulomb vertices are comparable and band 2 is narrow this yields $[E_{\text{gap}}/(\lambda - E_{\text{gap}})]^2$ and may become of the order of 1, leading to a rather small isotope effect.

We now comment upon the derivation of equations (1) and (5). The starting point is the BCS-reduced Hamiltonian in the two-band representation

$$H_R = \sum_{k,k'} \sum_{i,j} \Gamma_{ij}(\boldsymbol{k}, \boldsymbol{k}') a^+_{ik\uparrow} a^+_{i-k\downarrow} a_{j-k'\downarrow} a_{jk'\uparrow} \tag{7}$$

in which a_i^+ (a_i) creates (destroys) an electron in the ith band, $i = 1$ or 2. Employing the

Bogoliubov transformation in both bands, the self-consistent equations for the gap parameters at T_c read

$$\varphi_i(\boldsymbol{k}) = -\tfrac{1}{2}\sum_{\boldsymbol{k}'}\sum_j (-1)^{i+j}\Gamma_{ij}(\boldsymbol{k},\boldsymbol{k}')\frac{1-2f_j(\boldsymbol{k}')}{\varepsilon_j(\boldsymbol{k}')}\varphi_j(\boldsymbol{k}') \qquad i,j=1,2. \tag{8}$$

Here $\varepsilon_i(\boldsymbol{k})$ is the single-electron energy in the ith band, measured from the Fermi energy, and $f_i(\boldsymbol{k})$ is the corresponding Fermi function. Equations (8) are solved with the following assumptions: $\Gamma_{12}(\boldsymbol{k},\boldsymbol{k}') \equiv \Gamma_4$ and $\Gamma_{22}(\boldsymbol{k},\boldsymbol{k}') \equiv \Gamma_2$, independent of the momenta. The vertex of band 1, $\Gamma_{11}(\boldsymbol{k},\boldsymbol{k}')$ is assumed to take the values $-\lambda + \Gamma_1$ for $|\varepsilon_1(\boldsymbol{k})|, |\varepsilon_1(\boldsymbol{k}')| < \hbar\omega$ and Γ_1 otherwise. Correspondingly, the gap parameter Φ_2 of band 2 is independent of $\boldsymbol{k}$, while the gap parameter of band 1, $\varphi_1(\boldsymbol{k})$, assumes the values $\varphi_1^{(1)}$ for $|\varepsilon_1(\boldsymbol{k})| < \hbar\omega$ and $\varphi_1^{(2)}$ otherwise. One is left with the various sums of the form $\Sigma_k(1-2f_i(\boldsymbol{k}))/\varepsilon_i(\boldsymbol{k})$. These are carried out approximately by assuming a constant density of states in both bands and that the thermal energy is small compared to the energies of the band-edges. The sum over the second band gives the quantity a and the sum over the first band gives $N_1 \ln(1.14\hbar\omega/k_B T_c)$ when $|\varepsilon_1(\boldsymbol{k})| < \hbar\omega$, and $N_1 \ln[(E_1E_2)^{1/2}/\hbar\omega]$ otherwise. Equations (8) then yield a 3×3 determinant, whose solution is (5), with the total repulsive interaction given by (1).

We demonstrate now that typical high-frequency molecular CuO_2 vibrations, e.g., $\hbar\omega \simeq 800$ K [16], are consistent via (5) with $T_c \simeq 10^2$ K, with quite reasonable parameters. We have seen that $V_{tot} \leqslant E_{gap}$. Choosing $N_1\lambda \simeq 0.9$, $N_1 V_{tot} \simeq 0.4$ (the corresponding numbers for Nb are about 0.45 and 0.1) will explain the T_c of $YBa_2Cu_3O_{7-\delta}$. These parameters will also yield the almost complete vanishing of the isotope effect. This does necessitate a large electron–phonon coupling constant (twice that of Nb) but it is reduced by a still larger Coulomb energy to a total coupling constant only 50% stronger than that of Nb. The rather high value of $\hbar\omega$ helps; this vibration is also less likely to become unstable due to the larger electron–phonon coupling. Obviously, these are just simple-minded weak-coupling estimates done to show that the parameters needed are large but not out of proportion. The mechanism can be confirmed or otherwise by the usual experiments such as tunnelling measurements of $\alpha^2 f$, which should agree with both T_c and the isotope shift.

We remark that the original paper by Kondo [7] considered the possibility that a large enough Γ_4 might lead to superconductivity without an attractive electron–phonon component. Practically, however, we feel that the electron–phonon interaction in the high-T_c oxides may be strong anyway. Finally, we remark that, as in the usual BCS theory, the idea here is to explain the *difference* between the superconducting and normal state without really dealing with the intriguing intricacies of the latter.

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