Study of penetration depth as a function of temperature, in-plane hopping and single particle tunneling in cuprate superconductors

Mahipal Singh* and Vikash Dubey#

*Department of Physics, Govt. P.G. College, Bageshwar (Uttarakhand)-263642, India
#Department of Physics, Govt.P.G. College, Ramnagar (Uttarakhand), India

Abstract
The present study deals with the study of penetration depth as a function of in-plane hopping matrix element, single particle tunneling between the layers and temperature in bilayer high temperature cuprate superconducting materials. For this purpose, a tight binding bilayer Hubbard Hamiltonian has been considered that includes the in-plane (within CuO$_2$ plane) and out-of-plane interactions. Employing Green’s function technique, the expressions for superconducting order parameters, carrier density and penetration depth are obtained. The numerical analysis shows that in bilayer cuprates the penetration depth depends on in-plane hopping matrix element, single particle tunneling as well as on temperature in an essential way. Finally, we have compared our theoretical results on penetration depth with that of recent experimental results and found to be in qualitative agreement.

Keywords: Cuprate superconductors, Single particle tunneling, In-plane hopping matrix element, Penetration depth

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INTRODUCTION

Almost all high-$T_c$ cuprate superconductors possess layered perovskite-like crystal structure which consists of stacks of conducting two dimensional CuO$_2$ planes separated by charge reservoir blocks. The electronic structure of YBa$_2$Cu$_3$O$_{6.8}$ (YBCO) system is quite complicated because there are two CuO$_2$ planes, approximately 3.2 Å apart, per unit cell and these planes are separated by a yttrium ion(1). Besides this, in YBCO, there are one dimensional CuO chains along b-direction(2). The CuO$_2$ planes work as superconducting electrodes separated by BaO, SrO or BiO type of layers which act as weak links or insulating barriers depending on doping. In the superconducting state, the intrinsic Josephson’s effect has been discovered in Bi$_2$Sr$_2$CaCu$_2$O$_8$ and later confirmed in YBa$_2$Cu$_3$O$_{6.8}$ bilayer system(3-5). The intrinsic Josephson’s coupling facilitates the transfer of Cooper pair from one layer to another layer in the superconducting state while in the normal state, the two CuO$_2$ planes are coupled through single particle tunneling. Therefore, it is interesting to study the electrical property like supercurrent density and hence penetration depth as a function of in-plane hopping matrix element, single particle tunneling between the layers and temperature under competitive Josephson’s tunneling parameters in these multilayer materials[since supercurrent density I$_c$ is related to penetration depth $\lambda$ as $I_c \propto 1/\lambda^2$ (6)].

Recently, many experiments have been done to measure the penetration depth of various cuprate superconductors like La$_2$Sr$_2$CuO$_4$, YBa$_2$Cu$_3$O$_{7-x}$ and Bi$_2$Sr$_2$La$_x$CuO$_6$, TbBa$_2$CuO$_{6+\delta}$ and HgBa$_2$CuO$_{6+\delta}$ provide useful information about the superconducting state. Panagopolous et al (7), Shibata et al (8), Zaleski et al (9) focused experiments on c-axis penetration depth and they suggested that the variation of c-axis penetration depth ($\lambda_c$) with temperature is qualitatively different from the temperature variation of ab-plane penetration depth ($\lambda_{ab}$). At low temperatures, $\lambda_c$ shows a weaker temperature dependence compared to that of the in-plane penetration depth ($\lambda_{ab}$). Bonn et al (10) measured the penetration depth of a twin-free crystal of YBa$_2$Cu$_3$O$_{6.85}$ and found the linear temperature dependence of the penetration depth at low temperatures rather than the exponentially activated behaviour of an s-wave BCS superconductor.

Very recently, Zhou et al (11) studied universal scaling relation for high-temperature cuprate superconductors and concluded that $\lambda_{ab}^{-2}$ varies linearly with ($T/ T_{c max}$)$^{0.53}$ where $\lambda_{ab}$ is the inplane London penetration depth, $T$, $T_{c max}$, $\sigma_{dc}$ and $T_c$ are pseudogap temperature, maximum transition temperature, dc conductivity and superconducting transition temperature. Zaitsev et al (12) studied experimentally the dependence of superconducting current density on interlayer thickness and concluded that the superconducting current density decreases linearly with the interlayer thickness.

The various theoretical models have been proposed to understand the behaviour of penetration depth in YBCO. Donovan et al (13), starting with a model of isolated planes coupled through a transverse matrix element, considered the possibility of intra as well as inter-plane pairing within a nearly antiferromagnetic Fermi-liquid model and discussed the temperature dependence and in-plane anisotropy of the penetration depth in YBCO. They found that the penetration depth remains linear in the temperature at low temperature. Radike et al (14) found a weak temperature dependence of the London penetration depth along the c-direction in the cuprates. Singh et al (15) studied the effect of temperature, in-plane hopping matrix element
and single particle tunneling between the layers on supercurrent density in bilayer cuprate superconductors and concluded that in bilayer cuprates, supercurrent density depends on in-plane hopping matrix element and single particle tunneling as well as on temperature in an essential way. Very recently, Singh(16) studied the influence of temperature on penetration depth in bilayer cuprate superconductors and concluded that in bilayer cuprates the penetration depth depends on temperature in an essential way.

The above facts have motivated us to study the penetration depth as a function of in-plane hopping matrix element, single particle tunneling between the layers in these bilayer materials by considering a microscopic tight binding bilayered Hubbard model.

**THEORETICAL MODEL FOR BILAYER CUPRATES**

We consider the cuprates like YBa$_2$Cu$_3$O$_y$, having two CuO planes per unit cell. As it is believed that the physics of superconducting CuO planes can be well captured by a two dimensional tight binding Hubbard model, hence we simulate the coupled CuO planes by a bilayer Hubbard model with an effective attractive interaction within the plane. In order to introduce the coupling between neighbour CuO planes within the unit cell, we will incorporate single particle tunneling as well as Josephson like Cooper pair tunneling terms in the model Hamiltonian and analyse the role of these couplings on the supercurrent density. This situation for the bilayered cuprates will just serve as a SIS junction(17) along with a sort of Josephson like coupling, where CuO planes are working as superconducting electrodes separated by BaO types of insulating layer. Thus the microscopic tight binding model Hamiltonian of our bilayer system is given by:

$$H_{\text{bilayer}} = H_{\text{ intra}} + H_{\text{inter}} \quad \ldots (1)$$

where,

$$H_{\text{ intra}} = -\sum_{\sigma, \sigma', \mathbf{r}, \mathbf{r}'} t_{\mathbf{r}, \mathbf{r}'} C_{\mathbf{r}, \sigma}^\dagger C_{\mathbf{r}', \sigma'} + U \sum_{\mathbf{r}, \sigma} n_{\mathbf{r}, \sigma} n_{\mathbf{r}, \sigma'} + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} W_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} n_{\mathbf{r}, \sigma} n_{\mathbf{r}', \sigma'} \quad \ldots (1a)$$

and

$$H_{\text{inter}} = \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma} \varepsilon_{\mathbf{r}} C_{\mathbf{r}, \sigma}^\dagger C_{\mathbf{r}', \sigma} + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \sigma, \sigma'} (C_{\mathbf{r}, \sigma} C_{\mathbf{r}', \sigma'} + h.c.) \quad \ldots (1b)$$

where $t_{\mathbf{r}}$ is the hopping matrix element within the plane and $\mu$ is the chemical potential. $U$ and $W$ are on-site and inter-site attractive interactions within CuO plane; $r$, $s$ are layer indices, with $r = 1(2)$, $s = 2(1)$ for the bilayer systems; $i$, $j$ are the hole sites; $\sigma(-\sigma)$ are the spin of holes, $C^\dagger(C)$ are the creation (annihilation) operator for holes within CuO planes. The $H_{\text{ intra}}$ part of the model Hamiltonian given by equation (1a) is just the BCS – Hamiltonian with an effective attractive interaction that comprises the on-site interaction $U$ and inter-site interaction $W$ within CuO planes. In our present attempts, we consider the on-site interaction $U$ to be attractive as we are interested in the physics of superconducting state. However, to study the interplay of magnetism and superconductivity a repulsive U term is important to take care of electron correlations that exist in cuprates.

The first term in the interlayer part of the model Hamiltonian given by equation (1b) is the single particle hopping between the planes. The second term contains tunneling parameter $Z$ that defines a Josephson like pair tunneling process between the two adjacent planes in the unit cell.

By performing Fourier transformation in the usual way, the model Hamiltonian can be written in the momentum space. Employing Green’s function many body technique and using standard procedure Govind et al (18) have obtained the expression for superconducting order parameter within the BCS framework for the above model, which is given as:

$$\Delta = \frac{\langle \bar{U} \Delta / N \rangle}{\sum_k \left[ \tanh\left( \frac{E_{1K} + E_{2K}}{4E_{\text{F}}K} \right) + \tanh\left( \frac{E_{1K} - E_{2K}}{4E_{\text{F}}K} \right) \right]} \quad \ldots (2)$$

where, $\Delta$ is the superconducting order parameter and $\bar{U} = U + W + Z$, is the effective attractive interaction within the plane. Here $Z$ is also negative (attractive nature) so that the effective interaction $\bar{U}$ is assumed to be attractive (negative) to gives rise to the pairing within the CuO planes. In the above,

$$E_{1K} = \left( E_{K} - \mu + (U + W) \langle n_{ab} \rangle \right) + \epsilon_{K, \perp};$$

$$E_{K, \perp} = -2t_{11} \left( \cos k_x a + \cos k_y a \right);$$

$$\langle n_{ab} \rangle = \frac{(\langle n_{a b} \rangle)}{\langle n_{\sigma} \rangle} \quad \ldots (3)$$

where, $\langle n_{ab} \rangle$ is the carrier density within the plane in the superconducting state. We have assumed that $\langle n_{ab} \rangle = \langle n_{\uparrow} \rangle = \langle n_{\downarrow} \rangle$ and ‘$a$’ is lattice parameter. The carrier density $\langle n_{\sigma} \rangle$ is given as:

$$\langle n_{\sigma} \rangle = \frac{1}{(N)} \sum_{\mathbf{k}} \left[ \varepsilon_{\mathbf{k}} \tanh\left( \varepsilon_{\mathbf{k}} / 2E_{\text{F}}K \right) + \varepsilon_{\mathbf{k}} \tanh\left( \varepsilon_{\mathbf{k}} / 2E_{\text{F}}K \right) \right] \quad \ldots (3)$$

In order to analyse the full temperature dependence of supercurrent density for coupled bilayered system which is equivalent to a SIS junction, we shall use the Ambegaoker-Baratoff microscopic result for a tunnel junction (SIS) (19) which is given by:

$$I_c R_n = \left( \pi \Delta(T)/2e \right) \tanh\left( \Delta(T)/2K \right) \quad \ldots (4)$$

where, $I_c$ is supercurrent density and $R_n$ is the junction resistance in normal state. At $T = 0$, Equation (14) reduces to

$$I_c R_n = \pi \Delta(0)/2e \quad \ldots (5)$$

Where $\Delta(0)$ and $\Delta(T)$ are superconducting order parameter at $T = 0$ and $T (< T_c)$.

Using equations (14) and (15) we can express the normalized supercurrent density as:

$$I_c R = \left\{ \Delta(T)/\Delta(0) \right\} \tanh\left( \Delta(T)/2K \right) \quad \ldots (6)$$

Here $\Delta(T)$ for our bilayered cuprate is given by equation (8) and at $T = 0$, it reduces to the superconducting order parameter $\Delta(0)$ given by:

$$\Delta(0) = -\frac{U \Delta(0)}{(1/N)} \sum_k \left[ 1/4E_{1K} + 1/4E_{2K} \right] \quad \ldots (7)$$

The supercurrent density $(I_c)$ is related to penetration depth $(\lambda_c)$ as $I_c \propto 1/\lambda_c^2$ (6). Therefore

$$\lambda_c^2/\lambda_0^2 = 1/ \{ \Delta(T)/\Delta(0) \} \tanh\left( \Delta(T)/2K \right)$$

or

$$\lambda_c/\lambda_0 = \left[ 1/ \{ \Delta(T)/\Delta(0) \} \tanh\left( \Delta(T)/2K \right) \right]^{1/2} \quad \ldots (8)$$

Using eqs.(2), (7) and (8) one can study the penetration depth as a function of temperature and various microscopic parameters of the model Hamiltonian given by eq.(1). A close examination of eq.s.(2), (3), (7) and (8) reveal that these are coupled integral equation and require a self consistent numerical computation.
RESULTS AND DISCUSSION

For the study of penetration depth as a function of in-plane hopping matrix element, single particle tunneling between the layers, temperature and other parameters of the model Hamiltonian of bilayered system considered here, we convert summation over k-values in equations (2) and (7) into an integration and perform numerical calculations self-consistently.

During the numerical calculations, we have taken \( n_{ab} = 0.085, \)
t\(_{11} = 200\ \text{meV},\ t_{ii} = 20\ \text{meV},\ \widetilde{U} = -600\ \text{meV}.\) The values of superconducting order parameter \( \Delta(T) \) and \( \Delta(0) \) have been calculated self-consistently numerically from equations (2) and (7) as a function of temperature and the parameters of the model Hamiltonian. Using these results, finally from equation (8), we have plotted normalized penetration depth \( \lambda / \lambda_0 \) as a function of normalized temperature \( T/T_c \) for different values of the model Hamiltonian parameters.

In figure (1), we have analysed \( \lambda / \lambda_0 \) vs \( T/T_c \) for different values of in-plane hopping matrix element\( t_{11} \). From fig. (1), it is clear that on increasing in-plane hopping matrix element\( t_{11} \): (a) \( t_{11} = 200\ \text{meV} \), (b) \( t_{11} = 250\ \text{meV} \), (c) \( t_{11} = 300\ \text{meV} \), keeping all other
parameters fixed (\(n_{ab} = 0.085, \ t_{||} = 20 \text{ meV}, \ \bar{\nu} = -600 \text{ meV})\), the normalized penetration depth increases sharply and its rate with normalized temperature also increases rapidly. The increasing rate of \(\lambda_c/\lambda_{c0}\) with increase in \(t_{11}\) may be due to increase in the in-plane bandwidth (\(\approx 8 \ t_{11}\)) because an increase in in-plane bandwidth may also give rise a decrease in electronic density of states at Fermi level and thereby a decrease in \(T_c\) as well as superconducting order parameter \(\Delta\), which implies a decrease in normalized supercurrent density and hence a increase in normalized penetration depth \(\lambda_c/\lambda_{c0}\) [since supercurrent density \(I_c\) is related to penetration depth \(\lambda\) as \(I_c \propto 1/\lambda^2\) (6)].

In fig. (2), the variation of \(\lambda_c/\lambda_{c0}\) vs \(T/T_c\) has been plotted for different values of single particle tunneling between the layers: (a) \(t_{||} = 20 \text{ meV}\), (b) \(t_{||} = 40 \text{ meV}\), (c) \(t_{||} = 55 \text{ meV}\) and keeping all other parameters fixed. It can be seen from fig. (2) that there is a sharp increase in normalized penetration depth \(\lambda_c/\lambda_{c0}\) on increasing \(t_{11}\). This variation of penetration depth with \(t_{11}\) can be explained on the basis of Cooper pair breaking tendency of single particle tunneling in the superconducting state of bilayer cuprates(20).

**CONCLUSIONS**

Finally, in conclusion we have shown, using tight binding bilayer Hubbard model within simple BCS formalism that the normalized penetration depth depends on in-plane hopping matrix element, single particle tunneling between the layers as well as on temperature in an essential way. However, in the present calculation we have not included d-wave type superconducting order parameter and momentum dependence of the interlayer hopping parameter as suggested by Feng et al (21) through ARPES experiment in Bi 2212 system and theoretically studied by Chakravarty et al (22). Therefore the inclusion of these parameters will further improve the present theoretical results on YBCO system.

**REFERENCES**