Coupling Between Planes and Chains in YBa$_2$Cu$_3$O$_7$: A Possible Solution for the Order Parameter Controversy

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Abstract

We propose to explain the contradictory experimental evidence about the symmetry of the order parameter in YBa$_2$Cu$_3$O$_7$ 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, and provides a natural explanation for all the contradictory experiments.

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The mechanism responsible for pairing 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 the formation of pairs, as in the case where the interaction is due to the exchange of spin fluctuations [2]. For this specific case the order parameter has a d-wave symmetry which implies in particular that it changes sign on the Fermi surface. On the other hand an attractive interaction between electrons leads to an order parameter which does not change sign on the Fermi surface, even if there is a sizeable 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 conventional or unconventional, is to look experimentally at the symmetry of the order parameter.

Very surprisingly, recent experiments performed in $YBa_2Cu_3O_7$ in order to settle this issue of the order parameter symmetry have given convincing, but contradictory, answers [1]. For example the observation of a sizeable Josephson current [3] in a c-axis tunnelling junction between $YBa_2Cu_3O_7$ 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 an s-wave interpretation. On the other hand the evidence for a $\pi$ shift in corner SQUID experiments [5] is a clear indication for a change of sign of the order parameter between the a and the b axis. 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 which show an evidence for low energy excitations at low temperature, such as tunnelling [7], linear temperature dependence of the penetration depth in YBCO crystals or films [8], or photoemission experiments in $Bi_2Sr_2CaCu_2O_8$ [9] 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 of the variety of these experiments. A more natural view is to look for an explanation which allows to reconcile these various results.

It is just our purpose in this paper to present such a model, which blends s-wave and d-wave features, and provides a natural explanation for all the contradictory experiments [1]. The basic ingredient of our model is the coupling between planes and chains. 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, which is 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 dependence rather than in the wavevector 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 [4]. These two sheets could be produced by the two bands corresponding to the two CuO$_2$ planes, or they could correspond to the plane band and the chain band. Here we will take the view that, due for example to Coulomb interaction, the order parameter has opposite sign on the plane band and on the chain band. For simplicity we will consider here a single plane band.

However, although this change of sign of the order parameter on different sheets of the Fermi surface can account for the experiments showing a $\pi$ 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 which point 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. We propose to explain 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 eigenstates 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 \[10\]. Naturally this coupling is fairly small, and it 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 all 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 it is also seen in band structure calculations \[10\]. 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 which corresponds physically to a chain electron. We will take the following Hamiltonian as a model for the band structure:

\[
H_0 = \sum_k \varepsilon_k c_k^+ c_k + \sum_k \varepsilon'_k d_k^+ d_k + \sum_k T c_k^+ d_k + h.c.
\]  

(1)

It describes semi-quantitatively all the features of the band structure which are important for us. Here \(c_k^+\) and \(d_k^+\) are creation operators in the plane and in the chain band respectively. We take \(\varepsilon_k = -2t_0 (\cos(k_x a) + \cos(k_y a)) + 2t_0 \cos(k_x a) \cos(k_y a) - \mu_0\) and \(\varepsilon'_k = -2t_1 \cos(k_y a) - \mu_1\), with \(t_0 = 0.33\text{ eV}, t_1 = 0.53\text{ eV}, \mu_0 = -0.46\text{ eV}, \mu_1 = -0.74\text{ eV}\), 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 \(k\) dependence of the plane-chain coupling \(T\), since this term is relevant only in a rather small region in \(k\) space. Our model is purely 2-dimensional and we have neglected any 3-dimensional effect, since they are inessential for our purpose. The energy \(e_{\pm}\) of the eigenstates of Hamiltonian Eq.(1) are \(2 e_{\pm} = \varepsilon + \varepsilon' \pm \sqrt{ (\varepsilon - \varepsilon')^2 + 4 T^2 } \) and the corresponding Fermi surface \(e_{\pm} = 0\) is shown in Fig.1 for the
case $T = 0.1$ eV.

Let us now consider the superconducting state. In the planes we take a purely attractive pairing interaction, which can be for example of phononic origin. On the other hand the off-diagonal coupling between plane and chain is repulsive, as indicated above. Finally we have to consider for generality a pairing interaction in the chains. Neglecting all unnecessary wavevector dependence, this leads us in weak coupling to the following interaction (with singlet pairing understood): 

$$H_{\text{int}} = -g \sum_{k,k'} c_{k}^+ c_{-k'}^+ c_{-k} c_{k'} + K \sum_{k,k'} d_{k}^+ d_{-k}^+ c_{-k} c_{k} + h.c. + g' \sum_{k,k'} d_{k}^+ d_{-k}^+ d_{-k} d_{k} \tag{2}$$

where $g$ and $K$ are positive. This gives finally the following mean-field Hamiltonian:

$$H = H_0 + \Delta \sum_{k} c_{k}^+ c_{-k} + \Delta' \sum_{k} d_{k}^+ d_{-k} + h.c. \tag{3}$$

where we have set:

$$\Delta = -g \sum_{k} < c_{-k} c_{k}> + K \sum_{k} < d_{-k} d_{k}> \tag{4}$$

$$\Delta' = K \sum_{k} < c_{-k} c_{k}> + g' \sum_{k} < d_{-k} d_{k}> \tag{5}$$

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 $\Delta$ and $\Delta'$ (which correspond physically to the order parameter in the uncoupled planes and chains respectively) will have opposite sign. On the other hand, since (because of the anticrossing) when we move on a single sheet of the Fermi surface, we go continuously from a plane like 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 $\Delta$ on the plane like part, and to $\Delta'$ on the chain like 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 $E_{\pm}(k)$ for this spectrum:
where \( \eta = \epsilon^2 + \Delta^2 + T^2 \) and \( \eta' = \epsilon'^2 + \Delta'^2 + T^2 \), \( \delta = T (\Delta - \Delta') \) and \( \tau = T (\epsilon + \epsilon') \); \( \epsilon \) and \( \epsilon' \) are for \( \epsilon_k \) and \( \epsilon'_k \). One obtains indeed that \( E_{\pm} (k) = 0 \) if \( \epsilon |\Delta'| = \epsilon' |\Delta| = \pm [ |\Delta \Delta'| (T^2 - |\Delta \Delta'|)]^{1/2} \) and \( \Delta \Delta' < 0 \). The wavevectors 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 \( E_{\pm}^2 (k) = \epsilon^2 + \Delta^2 \) 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 takes then into account the pairing Hamiltonian, neglecting the coupling it induces between the bands \( e_{\pm} \). This leads naturally to the introduction of a \( k \) dependent order parameter \( \Delta_k \) 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, corresponding to each of the two bands. Since on a given sheet of the Fermi surface one goes from \( \epsilon >> \epsilon' \) to \( \epsilon << \epsilon' \), one sees explicitly that the order parameter goes continuously from \( \Delta \) to \( \Delta' \) or vice-versa, and therefore it changes sign for \( \Delta \Delta' < 0 \). Naturally the values of \( \Delta \) and \( \Delta' \) are obtained from the couplings \( g, g' \) and \( K \) by the gap equations Eq.(4) and (5). On Fig.2 we show the result for 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 will now consider 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 physics and from d-wave physics, and it 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 8 nodes instead of 4. 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 15th the chain electrons have their velocity essentially along the b-axis, they can naturally give the dominant contribution to tunnelling 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 $\pi$ shift in corner SQUID experiments [3], as well as for the spontaneous magnetization $\Phi_0/2$ found in 3-grain boundary junctions [3]. 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, tunnelling experiments, Raman scattering, NMR [4].
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 sizeable disorder in the chains, as produced for example by loss of 01 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 [11] (proving metallic behaviour 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 [12] or in tunnelling experiments. Our explanation for the behaviour of \( \lambda(T) \) is naturally consistent with the fact that \( \lambda(T) \) is BCS-like in \( Nd_{1.85}Ce_{0.15}Cu0_4 \) [13] where only \( Cu0_2 \) 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 Bi0 plane bands is coupled to the CuO plane bands [14] 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].

Finally 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 \( \mathbf{k} \) 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 therefore the physical reason for the reduction of \( T_c \) mostly disappears. In contrast non magnetic impurity scattering (as well as electron-phonon interaction) acts as a pair-breaker in d-wave [15], and the
insensitivity of $T_c$ requires more specific explanations. We note that we have used the same physical reason to restrict the attractive pairing interaction to the planes.

Let us conclude by some remarks on the dependence of the critical temperature $T_c$ on the repulsive interaction $K$. We have no experimental indication on whether the pairing interaction $g'$ is attractive or repulsive on the chains. Therefore let us take $g' = 0$ for simplicity. Since the summations over $k$ in Eq.(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 perform the calculation to zeroth order in the band coupling $T$. Introducing cut-off $\omega_\Delta$ and $\omega_c$ for the attractive and repulsive interactions $g$ and $K$, the weak coupling calculation leads to:

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

where $\lambda = N g$, $k = N K$ and $k' = N'K$, with $N$ and $N'$ being the density of states of the (uncoupled) plane band and chain band respectively. Naturally we find that the repulsive interaction increases the critical temperature, compared to the situation where we would only have the attractive s-wave coupling $\lambda$ at work. It is tempting to compare this increase with the increase of $T_c$ when the chains in YBCO are build-up upon adding oxygen. We may speculate for example that, at the 60 K plateau, only the attractive interaction is working, and that the increase up to 92 K is due to the progressive increase of the repulsive interaction caused by the chain construction, although there is also a contribution due to the variation of "doping". We can also make a rough estimate of the isotope effect from Eq.(7), which gives $(\delta\omega_D/\omega_D) / (\delta T_c/T_c) = 1 + 2 (kk'/\lambda) \ln (1.13\omega_c / T_c)$. As expected, the Coulomb repulsive interaction leads to a sizeable decrease in the isotope effect. This may explain the small oxygen isotope effect observed in $YBa_2Cu_3O_7$, while it is found to be much stronger for lower $T_c$ superconductors such as $La_{2-x}Sr_xCuO_4$. Therefore we obtain, in agreement with experiment, an increase of $T_c$ upon oxygenation while the isotope effect is decreasing at the same time. In this respect our model behaves as expected from a mixed mechanism where both electron-phonon interaction and Coulomb repulsion contribute to pairing.
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FIGURES

FIG. 1. Fermi surface in the Brillouin zone. The sign $\pm$ 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.

FIG. 2. Variation of the order parameter $\Delta_k$ on the two sheets of the Fermi surface for $k_x$ and $k_y > 0$, as a function of the angular position $\theta = \text{atan} (k_y / k_x)$. 
