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Condensation energy of the superconducting bilayer cuprates

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Abstract. In the present work, we report the interplay of single particle and Cooper pair tunnelings on the superconducting state of layered high-T_c cuprate superconductors. For this we have considered a model Hamiltonian incorporating the intra-planar interactions and the contributions arising due to the coupling between the planes. The interplanar interactions include the single particle tunneling as well as the Josephson tunneling of Cooper pairs between the two layers. The expression of the out-of-plane correlation parameter which describes the hopping of a particle from one layer to another layer in the superconducting state is obtained within a Bardeen–Cooper–Schriefer (BCS) formalism using the Green's function technique. This correlation is found to be sensitive to the various parameter of the model Hamiltonian. We have calculated the out-of-plane contribution to the superconducting condensation energy. The calculated values of condensation energy are in agreement with those obtained from the specific heat and the c-axis penetration depth measurements on bilayer cuprates.

Keywords. Superconducting bilayer cuprates; condensation energy; Cooper pair tunneling.

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1. Introduction

It is observed that the physical properties of single CuO_2 layer in single layer systems ($La_{2-x}Sr_xCuO_4$) are quite different from the multilayered systems in normal as well as in the superconducting state [1,2]. The superconducting transition temperature of these cuprates also depends on the number of CuO_2 layers per unit cell and the extent of doping. In a bilayer or multilayer cuprate the separation between adjacent CuO_2 planes within the unit cell is smaller than the adjacent layers in a single layer system; therefore it is natural to include interlayer coupling in multilayer/bilayer cuprates. The coupling between the planes within a unit cell in multilayer cuprates is important and should be included in a discussion of the superconducting behavior of these systems [3,4].

In order to describe the physical properties as well as the high superconducting transition temperature in cuprates, Anderson and his collaborators [4–7] have presented a mechanism of high-T_c superconductivity based on the tunneling of charge carriers between the layers; this model is known as the interlayer tunneling (ILT) model. These authors have suggested that the pairing mechanism within a given bilayer system can be amplified by allowing the Cooper pairs to tunnel to an adjacent layer, i.e., a sort of Josephson mechanism. The delocalization of these pairs gives rise to an enhancement in the pairing only if the incoherent single particle tunneling between the layers is blocked. This implies that in the superconducting state the single particle tunneling is replaced by 2D normal state to the coherent 3D superconducting state. This change in the c-axis kinetic energy of the electrons as they enter the superconducting state is known as the out-of-plane contribution to the superconducting condensation energy and a nonzero value of this energy makes the formation of Cooper pairs energetically favorable [7].

Recently, Ajay [8] and Ajay and Tripathi [9] have analyzed the role of single particle interlayer hopping on the superconducting state of layered cuprates within the BCS formalism. The author suggested that in the superconducting state the hopping of the holes between the layers gets suppressed. It is further argued that this is due to superconducting energy gap in the electronic state around the Fermi level and it is not possible for a single particle to overcome this gap. In the superconducting phase the states around the Fermi level are occupied by Cooper pairs and the possibility of tunneling of paired carriers is high. Hence, it is quite important to analyze how these two out-of-plane tunnelings couple with each other at or below the superconducting transition.

2. The model for bilayer cuprates

To study the interplay of single particle tunneling and Josephson-like Cooper pair tunneling in the superconducting state of layered cuprate superconductors, we consider the microscopic model Hamiltonian that incorporates the intra-planar interactions along with coupling between the planes in the form of the single particle tunneling as well as Cooper pair tunneling.

The model Hamiltonian of the system is given as

$$H_{\text{bilayer}} = H_{\text{intra}} + H_{\text{inter}} \tag{1}$$

where

$$\begin{aligned} H_{\text{intra}} = &-\sum_{rij\sigma}(t_{ij} - \mu)C^{+}_{ri\sigma}C_{rj\sigma} + U\sum_{ri\sigma} n_{ri\sigma}n_{ri-\sigma} \\ &+ \frac{1}{2}\sum_{ij\sigma,r} W_{ij}n_{ri\sigma}n_{rj-\sigma} \end{aligned} \tag{1a}$$

$$\begin{aligned} H_{\text{inter}} = &\frac{1}{2}\sum_{r\neq sij\sigma} t_{\perp}(C^{+}_{ri\sigma}C_{sj\sigma} + \text{h.c.}) \\ &+ Z\sum_{r\neq sij\sigma}[C^{+}_{ri\sigma}C^{+}_{ri-\sigma}C_{sj-\sigma}C_{sj\sigma} + \text{h.c.}] \end{aligned} \tag{1b}$$

where t_{ij} is the hopping matrix element within the plane, μ is the chemical potential, U is the on-site Coulomb repulsion and W is the intersite attractive interaction within CuO_2

plane. r, s are layer indices, with $r = 1(2)$, $s = 2(1)$ for the bilayer systems; i, j are the hole sites; σ is the spin of holes, $C^+(C)$ is the creation (annihilation) operator for holes within CuO_2 planes. In the interlayer part of the Hamiltonian given by eq. (1b) the first term describes the single particle hopping between the planes with $t_\perp$ as the hopping matrix element in the out-of-plane direction. The second term containing tunneling parameter Z defines a Josephson-like pair tunneling process between the two adjacent planes in the unit cell.

We write the Hamiltonian in k-representation by performing the Fourier transformation. In order to obtain expressions for the superconducting order parameter and the carrier density we employ the Green's function technique and use the standard procedure as described in our earlier work [8,10]. The Green's function equations contain the higher order Green's functions which are linearized into lower ones by employing a suitable decoupling scheme in which the various correlations like $\langle C^+_{rk\sigma} C^+_{r-k-\sigma}\rangle$ and $\langle C^+_{rk\sigma} C_{sk\sigma}\rangle$ important in the superconducting state of a bilayered cuprate system, are retained [9]. The following expression for the superconducting order parameter within the BCS framework can be obtained from the relevant Green's function.

$$\begin{aligned}\Delta &= \frac{1}{N}\sum_k \overline{U}\langle C^+_{1k\sigma}\,;\,C_{1-k-\sigma}\rangle \\ &= -\frac{\overline{U}\Delta}{N}\sum_k\left[\frac{\tanh(E_{1k}/2k_{\mathrm{B}}T)}{4E_{1k}} + \frac{\tanh(E_{2k}/2k_{\mathrm{B}}T)}{4E_{2k}}\right].\end{aligned} \tag{2}$$

Here, Δ is the superconducting order parameter and $\overline{U} = U + W + Z$ is the effective attractive pairing interaction within the plane. Here W and Z are negative (attractive nature) and U is the positive (repulsive nature), and the combined effective interaction $\overline{U}$ is assumed attractive (negative) to give rise to pairing within the plane. The expressions for the carrier density within the plane $\langle n_{ab}\rangle$ and the out-of-plane correlation parameter $\langle n_c\rangle$ which takes care of single particle tunneling in the superconducting state, are obtained:

$$\begin{aligned}\langle n_{ab}\rangle &= \frac{1}{N}\sum_k \langle C^+_{1k}; C_{1k}\rangle \\ &= -\frac{1}{N}\sum_k\left[\frac{\tilde{\varepsilon}_{1k}\tanh(E_{1k}/2k_{\mathrm{B}}T)}{4E_{1k}} + \frac{\tilde{\varepsilon}_{2k}\tanh(E_{2k}/2k_{\mathrm{B}}T)}{4E_{2k}}\right]\end{aligned} \tag{3}$$

and

$$\begin{aligned}\langle n_c\rangle &= \frac{1}{N}\sum_k \langle C^+_{1k}; C_{2k}\rangle \\ &= -\frac{1}{N}\sum_k\left[\frac{\tilde{\varepsilon}_{2k}\tanh(E_{2k}/2k_{\mathrm{B}}T)}{4E_{2k}} - \frac{\tilde{\varepsilon}_{1k}\tanh(E_{1k}/2k_{\mathrm{B}}T)}{4E_{1k}}\right].\end{aligned} \tag{4}$$

In the above $\varepsilon_{1,2k} = (\varepsilon_k - \mu + (W+U)\langle n_{ab}\rangle) \pm t_\perp$; $\varepsilon_k = -2t_{||}(\cos k_x a + \cos k_y a)$ and $E_{1,2k} = \sqrt{\tilde{\varepsilon}^2_{1,2k} + \Delta^2}$. Note that we have a tight binding band model in the ab-plane defined by plane hopping parameter $t_{||}$ and a is the lattice parameter. In the limit of $t_\perp \to 0$, i.e., when there is no single particle hopping between two planes, the electron motion in two planes becomes independent, i.e., $E_{1k} = E_{2k}$. A close examination of eqs (2)–(4) reveals that these are coupled equations and require a self-consistent solution. From eq. (2) one can study the superconducting order parameter as a function of doping as well as other parameters $t_{||}$ and Z of the model Hamiltonian.

3. Results and discussion

We study the behavior of the superconducting order parameter for different values of out-of-plane couplings. We convert the summations over k values in eqs (2)–(4) into an integration and set the limit $T \to 0$ to study $\Delta(0)$ and the out-of-plane correlation $\langle n_c \rangle_0$ at zero temperature. The numerical calculations are done self-consistently. In the limit $T \to T_c$, the superconducting order parameter $\Delta \to 0$. Under this limit the out-of-plane correlation at T_c can be obtained analytically from eq. (4) and we find

$$\langle n_c \rangle_{T_c} \approx \frac{t_\perp}{2k_B T_c} . \tag{5}$$

It is clear from eq. (5) that around superconducting transition temperature T_c, for a given interlayer hopping matrix element, the out-of-plane correlation is inversely proportional to the superconducting transition temperature T_c, i.e., on increasing the transition temperature the out-of-plane hopping correlation $\langle n_c \rangle_{T_c}$ decreases. This seems quite reasonable because if T_c is high the superconducting energy gap parameter will be large and it works like a barrier for single particle tunneling. Under such circumstances the single particle tunneling will diminish.

The kinetic energy of the particles moving in the out-of-plane direction can be calculated with the help of out-of-plane correlation. As the kinetic energy of the particles moving in the out-of-plane direction will be equivalent to the out-of-plane correlation at superconducting transition temperature $\langle n_c \rangle_{T_c}$ multiplied by out-of-plane hopping matrix element $t_\perp$ [4]. At very low temperatures below T_c the single particle tunneling gets blocked and is replaced by Josephson pair tunneling. From Anderson's ILT model as well as from the energy conservation principle, the change in the kinetic energy of the electrons in the out-of-plane direction at superconducting transition will serve as the out-of-plane contribution to the superconducting condensation energy to establish superconducting long range order. Hence, multiplying eq. (5) by $t_\perp$ one can calculate the out-of-plane contribution to the superconducting condensation energy which can be written in the form

$$E_b \approx \frac{t_\perp^2}{2k_B T_c} . \tag{6}$$

From eq. (6) one can see that for a given cuprate system if we have an estimate of the out-of-plane hopping matrix element $t_\perp$ (the magnitude of $t_\perp$ is 2–500 meV in cuprates) and the superconducting transition temperature, then the contribution of the out-of-plane coupling towards superconducting condensation energy can be estimated. For a typical value of $t_\perp = 2$ meV and $T_c = 90$ K, the superconducting condensation energy for bilayered cuprates, E_b, comes out to be approximately 3.2 K which is very close to the condensation energy (around 3 K) esimated from specific heat measurements for bilayer cuprate $YBa_2Cu_3O_7$ system by Loram *et al* [11]. This value is also in agreement with the estimates

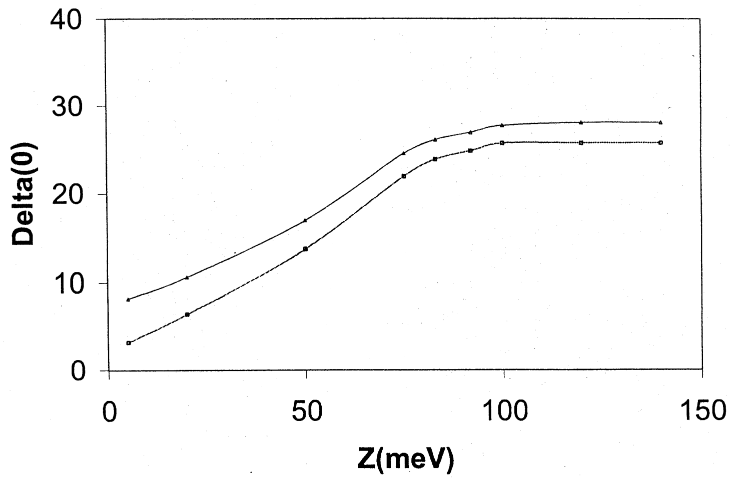

Figure 1. The variation of the superconducting order parameter $\Delta(0)$ (in meV) vs. pair tunneling parameter (Z) with (**a**) $\bar{U} = -0.25$ eV (triangles), (**b**) $\bar{U} = -0.2$ eV (squares). The other parameter values are taken to be $t_{||} = 250$ meV, $n_{ab} = 0.1$ and $t_{\perp} = 20$ meV.

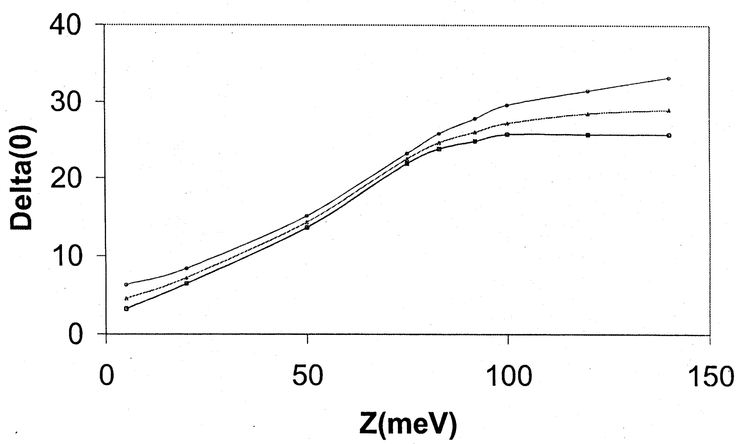

Figure 2. The variation of the superconducting order parameter $\Delta(0)$ (in meV) vs. pair tunneling (Z) with (**a**) $t_{\perp} = 10$ meV (circles), (**b**) $t_{\perp} = 15$ meV (triangles) and (**c**) $t_{\perp} = 20$ meV (squares). The other parameter values are $\bar{U} = -0.2$ eV, $t_{||} = 250$ meV and $n_{ab} = 0.1$.

of the condensation energy on the basis of c-axis electrodynamics within ILT theory due to Anderson [4,5].

In figure 1 we have plotted $\Delta(0)$ vs. Z, the Josephson pair tunneling parameter. It is clear from the figure that on increasing the magnitude of Josephson coupling between the layers, $\Delta(0)$ increases sharply initially and then saturates for higher values of Z. $\Delta(0)$ increases with the increase in the magnitude of effective attractive interaction within the layers and an increase in Z increases the effective attractive interaction. This implies that the increase in the coherent Cooper pair tunneling provides favorable conditions for the formation of Cooper pairs within the plane due to increase in the effective attractive interaction up to a certain value of Z. Here also the same Z for a large magnitude of $\overline{U}$, leads to larger $\Delta(0)$. To understand the Z-dependence of $\Delta(0)$, we have plotted the order parameter $\Delta(0)$ vs. Z for different values of $t_\perp$ in figure 2. The figure shows the interplay between the single particle hopping and the pair tunneling interaction. The pair tunneling interaction tries to enhance the superconducting order parameter whereas the single particle hopping tries to reduce it. For higher values of pair tunneling parameter and sufficiently large $t_\perp$ (single particle tunneling parameter) the two effects balance each other and order parameter $\Delta(0)$ saturates as seen in figure 1.

4. Conclusion

In conclusion, our present studies suggest that the coherent Josephson-type Cooper pair tunneling between the layers strengthens the superconducting long-range order. The out-of-plane contribution to the superconducting condensation energy is in agreement with the existing results on condensation energy calculated using specific heat measurements.

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