Coupling between Planes and Chains in $YBa_2Cu_3O_7$: A Possible Solution for the Order Parameter Controversy

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We propose to explain the contradictory experiments about the symmetry of the order parameter in $YBa_2Cu_3O_7$ by taking into account the coupling between planes and chains. This leads to an anticrossing of the plane and chain band. We include an attractive pairing interaction within the planes and a repulsive one between planes and chains, leading to opposite signs for the order parameter on planes and chains, and to nodes of the gap because of the anticrossing. Our model blends s-wave and d-wave features, providing a natural explanation for all the contradictory experiments.

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The pairing mechanism in high T_c superconductors is presently the subject of a vivid debate [1]. There is a high suspicion that some, if not all, high T_c compounds are unconventional. On one hand, a repulsive interaction between electrons can lead to pair formation, as in the case where the interaction is due to spin fluctuation exchange [2]. For this specific case the order parameter has a d-wave symmetry which implies that it changes sign on the Fermi surface. On the other hand, an attractive interaction leads to an order parameter which does not change sign on the Fermi surface, even if there is a sizable anisotropy of the gap. In this case the order parameter has an s-wave symmetry as for the conventional mechanism of phonon mediated pairing. Therefore, an efficient way to check the pairing mechanism, and to decide if high T_c superconductors are unconventional, is to look experimentally at the symmetry of the order parameter.

Very surprisingly, recent experiments performed in YBCO in order to settle this issue of the order parameter symmetry have given convincing, but contradictory, answers [1]. Indeed, the observation of a sizeable Josephson current [3] in a c-axis tunneling junction between YBCO and Pb is quite difficult to reconcile with a pure d-wave symmetry. Similarly, the absence of angular dependence and of sign change in the critical current of YBCO-YBCO grain boundary junctions in the a-b plane [4] is clearly in favor of s-wave symmetry. On the other hand, the evidence for a π shift in corner superconducting quantum interference device (SQUID) experiments [5] is a clear indication for a change of sign of the order parameter between the a and the b axes. Similarly, the observation of a spontaneous magnetization corresponding to a half magnetic flux quantum in 3-grain-boundary Josephson junctions [6] favors clearly d-wave symmetry. Finally, all the experiments giving evidence for low energy excitations at low temperature, such as tunneling [1], linear temperature dependence of the penetration depth in YBCO crystals or films [7], or photoemission experiments in $Bi_2Sr_2CaCu_2O_8$ [8] are also more naturally interpreted in terms of d-wave symmetry, although they are consistent with a strongly anisotropic s-wave order parameter. While there is always the possibility that one set of experiments is spoiled for obscure reasons, this is rather unlikely in view of the quality, the independence, and the variety of these experiments. A more natural view is to look for an explanation which allows one to reconcile these various results.

It is our purpose in this paper to present such a model, which blends s-wave and d-wave features, and provides a natural and intrinsic explanation for all the contradictory experiments [1]. The basic ingredient of our model is the coupling between planes and chains [9]. This is taken into account both in the band structure of YBCO (diagonal coupling), and in the (repulsive) pairing interaction between planes and chains (off-diagonal coupling). Indeed, in order to account for all the experiments in favor of a d-wave interpretation, we have to take an order parameter which changes sign. As in the spin fluctuation mechanism, the natural explanation for this is the existence of a repulsive interaction between electrons. Repulsive interactions are actually already present in conventional superconductivity because of the existence of the Coulomb repulsion between electrons, taken into account by the Coulomb pseudopotential. This leads indeed to a change of sign of the order parameter, but this occurs in the frequency rather than in the wave vector dependence. Therefore, if the Coulomb interaction is the dominant mechanism for scattering between some pieces of the Fermi surface, this can lead to a change of sign in the order parameter on the Fermi surface, in close analogy with the spin fluctuation mechanism. Similar ideas have been proposed very recently, pointing out that the sign of the order parameter could be opposite on two different sheets of the Fermi surface, due to repulsive interaction produced by spin fluctuation or by direct Coulomb interaction [10]. These two sheets could be produced by the two bands corresponding to the two CuO_2 planes, or they could correspond to the plane bands and the chain band. Here we take the view that, due, for example, to Coulomb interaction, the order parameter has opposite sign on the plane bands and on the chain band.

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However, although this change of sign of the order parameter on different sheets of the Fermi surface can account for the experiments showing a π shift in Josephson junctions, it does not explain a number of facts in favor of a d-wave-like interpretation. These are all the experiments pointing toward the existence of low lying excitations at low temperature [1,7,8], and therefore toward the presence of nodes of the gap on the Fermi surface. A possible explanation for these experiments has been proposed by Abrikosov [11]. We propose here another explanation of this feature by taking into account the coupling between plane and chain occurring in the band structure. This coupling is likely due to the O4 apical oxygen. Physically this means that an electronic eigenstate is never purely a plane electron or a chain electron. Rather it has a mixed nature with components on both plane and chain. This coupling is a well known feature in band structure calculations [12]. Naturally it is fairly small, and is of importance only when the plane and the chain band intersect, where it leads to a standard anticrossing feature in the dispersion relations found in band structure calculations. Similarly, wherever the (uncoupled) pieces of the Fermi surface related to plane and chain cross, the coupling leads to an anticrossing as also seen in band structure calculations [12]. This anticrossing has the important consequence that, when we move on a given sheet of the Fermi surface, we go from a part which corresponds physically to a plane electron, to a part corresponding physically to a chain electron.

More specifically, band structure calculations [12] give an anticrossing with the odd combination of the CuO_2 planes (except at $k_z = 0$ for symmetry reasons). The situation with respect to the even combination is not so clear, but this is unimportant for us. In order to explore the physical consequences of this anticrossing, we take a simplified model for the band structure which displays this feature (although it does not make any problem to take a full three-dimensional band structure); namely, we consider a single plane band anticrossing a chain band. Since the k_z dependence is not essential for our purpose, we omit it, which leads us to the following two-dimensional model Hamiltonian for the band structure:

$$\mathrm{H}_0 = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_k \varepsilon_k' d_k^\dagger d_k + \sum_k T c_k^\dagger d_k + \mathrm{H.c.} \tag{1}$$

It describes semiquantitatively all the band structure features which are important for us; $c_k^\dagger$ and $d_k^\dagger$ are creation operators in the plane and in the chain band respectively. As a simple model, we take $\epsilon_k = -2t_0[\cos(k_x a) + \cos(k_y a)] + 2t_0 \cos(k_x a)\cos(k_y a) - \mu_0$ and $\epsilon_k' = -2t_1 \cos(k_y a) - \mu_1$, with $t_0 = 0.33$ eV, $t_1 = 0.53$ eV, $\mu_0 = -0.46$ eV, and $\mu_1 = -0.74$ eV, in order to obtain a Fermi surface in reasonable agreement with band structure calculations, but this is not essential for our purpose. We neglect the $\mathbf{k}$ dependence of the plane-chain coupling T, since this term is relevant only in a rather small $\mathbf{k}$ space region. The energies $e_\pm$ of the eigenstates of H_0 are $2e_\pm = \epsilon + \epsilon' \pm [(\epsilon - \epsilon')^2 + 4T^2]^{1/2}$, and the corresponding Fermi surface $e_\pm = 0$ is shown in Fig. 1 for $T = 0.1$ eV.

Let us now consider interactions and, more precisely, their effect in the superconducting state. In the planes, we take a purely attractive pairing interaction, which may be of phononic origin. The off-diagonal coupling between plane and chain is repulsive, as indicated above. Finally we consider for generality a pairing interaction in the chains. Neglecting all unnecessary wave vector dependence, this leads us in weak coupling to the following pairing interaction (with singlet pairing understood):

$$\mathrm{H}_{\mathrm{int}} = -g \sum_{k,k'} c_{k'}^\dagger c_{-k'}^\dagger c_{-k} c_k + K \sum_{k,k'} d_{k'}^\dagger d_{-k'}^\dagger c_{-k} c_k + \mathrm{H.c.} + g' \sum_{k,k'} d_{k'}^\dagger d_{-k'}^\dagger d_{-k} d_k , \tag{2}$$

with g and K positive. This interaction is just the one studied in earlier work on two-band superconductivity [13]. This gives the following mean-field Hamiltonian :

$$\mathrm{H} = H_0 + \Delta \sum_k c_k^\dagger c_{-k}^\dagger + \Delta' \sum_k d_k^\dagger d_{-k}^\dagger + \mathrm{H.c.}, \tag{3}$$

where we have set

$$\Delta = -g \sum_k \langle c_{-k} c_k \rangle + K \sum_k \langle d_{-k} d_k \rangle , \tag{4}$$

$$\Delta' = K \sum_k \langle c_{-k} c_k \rangle + g' \sum_k \langle d_{-k} d_k \rangle . \tag{5}$$

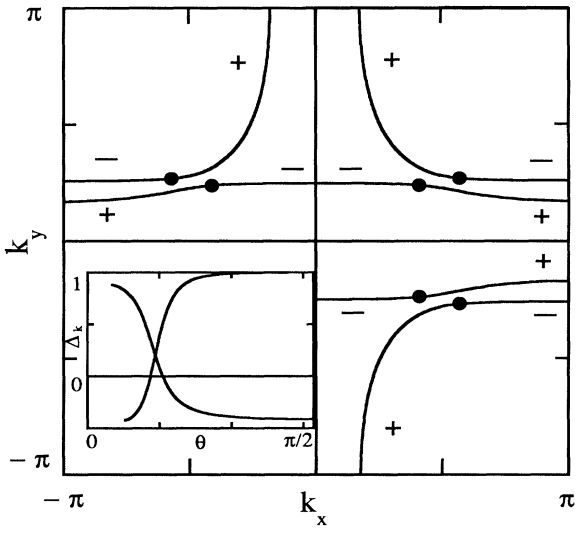

FIG. 1. Fermi surface in the Brillouin zone. The sign ± of the order parameter on the various parts of the Fermi surface is indicated. The filled circles give the positions of the nodes of the gap. Inset: variation of the order parameter Δ_k on the two sheets of the Fermi surface for k_x and $k_y > 0$, as a function of the angular position $\theta = a\tan(k_y/k_x)$.

It is now easy to see what happens physically. Because the pairing is attractive in the planes, but repulsive between plane and chain, the order parameters Δ and Δ' (which correspond physically to the order parameters in the uncoupled planes and chains, respectively) will have opposite sign. On the other hand (because of the anticrossing) when we move on a single sheet of the Fermi surface we go continuously from a planelike part to a chain like part, we see (Fig. 1) that on moving on this given sheet the order parameter will necessarily change sign, since it will be essentially equal to Δ on the planelike part and to Δ' on the chainlike part. This implies by continuity that the order parameter has necessarily a node on each sheet of the Fermi surface.

This is easily shown explicitly by solving exactly for the excitation spectrum of the Hamiltonian Eq. (3). One finds two branches $E_{\pm}(\mathbf{k})$ for this spectrum:

$$2E_{\pm}^2 = \eta + \eta' \pm \sqrt{(\eta - \eta')^2 + 4(\tau^2 + \delta^2)}, \quad (6)$$

where $\eta = \epsilon^2 + \Delta^2 + T^2$ and $\eta' = \epsilon'^2 + \Delta'^2 + T^2$, $\delta = T(\Delta - \Delta')$, and $\tau = T(\epsilon + \epsilon')$; ϵ and ϵ' are for ϵ_k and ϵ'_k. One obtains indeed that $E_-(\mathbf{k}) = 0$ if $\epsilon|\Delta'| = \epsilon'|\Delta| = \pm[|\Delta\Delta'|(T^2 - |\Delta\Delta'|)]^{1/2}$ and $\Delta\Delta' < 0$. The wave vectors of these zero energy excitations are actually slightly off the normal state Fermi surface, which is given by $\epsilon\epsilon' = T^2$. But the departure is small when the band coupling is large compared to the order parameter $T^2 \gg |\Delta\Delta'|$. On the other hand, it is very interesting to note that these zero energy excitations fuse at $\epsilon = \epsilon' = 0$ for $T^2 = |\Delta\Delta'|$, and they disappear for $T^2 < |\Delta\Delta'|$. However, in this regime $T^2 < |\Delta\Delta'|$, although there are no longer nodes in the gap, the coupling will produce a depression of the gaps of each band in the anticrossing regions. Naturally, one recovers for $T = 0$ the excitation spectrum $E_{\pm}^2(\mathbf{k}) = \epsilon^2 + \Delta^2$ and $\epsilon'^2 + \Delta'^2$ for uncoupled bands. In the regime $T^2 \gg |\Delta\Delta'|$, it is easier to first diagonalize the normal state Hamiltonian which leads to eigenstates with energies $e_{\pm}$. One then takes into account the pairing Hamiltonian, neglecting the coupling it induces between the bands $e_{\pm}$. This leads to the introduction of a $\mathbf{k}$ dependent order parameter Δ_k in each band. We find in this limit $\Delta_k = (\Delta\epsilon' + \Delta\epsilon')/(\epsilon + \epsilon')$, valid on the two sheets of the Fermi surface. Since on a given sheet one goes from $\epsilon \gg \epsilon'$ to $\epsilon \ll \epsilon'$, one sees explicitly that the order parameter goes continuously from Δ to Δ' or vice versa, and therefore changes sign for $\Delta\Delta' < 0$. Naturally, the values of Δ and Δ' are obtained from the couplings g, g', and K by the gap equations Eqs. (4) and (5). The inset shows the variation of the order parameter for the arbitrary choice $\Delta = 1$ and $\Delta' = -0.5$ (arbitrary units). The corresponding positions of the nodes of the gap are indicated in Fig. 1. We consider now the physical implications of our model, and show that it solves a number of problems, and accounts for many experiments.

Our model mixes features from s-wave and d-wave physics, and is therefore quite unconventional. It is d-wave-like because there are repulsive interactions between different parts of a given sheet of the Fermi surface, leading to a change of sign of the order parameter and nodes in the gap. The global result mimics closely d-wave pairing. However, in contrast with d-wave pairing, the nodes do not satisfy $k_x = \pm k_y$, since they are rather in the anticrossing regions (which happen to be not so far from $k_x = \pm k_y$ in YBCO). Because of the two sheets of the Fermi surface, we have eight nodes instead of four. On the other hand, our model is s-wave-like because the plane pairing is purely attractive. But, in contrast to standard superconductivity, the repulsive interaction contributes to raise T_c instead of destroying it. Finally, we obtain a strong anisotropy in the gap, although we do not need to invoke any anisotropy in the planes.

The c-axis Josephson experiment [3] is easily accounted for by our model, since the strengths $|\Delta|$ and $|\Delta'|$ of the order parameter with different signs are not related by any symmetry. Therefore, there is no reason for complete cancellation of the total current between different parts of the Fermi surface, while a partial cancellation may explain why the observed current is only 15% of the expected value. On the other hand, because the chain electrons have their velocity essentially along the b axis, they can naturally give the dominant contribution to tunneling in this direction, while only plane electrons (with opposite sign for the order parameter) will contribute to tunnelling along the a axis. Therefore, the situation is, in this respect, the same as with d-wave pairing, and our model accounts naturally for the π shift in corner SQUID experiments [5], as well as for the spontaneous magnetization $\Phi_0/2$ found in 3-grain-boundary junctions [6]. We provide also a possible explanation for the s-wave result of the hexagonal Josephson experiment [4]. Indeed, because of the specific choice of geometry, there is the possibility that no boundary is perpendicular to the b axis. This may imply that, because the chain electrons have their velocity along b, their contribution is strongly reduced (or at least overwhelmed by opposite sign contributions, in case of twinning, for example) leaving only the s-wave-like contribution from the plane electrons. Finally because of the nodes in the gap, our model explains naturally all the experiments in favor of low energy excitations ("states in the gap") such as the linear temperature dependence of the penetration depth, tunneling experiments, Raman scattering, and NMR [1].

The chain band is essential in our model in order to explain the peculiar properties of YBCO. It is clear that, if there is some sizable disorder in the chains, as produced, for example, by loss of O1 oxygen atoms, the anticrossing which occurs in specific regions of $\mathbf{k}$ space will be strongly perturbed or destroyed. We can model this effect by a decrease of the coupling T between plane and chain bands, since indeed the effect of the chain on the plane

will be reduced. As we have seen, this may lead to the disappearance of the nodes of the gap. And, indeed, only good YBCO crystals display a strong anisotropy of the penetration depth [14] (proving metallic behavior of the chains) and a linear T dependence of the penetration depth [7] (proving the existence of nodes). On the other hand, as we have seen, even if the nodes have disappeared, a local decrease of the gap will survive as a remnant if there is some coupling left. In this way our model provides a simple explanation for (strongly) anisotropic s-wave superconductivity. This may account for the observation of a small gap in penetration depth [15] or in tunneling experiments. Our explanation for the behavior of $\lambda(T)$ is naturally consistent with the fact that $\lambda(T)$ is BCS-like in $Nd_{1.85}Ce_{0.15}CuO_4$ [16], where only CuO_2 planes are present. Quite generally the systematic study of the effect of desoxygenation in YBCO will be a crucial test of validity for our model. We note in this respect that, in $Bi_2Sr_2CaCu_2O_8$, the BiO plane bands are coupled to the CuO plane bands [17], and that our model, where the role of the CuO chains would be played by the BiO planes, could also explain the strong anisotropy of the gap observed in photoemission experiments [8]. Naturally, this explanation will not work if the BiO bands are not metallic.

Our model accounts naturally for the fact that T_c in YBCO is rather insensitive to impurities [1] (except for magnetic ones). Indeed, since anticrossing occurs only in restricted regions of **k** space, we expect physically that impurity scattering is dominantly plane-plane or chain-chain, and not plane-chain. Therefore, electrons are not scattered between parts of the Fermi surface having order parameter with opposite sign, and the physical reason for the reduction of T_c mostly disappears. In contrast, nonmagnetic impurity scattering (as well as electron-phonon interaction) acts as a pair breaker in d wave [18], and the insensitivity of T_c requires more specific explanations.

We consider finally the dependence of T_c on the repulsive interaction K. Since we have no experimental indication of whether the pairing interaction on the chains g' is attractive or repulsive, we take $g' = 0$ for simplicity. Since the **k** summations in Eqs. (4) and (5) are over the whole Fermi surface, whereas anticrossing occurs only in restricted regions of **k** space, we can to a first approximation neglect the band coupling T. Introducing cutoffs ω_D and ω_c for the attractive and repulsive interactions, the weak coupling calculation gives

$$\frac{2}{\ln(1.13\omega_c/T_c)} = \frac{\lambda + \sqrt{\lambda^2 + 4kk'[1 + \lambda\ln(\omega_c/\omega_D)]}}{1 + \lambda\ln(\omega_c/\omega_D)}, \tag{7}$$

where $\lambda = Ng$, $k = Nk$, and $k' = N'K$, with N and N' the density of states of the (uncoupled) plane band and chain band. Naturally we find that the repulsive interaction increases T_c compared to having only attractive s-wave coupling λ. It is tempting to compare this with the increase of T_c when the chains in YBCO are built up upon adding oxygen. We may speculate that, at the 60 K plateau, only the attractive interaction is working, and that the increase up to 92 K is due to the increase of the repulsive interaction caused by the chain construction, though the variation of "doping" contributes also. We can also make an estimate of the isotope effect from Eq. (7): $(\delta\omega_D/\omega_D)/(\delta T_c/T_c) = 1 + 2(kk'/\lambda)\ln(1.13\omega_c/T_c)$. As expected, the repulsive interaction leads to a sizable decrease in the isotope effect. This may explain the small oxygen isotope effect observed in YBCO, while it is found to be much stronger for lower T_c superconductors such as LSCO. Therefore, we obtain, in agreement with experiment, an increase of T_c upon oxygenation while the isotope effect decreases at the same time.

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