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Orthorhombicity mixing of *s*- and *d*-gap components in $YBa_2Cu_3O_7$ without involving the chains

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Momentum decoupling develops when forward scattering dominates the pairing interaction. In this regime it is possible to obtain anisotropic *s*- or *d*-wave superconductivity even with isotropic pairing scattering. We show that in the momentum decoupling regime, the orthorhombic distortion of the CuO_2 planes is enough to explain the experimental reports for *s*- mixing in the dominantly *d*-wave gap of $YBa_2Cu_3O_7$. In the case of spin fluctuations mediated pairing instead, a large part of the condensate must be located in the chains in order to understand the experiments. [S0163-1829(98)51802-4]

The issue of the symmetry of the order parameter in the oxides has motivated intense investigations.[1] Advanced phase sensitive experiments allowed to establish that the order parameter in $YBa_2Cu_3O_7$ reverses its sign on the Fermi surface indicating *d*-wave symmetry.[2] This symmetry is generally believed to indicate spin fluctuation mediated superconductivity. The presence of nodes in the gap of $YBa_2Cu_3O_7$ is confirmed by the linear temperature dependence of the penetration depth in the low temperature regime.[3] However, there are also results that are in clear conflict with a simple *d*-wave picture.[4] In particular, *c*-axis Josephson tunneling experiments on $YBa_2Cu_3O_7$ indicated the existence of a significant *s* component.[5,6] It appears experimentally that the gap has a dominant *d*-wave component and also a significant *s*-wave component.[7] It has been argued that this behavior may indicate the existence of two different condensates.[8]

The mixing of *s* and *d* components arises naturally when the lattice is orthorhombically distorted.[9] Large orthorhombic distortions have therefore been invoked in order to understand the experimental conflicts in $YBa_2Cu_3O_7$.[10–12] However, the orthorhombic distortion of the CuO_2 planes in the case of $YBa_2Cu_3O_7$ is only a few percent ($\approx 3\%$) and such a small distortion cannot induce significant mixing of *s* components in a *d*-wave spin fluctuations mediated pairing. To reconcile the large orthorhombicity effects required by the phenomenology and spin fluctuations pairing, it has been argued that the Cu-O chains are involved in superconductivity and at least 25% of the condensate is located there.[12] Since the chain band concerns only one direction in the *ab* plane, if chains are involved, large in plane anisotropies are reasonable. Large anisotropies between the *a* and *b* directions are also reported in microwave penetration depth measurements.[13] A major involvement of the chains in the pairing[12] is supported by strong experimental arguments.[14] There are nevertheless equivalently strong arguments indicating that the pairing physics concerns mainly (if not only) the CuO_2 planes reviewed in Ref. 15. It can even been argued, on the basis of local-density approximation (LDA) calculations, that the chain bands do not contribute to the conductivity at all since oxygen vacancies disrupt the chains leaving purely localized electronic states.[16] Also, spin fluctuations are very sensitive on the dimensionality and is difficult to understand microscopically how they could mediate pairing simultaneously in the chains which are one-dimensional (1D) and in the planes which are 2D systems. Whether or not the chains contain a large fraction of the condensate is still an open issue. It is shown in the following that settling experimentally this issue will provide strong constraints on the structure of the pairing.

It has been proposed recently an alternative to spin fluctuations mechanism of anisotropies and gap symmetry transitions that involves isotropic scattering and has been named momentum decoupling (MD).[17–20] When the characteristic momenta exchanged in the pairing interaction are small compared to the characteristic momenta of the variations of the electronic density of states, there is tendency for decorrelation between the physical behavior in the different regions of the Fermi surface. In particular, couplings become proportional to the angular resolved electronic density of states (ARDOS) $N(E_F,\vec{k})=|v_F(\vec{k})|^{-1}$ at each region of the Fermi surface, and therefore anisotropies are driven by the electronic density of states and not by the scattering.[17] Taking into account the conventional Coulomb pseudopotential μ^* the *d*-wave and *s*-wave (both ARDOS driven anisotropic) states become energetically degenerate.[18] The presence of different gap symmetries in different oxides as well the *d*-*s* gap symmetry transition by overdoping $Bi_2Sr_2CaCu_2O_8$ (Ref. 21) are natural consequences of MD.[18,19] The temperature enhancement of the anisotropy[22] and the behavior of the anomalous dip above the gap in the electronic density of states[23] are qualitative puzzling aspects of the phenomenology of $Bi_2Sr_2CaCu_2O_8$ that also indicate MD.[17]

Dominance of forward scattering in the pairing could result from the vicinity of the strongly correlated electronic system to a phase separation instability[24] (which is an instability at $q\approx 0$). The interlayer tunneling mechanism proposed by Anderson is effectively $q\approx 0$ pairing and could be at the origin of MD.[25] The same for the charge transfer resonance pairing mechanism[26] which also concerns small momentum transfer process.[27] Notice that dominantly forward scattering has unexpected implications even for the normal state properties that have not yet been fully explored, like for

example, the possibility of linear T-dependent dc resistivity despite electron scattering with high energy phonons.[28] We report here that the orthorhombic distortion of the CuO_2 planes in $YBa_2Cu_3O_7$ (YBCO), produces an effect an order of magnitude larger in the case of MD than in the case of spin fluctuations pairing and could, therefore, explain the experimental reports of significant mixing of s components in the dominantly d-wave gap without need to involve the chains.

We solve the BCS equations on a two-dimensional lattice that might simulate the CuO_2 planes of YBCO. The gap is obtained by

$$\Delta(\vec{k}) = -\sum_{\vec{p},|\xi_{\vec{p}}|<\Omega_D} \frac{\Lambda(\vec{k}-\vec{p})\Delta(\vec{p})}{2\sqrt{\xi_{\vec{p}}^2+\Delta(\vec{p})^2}} \tanh\left(\sqrt{\frac{\xi_{\vec{p}}^2+\Delta(\vec{p})^2}{2T}}\right). \tag{1}$$

The materials characteristics enter through the dispersion $\xi_{\vec{k}}$. The effect of orthorhombicity on the CuO_2 plane is to make inequivalent the a and b axes and in $YBa_2Cu_3O_7$ the difference in these lattice constants is less than $\approx 3.5\%$. For such small variations we can consider that in a tight-binding dispersion the hoping along the two different axes will be inequivalent with differences of the same order. We consider in fact a simple next nearest neighbors tight binding fit to LDA calculations of the CuO_2 band in YBCO (Ref. 29)

$$\xi_{\vec{k}} = -2t[\cos(k_x)+(1+\beta)\cos(k_y)] - 4t'\cos(k_x)\cos(k_y) - \mu, \tag{2}$$

where $t=0.25$ eV, $t'/t=-0.45$, and $\mu=-0.44$ eV. This type of dispersion produces a van Hove peak in the density of states about 10 meV below the Fermi level (for the small distortions we consider here the singularity remains below the Fermi level). The relevant parameter for our discussion is β which characterizes the orthorhombic distortion.

The scattering amplitude $\Lambda(\vec{k}-\vec{p})$ in Eq. (1) contains the physics of the pairing mechanism. The two different situations of momentum decoupling and spin fluctuation pairing that we consider here correspond to two different characteristic structures of $\Lambda(\vec{k}-\vec{p})$. In the momentum decoupling regime the pairing scattering is isotropic taking at small momenta a Lorentzian form

$$\Lambda(\vec{k}-\vec{p}) = -\Lambda^o\left(1+\frac{|\vec{k}-\vec{p}|^2}{q_c^2}\right)^{-1} + \mu^*, \tag{3}$$

where the first term concerns the pairing and q_c plays the role of a momentum cutoff. This type of Lorentzian form is found to occur in the scattering of the electronic system with any bosonic system including phonons, provided the electronic system is close to the phase separation instability. This analysis will be presented in a forthcoming paper. The Coulomb pseudopotential μ^* is the effective repulsion of the paired electrons and is not necessarily momentum independent. We are in the MD regime provided the characteristic momenta of the variations of μ^* are large compared to q_c.

The interaction of Eq. (3) leads to either s- or d-wave superconductivity, depending on marginal for the pairing parameters like the magnitude of μ^* and its characteristic mo-

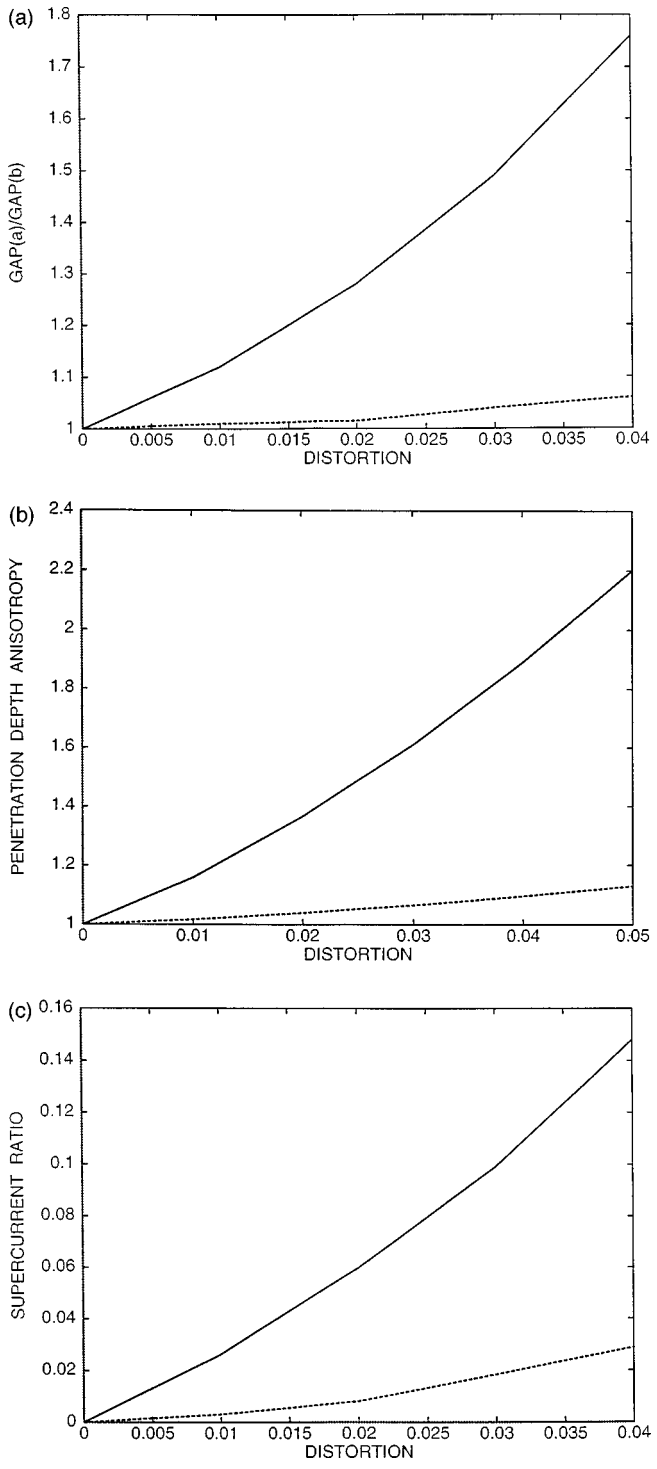

FIG. 1. (a) The ratio of the gaps along the a and b directions Δ_a^2/Δ_b^2 as a function of the distortion parameter β. (b) The London penetration depth in-plane anisotropy λ_b^2/λ_a^2 as a function of the distortion parameter β. (c) The ratio of supercurrent obtained from a Josephson junction of Pb with anisotropic YBCO over that expected from a junction of lead with isotropic YBCO with gap magnitude $(1/2)(|\Delta_a|+|\Delta_b|)$. In all cases the full lines correspond to the MD regime as described in the text and dashed lines to the MMP spin fluctuations scattering amplitude with the same dispersion conditions.

mentum range. Considering for μ^* a Lorentzian structure as that of the pairing amplitude we were able to plot a phase diagram of the energetically favorable (having the lowest free energy) gap symmetry (s-wave or d-wave) on a plane defined by the ratio of the characteristic cut-off of μ^* over that of the pairing amplitude and the magnitude of μ^* for an electronic structure similar to that of the oxides.[18,19] What is relevant for our discussion here is that a dominantly d-wave gap as reported by phase sensitive and node sensitive experiments on YBCO arises naturally for conventional values of μ^* with a pairing amplitude as in Eq. (3).[18,19]

The alternative ''conventional'' mechanism for d-waves is the scattering with spin fluctuations that has been extensively discussed in the literature. As an example of this second approach we consider the phenomenological Millis, Monien, and Pines (MMP) scattering with spin fluctuations[30] in the static limit

$$\Lambda(\vec{k}-\vec{p}) \approx \frac{\Lambda_o}{1+\xi_M^2(\vec{k}-\vec{p}-\vec{Q})^2}, \tag{4}$$

where $\vec{Q}=(\pi,\pi)$, the coherence range of the antiferromagnetic spin fluctuations ξ_M is taken on the order of three lattice spacings as in the experiment[30] and Coulomb pseudopotential is neglected.

In the orthorhombically distorted case a and b directions are not equivalent and since the Fermi velocities are different in these two directions one would expect different magnitudes of gap. The difference between the absolute values of the gap along a and along b is therefore a measure of the orthorhombicity effect. We plot in Fig. 1(a) the evolution of the ratio Δ_a^2/Δ_b^2 with β. In the tetragonal case $\beta=0$ this ratio is of course equal to unity. However, as we switch on the distortion β the maximum absolute values of the gap we obtain near the $(0,\pi)$ and $(\pi,0)$ points are appreciably different. Full line in Fig. 1(a) corresponds to the MD regime with a scattering amplitude as in Eq. (3) and dashed line to the MMP scattering amplitude given in Eq. (4). In both cases the energetically favorable d-wave channel is considered (in the MD case we take $q_c=\pi/10$ and $\mu^*/\Lambda^o=0.075$) and therefore the gap changes sign between $(0,\pi)$ and $(\pi,0)$. We can already conclude from Fig. 1(a) that in the case of MD the effect of orthorhombicity is an order of magnitude larger than in the case of spin fluctuations. In fact, the MMP interaction [Eq. (4)], contrary to the MD interaction [Eq. (3)], allows important scattering between the Fermi surface regions in the a and b directions cancelling the orthorhombicity effects.

Let us illustrate now that, in the MD case, the distortion of the CuO_2 planes may be sufficient to understand the experiments. We first consider the London penetration depth along the two different directions at zero temperature

$$\lambda_{k_{x(k_y)}}^{-2} \propto \sum_{\vec{k}} v_{k_{x(k_y)}}^2 [\partial f(E_{\vec{k}})/\partial E_{\vec{k}}], \tag{5}$$

where $E_{\vec{k}}=\sqrt{\xi_{\vec{k}}^2+\Delta_{\vec{k}}^2}$. The experimental results of Ref. 13 indicate large in-plane anisotropy of the penetration depth $\lambda_a/\lambda_b \approx 1.6$. We show in Fig. 1(b) the dependence of the penetration depth in plane anisotropy $\lambda_a^{-2}/\lambda_b^{-2}$ on the distortion parameter β. The full line corresponds to the MD regime while the dashed line to the MMP spin-fluctuation scattering. We see that in the MD regime the in plane distortion expected on the order $\beta \approx 0.03-0.04$ could be sufficient to produce the experimental in-plane anisotropy of the penetration depth, while for an MMP interaction, the calculated in plane anisotropy of λ is an order of magnitude smaller than in the experiment.

The same can be said for the c-axis Josephson tunneling results of Dynes and collaborators.[5,6] In fact, they observed Josephson tunneling currents on c-axis Pb/insulator/$YBa_2Cu_3O_7$ tunnel junctions. According to Ambegaokar and Baratoff[31] the Josephson current is given by

$$JR = \frac{2\pi T}{N_1 N_2} \frac{1}{\pi} \sum_{n=0}^{\infty} \sum_{\vec{k}} \frac{\Delta_1(\vec{k})}{\xi_1(\vec{k})^2+\Delta_1(\vec{k})^2+\omega_n^2} \sum_{\vec{k}'} \frac{\Delta_2(\vec{k}')}{\xi_2(\vec{k}')^2+\Delta_2(\vec{k}')^2+\omega_n^2}. \tag{6}$$

At zero temperature the sum over the fermion Matsubara frequencies is becoming an integral that can be performed straightforwardly, leading to the following expression for the Josephson current at $T=0$:

$$J(T=0)R = \frac{1}{2\pi} \frac{1}{N_1 N_2} \sum_{\vec{k}\vec{k}'} \Delta_1(\vec{k})\Delta_2(\vec{k}') \frac{1}{\sqrt{\xi_1(\vec{k})^2+\Delta_1(\vec{k})^2}\sqrt{\xi_2(\vec{k}')^2+\Delta_2(\vec{k}')^2}} \frac{1}{\sqrt{\xi_1(\vec{k})^2+\Delta_1(\vec{k})^2}+\sqrt{\xi_2(\vec{k}')^2+\Delta_2(\vec{k}')^2}}, \tag{7}$$

where R is the junction resistance and $N_i(0)$ the densities of states on the Fermi level. It is clear that if Δ_1 and Δ_2 are orthogonal (they belong to different irreducible representations of the point group), there should not be any Josephson current in the junction. Therefore, since the gap of Pb is known to be s wave, the observation of the Josephson current seems to exclude a purely d-wave gap in YBCO and a significant part of s component is necessary in order to have Josephson coupling between the two condensates. For the Pb/insulator/YBCO junction, if we suppose that the Pb gap is isotropic then in Eq. (6) the sum over k for the isotropic case is becoming trivial leading to a term proportional to the density of states of lead. At zero temperature the Matsubara frequency sum is becoming a frequency integral taking here

the form $\int_0^\infty d\omega F(\omega)G(\omega)$ where $F(\omega)=(\Delta_{\rm Pb}^2+\omega^2)^{-1/2}$ and $G(\omega)=(\xi_Y(\vec{k})^2+\Delta_Y(\vec{k})^2+\omega^2)^{-1}$. This integral is calculated numerically.

In Ref. 5 is reported a Josephson current along the *c* axis that was about 10% of what it should be expected from the isotropic Ambegaokar-Baratoff formula[31] if for YBCO the gap were taken equal to $1.76T_c$ as expected in weak coupling BCS theory. These experiments were repeated on untwinned crystals yelding very similar results and ruling out any possibility of second-order tunneling.[6] The weakness of the supercurrent could show that the *d* components are dominant in YBCO.[32] To our approach the gap in YBCO is indeed dominantly *d* wave yet because of the orthorhombic distortion there is also an *s* component that is responsible for the Josephson coupling with the condensate of lead. To show that this approach could reasonably account for the results of Refs. 5 and 6 we take two different cases. In the first case we consider the gap of YBCO to be isotropic and in the second case we obtain the gap from the solution of the BCS equations as previously. In both cases we adjust the YBCO gap to a value about 15 times larger than the gap of Pb. We also adjust the isotropic gap we take for YBCO in the first case to be equal to $(1/2)(|\Delta_a|+|\Delta_b|)$. What would be comparable to the findings of Ref. 5 is the ratio of the Josephson current that results using the anisotropic gap we obtain in the MD regime solving the BCS equations as previously over the supercurrent obtained in the isotropic case and which should correspond to the Ambegaokar-Baratoff expectations. We plot in Fig. 1(c) the evolution of this ratio with the distortion parameter β. When $\beta=0$ we have no Josephson supercurrent and as the distortion parameter reaches values as high as $\beta=0.04$ in the case of MD (full line) we can have appreciable supercurrents of the order of 15% of what should be expected in a junction between isotropic superconductors in agreement with the results of Ref. 5. With the MMP interaction instead the supercurrent is about an order of magnitude smaller than the experimental report.

It emerges therefore a fundamental qualitative difference between MD and spin fluctuations pairing. In the latter case, if the orthorhombic distortions interpretation of the *s* and *d* mixing in YBCO makes sense, the chains participate fundamentally in the pairing and at least about 25% of the condensate should be located there. On the other hand, in the case of MD, the orthorhombic distortion of the CuO_2 planes is sufficient to explain the puzzle of significant *s*-wave components in the dominantly *d*-wave gap of $YBa_2Cu_3O_7$.

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