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Effect Of Single Particle Hopping And Out Of Plane Magnetic Impurity On Coupled Planar Superconductors

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Abstract

It is shown that the single particle band motion along the c axis is harmful for superconductivity in anisotropic systems. Variation of T_c with c axis hopping parameter is shown for both the conventional Josephson coupled, planar superconductors and for interlayer pair tunneling mechanism of Wheatley Hsu and Anderson(WHA).Effect of out of plane magnetic impurity substitution is shown to suppres T_c more for conventional superconductors whereas there is very sharp decrease of T_c in the WHA mechanism at larger concentrations.

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All normal state properties of the high T_c materials are highly anisotropic in nature. For example, resistivity anisotropy ρ_c/ρ_{ab} is about 10^3 to 10^5 in Bi compounds [1]. On the other hand the typical anisotropies in the superconducting phase like λ_{ab}/λ_c and ξ_{ab}/ξ_c are much smaller (of the order of 5-10). This shows that the superconductivity is a real 3 dimensional phenomena, with the coupling between the CuO planes being a very relevent parameter. The normal to superconductor transition is at the same time a two to three dimensional transition.

Most theories of high T_c materials are purely two dimensional in nature, where the coupling between the planes is ignored to begin with. The large semiconducting type c axis resistivity (greater than Mott limit al low temperatures) is shown as a proof, that the electrons have no band motion along the c axis [2]. In other words c axis motion is fully incoherent. Invoking localisation along the c axis is meaningless, because electrons cannot localise along one direction only [2]. It has been emphasized by Anderson [2], that the single particle band term along the c axis is inoperative in the normal state, and in the superconducting state as well. On the other hand recently it has been argued by Rojo et. al, [3] that the large c-axis resistivity is not inconsistent with a finite hopping amplitude between the planes, because the off-diagonal disorder has a delocalization effect. For the superconducting state, at a phenomenological level they are described by a Lorence-Doniach kind of model [4]. Here the two adjacent CuO layers (who are individually superconducting , coming from any of the existing purely 2-d mechanisms) have a Josephson coupling between them. This coupling further enhances the transition temperature of the individual layers. A Josephson coupling between the planes tunnels pairs of electrons between the planes. One starts from an effective BCS hamiltonian for the two planes, and switches on a single particle hopping term in the c-direction. Josephson coupling occurs between the planes in second order of this single particle hopping amplitude.

We explicitly show here that, having a single particle tunneling term in the c-direction is harmful for superconductivity. This is because, as far as one plane is concerned, this acts as a pair breaking perturbation. So even though, the Josephson coupling leads to real 3-d coherence and an apparent increase in transition temperature, the single particle hopping between the planes ($t_\perp$) tries to destory superconductivity, and the T_c is very much suppresed compared to the purely decoupled 2-d superconductors, because the single particle and pair tunneling have opposite effects on T_c. We find that, for the model where, two planar BCS superconductors are coupled by both single particle and josephson tunneling, the T_c decreases with increase of $t_\perp$ slowly at first and very steeply at larger values. It is a monotonous decrease of T_c , in other words,single particle tunneling and consequent reduction of T_c due to pair breaking always plays a dominant role.

On the other hand , in the interlayer pair tunneling mechanism of Wheatley , Hsu and Anderson [5](WHA), it is argued that in the normal state there is no band motion of electrons in the c-direction, even though the hopping amplitude $t_\perp$ is quite substantial as many band theory calculations shows. This is so, because of the underlying assumpsion of spin-charge decoupling of the electronic system in the 2-d plane due to strong correlation. Therefore, even though $t_\perp$ is quite large , it is not effective in tunneling electrons in the c-direction simply because there are no low energy electron like quasiparticle near the Fermi surface in the 2-d plane (c-direction conduction is supposed to be purely incoherent in nature). In this mechanism, it is proposed that even in the superconducting phase single particle band motion is absent. The first channel of c- axis conductivity occurs in the second order in $t_\perp$, that is through Josephson pair tunneling. Incoherent motion of single electrons , but coherent tunneling of pairs of electrons is shown to be possible in model hamiltonian by Muthukumar et al [6] Here T_c increases with increase in $t_\perp^2$ unlike in the earlier case where T_c decreases with increase in $t_\perp$.

Next we consider the effect of magnetic impurity substitution out of the plane . There is a dramatic suppression of T_c upon substituting Y by Pr in YBCO compound , where Pr ions show a net magnetic moment ($\approx 2.7\mu_B$) as has been observed in the high temperature susceptibility data [7]. We consider the case , where out of plane magnetic impurity have no direct exchange coupling (of the local Kondo kind) with the conduction electrons in the plane. Also there is no hybridization of the impurity levels with the O or Cu orbitals. In other words , the presence of the moment does not change the in plane electronic parameters. In contrast, Fehrenbacher et. al, [8] has proposed that Pr electronic levels hybridize with the planar Oxygen leading to a decrease in the inplane hopping amplitude.

In the present situation, we show that for more conventional theories , where single particle motion in the c-direction is operative, there will be, (1) strong suppresion of T_c due to spin flip scattering by the impurity moment with the electrons moving along c-axis. (2) The second channel of conduction along the c-axis, that is the pair tunneling process, will also be affected by the magnetic impurity. The effect can be modelled , as if the Cooper pairs get a phase slip of π while travelling through the impurity center [9]. This will reduce effective pairing potential and hence reduce T_c. We will show that the first process of reduction of T_c is more dominant than the second one, because for moderate values of $t_\perp$, the Josephson tunneling between the planes, even in the absence of impurity increases T_c very slowly with increase of $t_\perp$. However, in the Wheatley Hsu Anderson mechanism(WHA)

, the single particle tunneling is absent. Only the interlayer pair tunneling , will be affected by the presence of the moments. In the WHA mechanism, the pair tunneling term is peculiar, in the sense that, in the process of pair tunneling, the individual momenta of the partners of the cooper pairs are conserved. So the pairing term in the hamiltonian there is only one momentum sum rather that the conventional two momenta sum. The pairing potential is extremely local in momentum space. This has a remarkable effect on T_c. The T_c increases with increase of pair tunneling amplitude(which is quadratic in $t_\perp$) much more steeply compared to the usual Josephson coupling case. Theoretically it is argued that, the pequliar momenta conserving pair tunneling is a consequence of the normal state being a Luttinger liquid [2]. This Josephson coupling will decrease with increase of magnetic impurity concentration due to phase slippage leading to decrease of T_c. We find that for low impurity concentration the T_c falls faster with impurity concentration in the conventional planar models, but at larger concentrations ,T_c falls faster in the WHA mechanism.

To begin we consider the hamiltonian,

$$\begin{aligned} H &= \sum_k ((\epsilon_k - \mu) c^{1\dagger}_{k\sigma} c^1_{k\sigma} + 1 \rightarrow 2) + t_\perp \sum_k (c^{1\dagger}_{k\sigma} c^2_{k\sigma} + h.c.) \\ &+ \sum_{kk'} (V_{kk'} c^{1\dagger}_{k\alpha} c^{1\dagger}_{-k\beta} c^1_{-k'\beta} c^1_{k'\alpha} + 1 \rightarrow 2) + \frac{t_\perp^2}{t} \sum_{kk'} (c^{2\dagger}_{k\alpha} c^{2\dagger}_{-k\beta} c^1_{-k'\beta} c^1_{k'\alpha} + 1 \rightarrow 2) \end{aligned} \tag{1}$$

Here all momenta are 2-d momenta. We consider a 2 layer per unit cell material. c^1_k and c^2_k are electron annihilation operators in layer 1 and 2. ϵ_k is the free dispersion in the plane and $t_\perp$ is the c-axis hopping amplitude. $V_{kk'}$ is a BCS type pairing potential in the plane, coming from any conventional mechanism, details of which are of no consequence for our purpose. $\frac{t_\perp^2}{t}$ is the Josephson coupling term. We have not taken any momentum dependence of the hopping amplitude $t_\perp$ along the c axis. $V_{kk'}$ is assumed to have the form,

$$V_{kk'} = \begin{cases} -V \;, & \text{for} \quad \epsilon_F - \hbar\omega_c \langle |\epsilon_k|, |\epsilon_{k'}| \langle \epsilon_F + \hbar\omega_c \\ 0 \;, & \text{otherwise} \end{cases} \tag{2}$$

Where $\hbar\omega_c$ is the cutoff energy coming from a more microscopic origin. We assume that the in-plane pairing interaction comes from electron phonon interaction. So ω_c will be the Debye frequency. For simplicity we assume that there is only one cutoff in the theory set by the in plane BCS coupling, and Josephson coupling also operates within the same cutoff.

Now we do the mean field, by putting in the pairing ansatz

$$\langle c^{1\dagger}_{k\uparrow} c^{1\dagger}_{-k\downarrow} \rangle = \langle c^{2\dagger}_{k\uparrow} c^{2\dagger}_{-k\downarrow} \rangle = \Delta^*$$

Then the third and fourth term can be combined into

$$(V + \frac{t_\perp^2}{t}) {\sum_k}' (\Delta^* c^1_{k\downarrow} c^1_{k\uparrow} + \Delta c^{1\dagger}_{k\uparrow} c^{1\dagger}_{-k\downarrow} + 1 \rightarrow 2)$$

Where the prime over the summation represents a restricted sum within the Debye Cut-off. To take into account the single particle hopping between the planes, we define two kinds of fermions

$$c^1_{k\sigma} = \frac{1}{2}(\phi_{k\sigma} + \psi_{k\sigma}) \text{ and } c^2_{k\sigma} = \frac{1}{2}(\phi_{k\sigma} - \psi_{k\sigma})$$

In terms of them the mean field hamiltonian will be

$$\sum_k (\epsilon_k - \mu + t_\perp) \phi^\dagger_{k\sigma} \phi_{k\sigma} + \sum_k (\epsilon_k - \mu - t_\perp) \psi^\dagger_{k\sigma} \psi_{k\sigma} + (V + \frac{t_\perp^2}{t}) \sum_k [(\Delta^* \phi_{-k\downarrow} \phi_{k\uparrow} + \Delta \phi^\dagger_{k\uparrow} \phi^\dagger_{-k\downarrow}) + \tag{3}$$

ϕ and ψ fermions describes the electrons in the bonding and antibonding bands. The hamiltonian looks like a sum of two BCS reduced hamiltonins for the bonding and antibonding electron systems. The generalised gap equation will be

$$\frac{1}{(V + \frac{t_\perp^2}{t})} = \frac{1}{2}\sum_k \frac{tanh(\beta E_k^\phi/2)}{2E_k^\phi} + \frac{1}{2}\sum_k \frac{tanh(\beta E_k^\psi/2)}{2E_k^\psi} \qquad (4)$$

where,

$$E_k^{\phi,\psi} = \sqrt{(\epsilon_k \pm t_\perp)^2 + \Delta^2}$$

Note that the summations over momenta in the first and second term are over two different energy shells centered around $\mu \pm t_\perp$. Going from summation to integral and converting to energy variables it is not very difficult to see that the T_c is given by

$$k_B T_c = \sqrt{\omega_c^2 - t_\perp^2}\,\frac{2e^\gamma}{\pi} e^{-\frac{1}{N(0)(V + t_\perp^2/t)}} \qquad (5)$$

for small values of $t_\perp$, where $e^\gamma = 1.781$. It is clear that the T_c decreases with increase in $t_\perp$ or more or less insensitive to it depending on the magnitude of ω_c and the in plane BCS coupling. Major effect of the out of the plane single particle hopping is to shrink the cutoff of the effective BCS interaction potential. Physically one should think of the single particle hopping in the c-direction acting as a pair breaking mechanism, and thereby destroying superconductivity. Energetically the condensation energy lost by losing superconductivity can be compensated by the gain in the single particle kinetic energy in the C direction. For larger values of $t_\perp$, band splitting will be larger and the chemical potential will be very near the band edge of one of the subbands, for low doping, while the other band will be submerged much below the Fermi surface. This kind of scenario has been proposed by Levin and Quader [11] to explain the transport properties in the normal state of the two layer materials. We do not consider this limit.

Next we consider the case where, there is some magnetic impurity in between the planes. Within the 1-band $t-J$ model scenario [10], the tunneling process in the c-direction is a two step process, where the inplane hole(Zhang -Rice singlet) moves over to the Y 6s orbital(for 123 compound) and from there to the ZR singlet in the upper plane. If one substitutes the Y atom by some other atom having a net magnetic moment, then this will scatter the electrons moving along the c direction. One can model the effect of the impurity by the interaction hamiltonian,

$$H' = U_2 \vec{S} \cdot \vec{\sigma} \qquad (6)$$

Where $\vec{S}$ denotes the impurity spin and $\vec{\sigma}$ the electron spin density. This will flip the spin of the electrons travelling along the c direction. We can rewrite the above Hamiltonian in the form

$$H' = \sum_{kk'} U(k-k')[(c_{k\uparrow}^{2\dagger} c_{k'\downarrow}^{1} + c_{k\downarrow}^{2\dagger} c_{k'\uparrow}^{1}) + 1 \rightarrow 2] \qquad (7)$$

It is reasonable to assume that the scattering will be predominantly in the forward or backward direction only. Also since the translational symmetry is broken only in the c direction , the inplane momenta should be conserved. So the interaction hamiltonian will be,

$$U(0)\sum_k (c_{k\uparrow}^{2\dagger} c_{k\downarrow}^{1} + c_{k\downarrow}^{2\dagger} c_{k\downarrow}^{1} \quad + \quad 1 \rightarrow 2)$$

for the forward scattering and similarly, there will be backward scattering terms like,

$$U(2k)\sum_k (c_{k\uparrow}^{1\dagger} c_{k\downarrow}^{1} + c_{k\downarrow}^{1\dagger} c_{k\downarrow}^{1} \quad + \quad 1 \rightarrow 2)$$

Going to the ϕ and ψ fermion representation, we get

$$H' = U_{eff} \sum_k (\phi_{k\uparrow}^\dagger \phi_{k\downarrow} + \phi_{k\downarrow}^\dagger \phi_{k\uparrow} + \phi \rightarrow \psi$$

Where $U_{eff} = U(0) + U(2k)$. In terms of these fermions, the interaction hamiltonian looks like *a direct exchange coupling of the impurity moment with the bonding and antibonding band* *electrons.* This will lead to a further reduction in the transition temperature as discussed by Maki [12]. The modified T_c will be, $T_c = T_{c0} - \frac{\pi}{4}\frac{1}{\tau_2}$, where

$$\frac{1}{\tau_2} = 2\pi U_{eff}^2 n N(0) S(S+1)$$

where n, $N(0)$ and S are the impurity density, conduction electron density of states near the Fermi surface and the impurity magnetic momont respectively. As discussed by Maki, not only the T_c will be suppressed and superconductivity destroyed beyond a certain concentration of impurity, but also , for moderate density of moments one will see a finite density of states within the gap. This could be observed in the tunneling and photoemission experiments.

Moving over to the pair tunneling from layer to layer, the tunneling hamiltonian can be written in the form,

$$\sum_{kk'} t_{\perp kk'}\delta_{ss'} + U_{kk'}\sigma_{ss'}S_i)c^{1\dagger}_{k\sigma}c^{2}_{k'\sigma'} + h.c$$

S_i is the operator for the local moment at site i and σ s are the Pauli matrices. It is not difficult to see that , whenever the cooper pair encounters a magnetic moment while travelling along the C axis, the corresponding pair tunneling amplitude gets reduced from $\frac{t_\perp^2}{t}$ to $\frac{(t_\perp^2 - U_{eff}s(s+1))}{t}$. The mean field pair tunneling hamiltonian will be after impurity average.

$$\frac{(t_\perp^2 - nU_{eff}^2 s(s+1))}{t}\sum_k(\Delta^* c_{-k\downarrow}c_{k\uparrow} + \Delta c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow} + 1 \to 2$$

where n is the concentration of magnetic impurity substituted in between the planes. Corresponding gap equation will be,

$$\frac{1}{V_{eff}} = \frac{1}{2}\sum_k \frac{\tanh(\beta E_k^{\rho}/2)}{2E_k^{\rho}} + \frac{1}{2}\sum_k \frac{\tanh(\beta E_k^{\gamma}/2)}{2E_k^{\gamma}} +$$

where $V_{eff} = V + t_\perp^2/t - nU_{eff}^2 s(s+1)/t$, remembering of course that with the introduction of single particle hopping the T_c will be further reduced the way we indicated before.

In the case of WHA mechanism, modified recently by Chakraborty et al [13], The full hamiltonian in absence of impurity is,

$$\sum_k(\epsilon_k - \mu)c^{1\dagger}_{k\sigma}c^1_{k\sigma} + 1 \to 2 + V\sum_{kk'} c^{1\dagger}_{k\uparrow}c^{1\dagger}_{-k\downarrow}c^2_{-k'\downarrow}c^2_{k'\uparrow} + h.c + 1 \to 2 \qquad (8)$$

$$+ t_\perp^2/t\sum_k c^{1\dagger}_{k\uparrow}c^{1\dagger}_{-k\downarrow}c^2_{-k\downarrow}c^2_{k\uparrow} + h.c + 1 \to 2 \qquad (9)$$

Notice the difference in the Josephson tunneling term in Chakraborty et al's hamiltonian from the conventional Josephson terms. The gap equation will be,

$$\Delta_k = \frac{t_\perp^2}{t}\frac{\Delta_k}{2E_k}\tanh(\beta E_k/2) + V\sum_q \frac{\Delta_q}{2E_q}\tanh(\beta E_q/2)$$

where $E_q = \sqrt{E_q^2 + \Delta_q^2}$ In the presence of magnetic impurity the gap equation will be modified to.

$$\Delta_k = \frac{(t_\perp^2 - nU_{eff}^2 s(s+1))}{t}\frac{\Delta_k}{2E_k}\tanh(\beta E_k/2) + V\sum_q \frac{\Delta_q}{2E_q}\tanh(\beta E_q/2)$$

We have solved all the gap equations numerically to locate the T_c.

We take the inplane dispersion to be $\epsilon_k = -2t(\cos k_x + \cos k_y) + 4t'\cos k_x \cos k_y - \mu$, with $t = 0.3$ eV, $t' = 0.1125$ eV, $\mu = -0.45$ eV, $v = 0.27$ eV and $t_\perp = 0.1$ eV. In Fig.1 we show the T_c variation with $t_\perp$ for interlayer tunneling mechanism and the usual Josephson coupled superconductors , with and without the band term along c axis. We find that, (1) For the interlayer tunneling mechanism the T_c rises with increase in $t_\perp$ very steeply. For example, with $t_\perp = 0.0$ we fix $V = 0.22$ to get a T_c of 5 degrees. But for $t_\perp = 0.1$ the T_c increase to 85 degrees. (2) For the usual Josephson coupled superconductor without single particle hopping, T_c rises very slowly with $t_\perp$. T_c is only 35 degrees for $t_\perp = 0.1$. (3)

With single particle hopping term included, remarkably the T_c decreases with increase in $t_\perp$. We emphasize that, there is no obvious reason why the single particle hopping along the c axis should be absent in conventional fermi liquid theories.. This is one of the important differences between the conventional Josephson coupling and Anderson's Josephson term.

In Fig.2 , we show the T_c variation with the pair breaking parameter $\alpha = U_{eff}^2 ns(s+1)$, which is directly proportional to the magnetic impurity concentration. Clearly the T_c in the interlayer tunneling mechanism falls slower than usual Josephson coupled superconductors for low concentration of impurity, but at larger concentrations it falls very steeply to zero The critical concentration of impurity is much smaller in the interlayer mechanism.

In conclusion , we have pointed out that even though Josephson coupling between plane increases T_c, the single particle hopping between the planes reduce T_c. For larger values of $t_\perp$, the increase of T_c by Josephson tunneling is taken over by the single particle hopping between the planes at any finite temperatures, and T_c will decrease with increase of $t_\perp$. Next we considered the effect on T_c by magnetic impurity substitution out of the plane, where the magnetic moment does not have any direct exchange coupling with the conduction electrons in the plane, and it does not change the inplane electronic parameters appreciably like Pr doping at Y sites does in the $YBCO$ compounds. In the case of purely planar models, there should not be any suppresion of T_c, but with a non zero effective band term along the c axis, superconductivity will be suppresed due to both by spin flip scattering by the moment as well as due to phase slip processes coming from the travelling cooper pairs along the c direction. For the WHA mechanism, only the second process is operative. We have done a quantitative prediction that, for small impurity concentration, the fall of T_c with impurity concentration in conventional planar superconductors is faster than in WHA case. At larger concentration of impurity , on the other hand T_c falls very sharply in WHA mechanism. This is so, because in the WHA mechanism even though the band motion of single quasiparticle motion along c axis is prevented, and hence the first channel of T_c reduction process is absent, but due to its peculiar momentum conserving nature of pair tunneling the T_c is a very sensitive function of the pair tunneling amplitude.

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Figure Captions

All the results were obtained with the following choice of parameters : t = 0.25 eV, t' = 0.1125 eV, ϵ_F = -0.45 eV, $t_\perp$ = 0.092 eV, V_{BCS} = 0.086 eV and $\hbar\omega_D$ = 0.02 eV.

1. T_c versus the interlayer hopping parameter $t_\perp$ for, Interlayer tunneling mechanism (dashed lines with open circles), Josephson coupled superconductors with and without single particle hopping term along c axis (dashed and solid line).

2. The variation of T_c with the pair breaking parameter α for a Josephson coupled BCS superconductor (dashed line) and in the interlayer tunneling mechanism (solid line). T_c is different for the two mechanisms for same values of parameters.

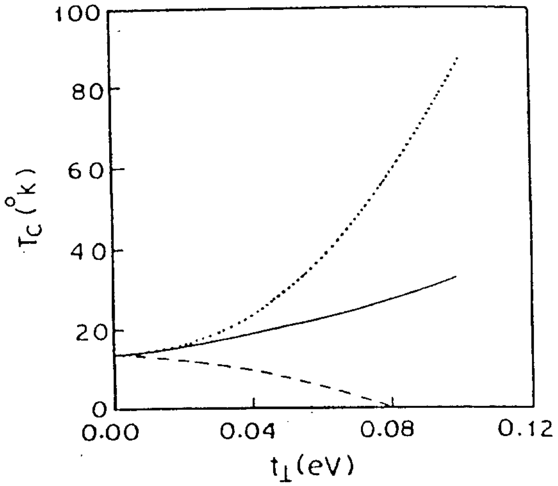
100
80
60
40
20
0
0.00
0.04
0.08
0.12
t⊥(eV)
Tc (°k)

Fig.1

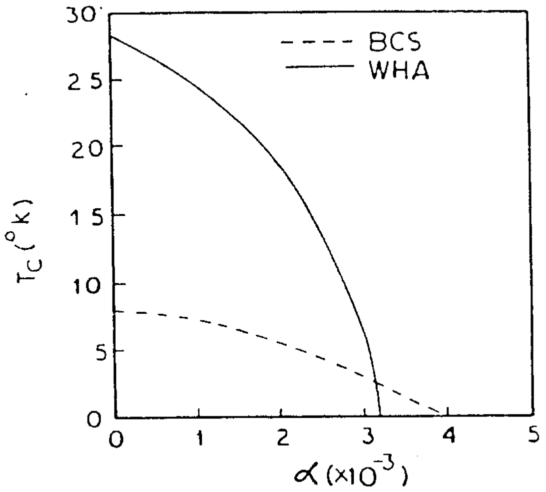
30
25
20
15
10
5
0
0
1
2
3
4
5
α (×10⁻³)
Tc (°k)
BCS
WHA

Fig.2