

Influence of C-Axis Inter Unit Cell Resonant Tunneling on the Spectral Function in Bilayer Cuprates

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Abstract

The role of intra unit cell coupling along with inter unit cell resonant tunneling between the copper-oxygen planes on the electronic spectral function in normal state of bilayer high T_c cuprates like $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ is investigated. The Hubbard model including terms representing hopping between the planes within the unit cell, and resonant tunneling between the planes in two adjoining cells is used along with the Green's function equation of motion approach to obtain an expression of spectral function. The spectral function at $(\pi, 0)$ point of the Brillouin zone is numerically calculated. It is found that the intra unit cell coupling lead to splitting of spectral peak especially close to $(\pi, 0)$ point, while the inter unit cell resonant tunneling lead to a broadening in the spectral function and suppression of bilayer splitting in the normal state. In the presence of finite electron correlations the inter unit cell tunneling induce strong broadening in the spectral features. The electron correlations and inter unit cell tunneling is important in determining the shape of the spectral function in doped bilayer cuprates. These results are viewed in terms of the existing ARPES measurements on bilayer cuprates.

Keywords: Multilayer Superconductors, Electronic Structure, Strongly Correlated Systems

1. Introduction

The angle resolved photoemission spectroscopic (ARPES) measurements [1,2] have emerged as dependable and useful tools for understanding the electronic structure of layered cuprates. In comparison to the single layer per unit cell material such as $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, the ARPES spectra of bilayer cuprates such as $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ (Bi-2212) showed a splitting of spectral function along the antinodal point of the Brillouin zone. A number of experiments are performed to study the band splitting in Bi-2212 which has two Cu-O planes within its unit cell [3-6]. The splitting is found to be large in normal state, with the maximum splitting (~ 110 meV) at $(\pi, 0)$ point of the Brillouin zone. It is also pointed out that the normal state of cuprates shows broadening in the spectral function while sharp and prominent spectral features are observed in the superconducting state. The splitting in the electronic states is attributed to the coupling between the Cu-O planes within the

unit cell. The absence of band splitting in cuprates having only one Cu-O layer per unit cell gives credence to the hypothesis that there must be some sort of out-of-plane effect on account of interlayer coupling in cuprates where there are more than one Cu-O planes per unit cell.

Several authors have emphasized [7-10] the role of intra cell coupling on the electronic spectra of the bilayer cuprates within the framework of a bilayer tight binding Hubbard Hamiltonian. Based on bilayer electronic band structure calculations Chakravarty and collaborators [11] have estimated a highly anisotropic intra cell coupling having the planar momentum dependence of the form

$$\varepsilon_{k\perp} = -\frac{t_{\perp}}{4} (\cos k_x a - \cos k_y a)^2,$$

which gives maximum bilayer splitting at $(\pi, 0)$ point of the Brillouin zone.

The influence of third dimension on the photoemission spectra of two dimensional materials has also been pointed out recently. Bansil *et al.* [12] have analyzed the

intercell coupling on the basis of simulated ARPES line-shapes in Bi-2212 and concluded that the inter cell hopping induces a broadening to the photoemission spectra which have a characteristic dependence on the momentum \vec{k} . Markiewicz *et al.* [13] have also analyzed the effect of intercell coupling and the resulting k_z dispersion in the cuprates within the framework of the one-band tight binding (TB) model Hamiltonian. These authors have obtained various values of tight binding parameters by fitting to the first principles local density approximation (LDA) based band structures, and also with experimental Fermi surfaces obtained by ARPES experiments in optimally doped and overdoped single layer cuprates, $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ and bilayer cuprate Bi-2212.

The out-of-plane coupling not only connects the Cu-O planes within the unit cell (intra unit cell) but also Cu-O planes of the adjacent unit cells (inter unit cell). In bilayer cuprates due to small separation (of the order of 3.2 Å) between two Cu-O planes within the unit cell, the intra unit cell coupling between two Cu-O bilayers results in the band splitting as observed in ARPES measurements. On the other hand, the inter unit cell coupling that connects the two adjacent Cu-O planes in different unit cells is believed to be weaker due to greater separation (of the order of 12 Å in Bi-2212 cuprates) between Cu-O planes of two adjacent unit cells. Because of very low strength of inter unit cell interaction between Cu-O planes, their effect shows up only in recent high resolution ARPES measurements of Chuang *et al.* [5,14] on Bi-2212 system.

Several mechanisms have been proposed so far to explain the out of plane (c-axis) electronic conduction in multilayer cuprates [15,16] and we are still far from a clear understanding of c-axis electronic conduction in cuprates.

Recently, the influence of inter unit cell resonant tunneling between the copper-oxygen planes on c-axis electronic conductivity in normal state of optimally doped bilayer cuprates is investigated [17]. It is concluded that the c-axis conductivity increases with the increment in intercell resonant tunneling and this effect becomes more prominence at low temperatures ($T < 300^\circ\text{K}$). Therefore, the resonant tunneling mechanism is able to account for out of plan (c-axis) electronic conduction processes in

systems like Y-123 and Bi-2212. Most of the recent theoretical studies related to ARPES electronic spectra are based on the two dimensional tight binding Hubbard model and its extension within numerical and analytical approaches and the role of third dimensional coupling on the spectra in the presence of electrons correlation effect has not been clearly understood so far. Therefore, it would be interesting to study the effect of intra cell coupling, inter unit cell resonant tunneling, and electronic correlations simultaneously on the spectral function in doped multilayer cuprates in normal state.

2. Theoretical Formulation

For the system like Bi-2212 and Y-123 which have two Cu-O planes per unit cell, we have proposed a model Hamiltonian that incorporates the intra cell coupling, inter cell resonant tunneling alongwith strong Coulomb interaction that exist in cuprates.

The mechanism of inter unit cell resonant tunneling is schematically depicted in **Figure 1** for Bi-2212 and Y-123 systems. The model Hamiltonian for cuprates with two Cu-O planes per unit cell which incorporates inter cell resonant tunneling is given below: (Equations 1(a) and (b)) where, m is unit cell indice and r, s are layer indices within a unit cell (where $r = 1, s = 2$ and vice-versa). $c_{mrk\sigma}^+$ ($c_{mrk\sigma}$) are creation (annihilation) operator for the holes of m^{th} unit cell, r^{th} Cu-O plane with wave vector k and spin σ . The 1st term in 1(a) is kinetic energy of charge carrier (holes) within the Cu-O plane. The in plane band dispersion ε_{rk} having the contribution of nearest neighbour hopping (t) and next nearest neighbour hopping (t') is taken as

$$\{-2t(\cos k_x a + \cos k_y a) - 4t'(\cos k_x a \cos k_y a)\}$$

It also includes the chemical potential of coupled bilayer system and therefore, initially we have taken Fermi energy $E_F = 0$ for our calculations. The 2nd term in 1 (a) is the on site Coulomb energy at $\text{Cu}3d^9$ site and in cuprates this energy is quiet large (in the range 5 to 10 eV) as compared to hopping energy. The 3rd term in 1(a) is the single particle coupling between the bilayers within the unit cell and we have assumed momentum dependent of the form:

$$H = H_{\text{intracell}} + H_{\text{intercell}}, \text{ Here, } H_{\text{intracell}} = \sum_{m=1,2} \left[\sum_{k,\sigma} \varepsilon_{rk} c_{mrk\sigma}^+ c_{mrk\sigma} + U \sum_{k,k',q,r} c_{mrk+q\uparrow}^+ c_{mrk'\uparrow} c_{mrk'-q\downarrow}^+ c_{mrk\downarrow} + \sum_{r \neq s, k, \sigma} \varepsilon_{k\perp} (c_{mrk\sigma}^+ c_{msk\sigma} + c_{msk\sigma}^+ c_{mrk\sigma}) \right] \quad 1(a)$$

$$H_{\text{intercell}} = \varepsilon_0 \sum_l b_l^+ b_l + \sum_{m,r,s,k,\sigma,l} T_{rs}(m, m+1) \left[(c_{mrk\sigma}^+ b_l + b_l^+ c_{m+1sk\sigma}) + (c_{m+1sk\sigma}^+ b_l + b_l^+ c_{mrk\sigma}) \right] \quad 1(b)$$

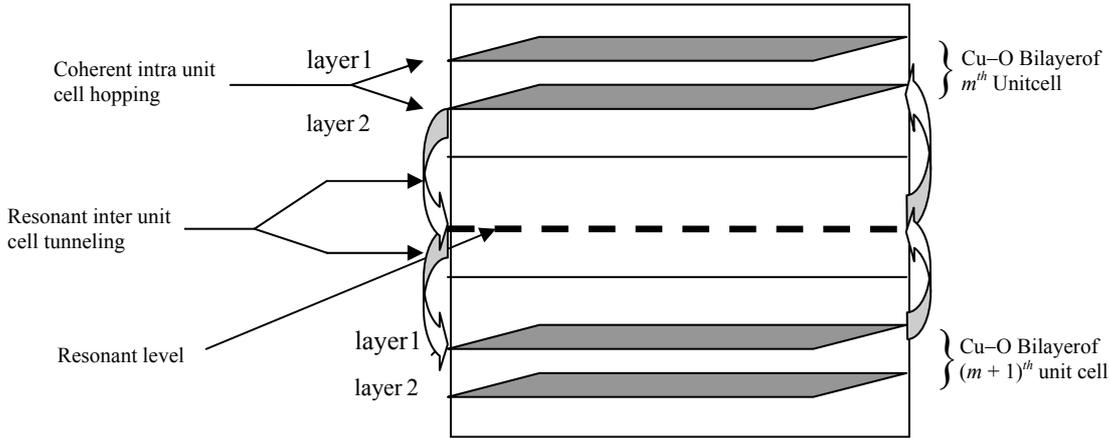


Figure 1. Schematic presentation of intra cell coupling and inter unit cell resonant tunneling in bilayer cuprates (Bi-2212 and Y-123).

$$\varepsilon_{k\perp} = -\frac{t_{\perp}}{4} (\cos k_x a - \cos k_y a)^2$$

as suggested by band structure calculation [11] and ARPES measurements [3,4,12,13].

The 1st term in 1(b) represents the energy of the resonant level due to oxygen deficient BiO chain which lies mid way between the two Cu-O planes lying in adjoining unit cells. The 2nd term in 1(b) represents the single particle resonant tunneling from lower layer (say r^{th} layer) of m^{th} unit cell to upper layer (say s^{th} layer) of adjacent $(m + 1)^{th}$ unit cell and vice-versa. The parameter $T_{rs}(m, m + 1)$ represent the inter unit cell resonant tunneling

matrix element for the case when tunneling probability between two Cu-O planes in different unit cells is of the order of unity [18]. During the theoretical calculation $T_{rs}(m, m + 1)$ is taken as T_{12} for the case of nearest CuO planes in adjacent unit cells (**Figure 1**). To obtain an expression for the corresponding Green's function $G_{11}(k, \omega) = \langle\langle c_{11k\sigma} | c_{11k\sigma}^+ \rangle\rangle$ and hence planar single particle spectral function $A(k, \omega)$ for the model Hamiltonian (1), we have employed Green's function equations of motion approach [9,15,16]. Finally, we derived a set of coupled equations having higher order Green's functions as:

$$(\omega - \varepsilon_k) \langle\langle c_{11k\sigma} | c_{11k\sigma}^+ \rangle\rangle = \frac{1}{2\pi} + \sum_{k'q} U \langle\langle c_{11k'\sigma} c_{11k'-q-\sigma}^+ c_{11k-q-\sigma} | c_{11k\sigma}^+ \rangle\rangle + \varepsilon_{k\perp} \langle\langle c_{12k\sigma} | c_{11k\sigma}^+ \rangle\rangle + T_{12} \langle\langle b_1 | c_{11k\sigma}^+ \rangle\rangle \tag{2}$$

$$(\omega - \varepsilon_k) \langle\langle c_{12k\sigma} | c_{11k\sigma}^+ \rangle\rangle = \varepsilon_{k\perp} \langle\langle c_{11k\sigma} | c_{11k\sigma}^+ \rangle\rangle + \sum_{k'q} U \langle\langle c_{12k'\sigma} c_{12k'-q-\sigma}^+ c_{12k-q-\sigma} | c_{11k\sigma}^+ \rangle\rangle \tag{3}$$

$$(\omega - \varepsilon_0) \langle\langle b_1 | c_{11k\sigma}^+ \rangle\rangle = T_{12} (\langle\langle c_{22k\sigma} | c_{11k\sigma}^+ \rangle\rangle + \langle\langle c_{11k\sigma} | c_{11k\sigma}^+ \rangle\rangle) \tag{4}$$

$$(\omega - \varepsilon_k) \langle\langle c_{22k\sigma} | c_{11k\sigma}^+ \rangle\rangle = \varepsilon_{k\perp} \langle\langle c_{21k\sigma} | c_{11k\sigma}^+ \rangle\rangle + \sum_{k'q} U \langle\langle c_{22k'\sigma} c_{22k'-q-\sigma}^+ c_{22k-q-\sigma} | c_{11k\sigma}^+ \rangle\rangle + T_{12} \langle\langle b_1 | c_{11k\sigma}^+ \rangle\rangle \tag{5}$$

and

$$(\omega - \varepsilon_k) \langle\langle c_{21k\sigma} | c_{11k\sigma}^+ \rangle\rangle = \varepsilon_{k\perp} \langle\langle c_{22k\sigma} | c_{11k\sigma}^+ \rangle\rangle + \sum_{k'q} U \langle\langle c_{21k'\sigma} c_{21k'-q-\sigma}^+ c_{21k-q-\sigma} | c_{11k\sigma}^+ \rangle\rangle \tag{6}$$

In order to take into account the electronic correlation effects that exist in cuprates, the equations of motion of higher order Green's functions appearing in Equations

(2-6) can be rewritten and the decoupling in higher order Green's functions in these equations of motion is made at second stage. During the decoupling of higher order

Green's function, it is also assumed that the system is paramagnetic. This makes the equations tractable and avoids complications. With these approximations and

simplification the higher order Green's functions that exist in equations can now be written as:

$$\begin{aligned}
 (\omega - \varepsilon_{k'}) \left\langle \left\langle c_{11k'_\sigma} c_{11k'_-q-\sigma}^+ c_{11k-q-\sigma} \middle| c_{11k\sigma}^+ \right\rangle \right\rangle &= \frac{\delta_{k'k}}{2\pi} \left\langle c_{11k'_-q-\sigma}^+ c_{11k-q-\sigma} \right\rangle + \varepsilon_{k'_\perp} \left\langle \left\langle c_{11k'_-q-\sigma}^+ c_{11k-q-\sigma} c_{12k'_\sigma} \middle| c_{11k\sigma}^+ \right\rangle \right\rangle \\
 &+ T_{12} \left\langle \left\langle c_{11k'_q\sigma}^+ c_{11kq\sigma} b_1 \middle| c_{11k\sigma}^+ \right\rangle \right\rangle \\
 - \sum_{k'q} U \left\langle \left\langle c_{11k'_-q-\sigma}^+ c_{11k'_-q-\sigma} c_{11k'_\sigma}^+ c_{11k'_-q-\sigma} c_{11k-q-\sigma} \middle| c_{11k\sigma}^+ \right\rangle \right\rangle & \tag{7}
 \end{aligned}$$

The other higher order equations are also obtained and after truncating the hierarchy of still higher order Green's function in the Hartree Fock approximation, we finally obtained set of linear coupled equations of Green's functions. It is assumed that the charge carriers

in Cu-O planes are equally distributed and also used a paramagnetic situation (*i.e.* carriers with up spin are equal to carriers with down spin). Solving the above coupled equations, one derives the Green's function $G_{11}(k, \omega)$ as follows;

$$\begin{aligned}
 G_{11}(k, \omega) &= \frac{1}{2\pi} (\omega - \varepsilon_k) (1 + F_{k\omega}) \times \\
 &\left[\frac{(\omega - \varepsilon_k)^2 (\omega - \varepsilon_0) - \varepsilon_{k\perp}^2 (\omega - \varepsilon_0) (1 + F_{k\omega})^2 - T_{12}^2 (\omega - \varepsilon_k) (1 + F_{k\omega})}{\left\{ (\omega - \varepsilon_k)^2 - \varepsilon_{k\perp}^2 (1 + F_{k\omega})^2 \right\} \left\{ (\omega - \varepsilon_k)^2 (\omega - \varepsilon_0) - \varepsilon_{k\perp}^2 (\omega - \varepsilon_0) (1 + F_{k\omega})^2 - 2T_{12}^2 (\omega - \varepsilon_k) (1 + F_{k\omega}) \right\}} \right] \tag{8}
 \end{aligned}$$

In the absence of Coulomb energy term (*i.e.* $U = 0$), the

Equation (8), can be written in the following form.

$$\begin{aligned}
 G_{11}(k, \omega) &= \left\langle \left\langle c_{11k\sigma} \middle| c_{11k\sigma}^+ \right\rangle \right\rangle \\
 &= \frac{1}{2\pi} (\omega - \varepsilon_k) \times \left[\frac{(\omega - \varepsilon_0) \left\{ (\omega - \varepsilon_k)^2 - \varepsilon_{k\perp}^2 \right\} - T_{12}^2 (\omega - \varepsilon_k)}{\left\{ (\omega - \varepsilon_k)^2 - \varepsilon_{k\perp}^2 \right\} \left[(\omega - \varepsilon_0) \left\{ (\omega - \varepsilon_k)^2 - \varepsilon_{k\perp}^2 \right\} - 2T_{12}^2 (\omega - \varepsilon_k) \right]} \right] \tag{9}
 \end{aligned}$$

If, in the above expression of $G_{11}(k, \omega)$, the resonant tunneling is taken as zero ($T_{12} = 0$), we obtain the propagator for bilayer system having intra cell coupling only, and Equation (8) reduced to the following:

$$G_{11}(k, \omega) = \frac{1}{2\pi} \left[\frac{\omega - \varepsilon_k}{(\omega - \varepsilon_k)^2 - \varepsilon_{k\perp}^2} \right] \tag{10}$$

One can check from above Equation (10) that there are two quasiparticle energy branches (*i.e.* $\omega_{1,2} = \varepsilon_k \pm \varepsilon_{k\perp}$): a manifestation of intrabilayer coupling between two CuO_2 planes within the unit cell. On simplification one can rewrite the Equation (8) as:

$$G_{11}(k, \omega) = \frac{1}{2\pi} (\omega - \varepsilon_k) (1 + F_{k\omega}) \left\{ \frac{\omega^3 + A\omega^2 + B\omega + C}{\omega^5 + D\omega^4 + E\omega^3 + F\omega^2 + G\omega + H} \right\} \tag{11}$$

where,

$$\begin{aligned}
 A &= -(\varepsilon_0 + 2\varepsilon_k) \\
 B &= 2\varepsilon_k \varepsilon_0 + \varepsilon_k^2 - \varepsilon_{k\perp}^2 (1 + F_{k\omega})^2 - T_{12}^2 (1 + F_{k\omega}) \\
 C &= -\left\{ \varepsilon_k^2 \varepsilon_0 - \varepsilon_{k\perp}^2 \varepsilon_0 (1 + F_{k\omega})^2 - \varepsilon_k T_{12}^2 (1 + F_{k\omega}) \right\} \\
 D &= -(\varepsilon_0 + 4\varepsilon_k)
 \end{aligned}$$

$$\begin{aligned}
 E &= 4\varepsilon_k \varepsilon_0 + 6\varepsilon_k^2 - 2\varepsilon_{k\perp}^2 (1 + F_{k\omega})^2 - 2T_{12}^2 (1 + F_{k\omega}) \\
 F &= -\left\{ 6\varepsilon_k^2 \varepsilon_0 + 4\varepsilon_k^3 - 4\varepsilon_k \varepsilon_{k\perp}^2 (1 + F_{k\omega})^2 - 2\varepsilon_0 \varepsilon_{k\perp}^2 (1 + F_{k\omega})^2 - 6\varepsilon_k T_{12}^2 (1 + F_{k\omega}) \right\} \\
 G &= \left\{ \begin{aligned} &4\varepsilon_k^3 \varepsilon_0 - 2\varepsilon_k^2 \varepsilon_{k\perp}^2 (1 + F_{k\omega})^2 + \varepsilon_k^4 - 4\varepsilon_k \varepsilon_0 \varepsilon_{k\perp}^2 (1 + F_{k\omega})^2 - 6\varepsilon_k^2 T_{12}^2 (1 + F_{k\omega}) + \\ &\varepsilon_{k\perp}^4 (1 + F_{k\omega})^4 + 2T_{12}^2 \varepsilon_{k\perp}^2 (1 + F_{k\omega})^3 \end{aligned} \right\}
 \end{aligned}$$

and

$$H = -\left\{ \begin{aligned} &\varepsilon_k^4 \varepsilon_0 - 2\varepsilon_k^2 \varepsilon_0 \varepsilon_{k\perp}^2 (1 + F_{k\omega})^2 - 2\varepsilon_k^3 T_{12}^2 (1 + F_{k\omega}) + \varepsilon_{k\perp}^4 \varepsilon_0 (1 + F_{k\omega})^4 \\ &+ 2\varepsilon_{k\perp}^2 (1 + F_{k\omega})^3 \varepsilon_k T_{12}^2 \end{aligned} \right\}$$

Using simple algebra above Equation (12) can be rearranged as:

$$G_{11}(k, \omega) = \frac{1}{2\pi} \sum_{i=1}^5 \frac{A_i}{(\omega - \alpha_i)} \quad (12)$$

where, $\alpha_1, \dots, \alpha_5$ are the five quasi-particle energies which have been computed numerically. The planar single particle spectral function $A(k, \omega)$ can be calculated from the above Green's function $G_{11}(k, \omega)$ numerically by using the relationship:

$$A(k, \omega) = -\frac{1}{\pi} \text{Im} G_{11}(k, \omega), \quad (13)$$

where Im stands for imaginary part of Green's function. Using Equations (12) and (13) the expression for planar electronic spectral function can be written in the following form:

$$A(k, \omega) = \frac{1}{\pi} \sum_{i=1}^5 \frac{\Gamma A_i}{\Gamma^2 + (\omega - \alpha_i)^2} \quad (14)$$

To fit the line shape of the photoemission experimental results, we need to solve δ -functions involved in the spectral function (Equation (14)). The calculation of $A(k, \omega)$ would give a broadening of the quasiparticle peak. A Lorentzian type of broadening is used as given below:

$$\delta(\omega - \tilde{\varepsilon}_k) \cong \lim_{\Gamma \rightarrow 0} \frac{1}{\pi} \frac{\Gamma}{(\omega - \tilde{\varepsilon}_k)^2 + \Gamma^2} \quad (15)$$

The phenomenological broadening parameter Γ takes care of quasi-particle scattering rate and initially taken to be independent of k and ω [19,20] as we are interested in the influence of inter unit cell resonant tunneling on photoemission spectral function. The line shape of the peak in the ARPES spectral function $A(k, \omega)$ can be analyzed using Equation (14) numerically.

3. Results and Discussion

The spectral function $A(k, \omega)$ is measured by angle resolved photoemission spectroscopy. The measured

$A(k, \omega)$ can be numerically analyzed using Equations (13-15). The $A(k, \omega)$ is analyzed especially at $(\pi, 0)$ points of the Brillouin zone, where the splitting in the ARPES spectra of Bi2212 is found to be maximum in normal state. These calculations would be relevant to bilayer cuprates, Bi-2212, because the range of various intra and inter cell parameters used in the present analysis have been taken from recent electronic band structure calculations [10,11] and works on electronic spectra of Bi2212 cuprates [3,4,12,13].

In **Figure 2**, one can observe the spectral function $A(k, \omega)$ against energy (ω) for different intra cell coupling strength in optimal doped regime of Bi-2212 in the normal state in the presence of inter cell resonant tunneling ($T_{12} = 0.1$ eV) and for the case $U = 0.0$ eV). The variation of $A(k, \omega)$ versus band energy (ω) at $(\pi, 0)$ point of Brillouin zone shows a splitting in the spectral function in the presence of intra cell coupling between the planes ($t_{\perp} = 0.2$ eV). Such a bilayer splitting in Bi-2212 at $(\pi, 0)$ point is also observed in recent ARPES measurements [4-7]. On introducing the inter unit cell resonant tunneling ($T_{12} = 0.05$ eV, 0.075 eV and 0.1 eV and keeping $t_{\perp} = 0.1$ eV), one can point out a broadening in the spectral function (**Figure 3**). Also, the bilayer splitting in the spectral function disappeared due to broadening in the spectra on increasing inter cell resonant tunneling term ($T_{12} = 0.1$ eV to 0.15 eV) (**Figure 4**). Such broadening in the normal state spectra has also been predicted by simulated ARPES line shapes in Bi-2212 bilayer systems as manifestation of third dimensional inter unit cell coupling [12,13]. On comparing Fig. 2 and **Figure 4** one can observe that intra cell coupling (t_{\perp}) leads the bilayer splitting in the spectral function, while inter unit cell resonant tunneling (T_{12}) suppresses the bilayer splitting and induces broadening in the spectral peak close to Fermi level.

One can also analyze the influence of inter cell resonant tunneling term (T_{12}) on the spectral function at $(\pi, 0)$ point in the presence of Coulomb correlation (U), keeping other parameters fixed, and using Green's func-

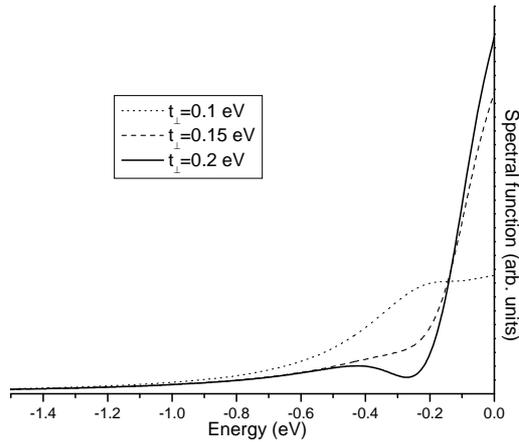


Figure 2. Spectral function versus energy at $(\pi, 0)$ point of the Brillouin zone keeping $t = 0.4$ eV, $T_{12}=0.1$ eV, $U = 0.0$ eV, $n = 0.2$, $\Gamma = 0.25$ eV, and $\varepsilon_0 = 0.05$ eV.

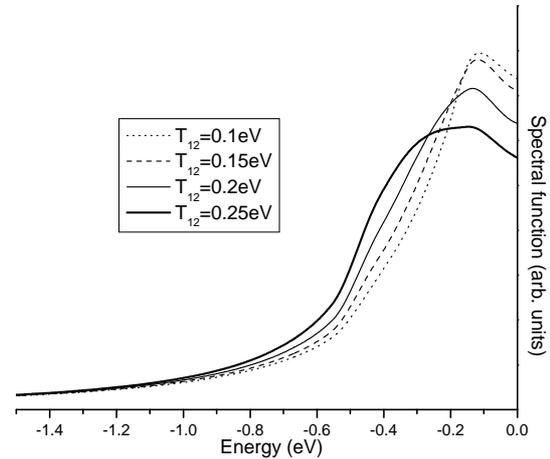


Figure 5. Spectral function versus energy at $(\pi, 0)$ point of the Brillouin zone keeping $t = 0.4$ eV, $t_{\perp} = 0.2$ eV, $U = 3.0$ eV, $n = 0.2$, $\Gamma = 0.25$ eV, and $\varepsilon_0 = 0.05$ eV.

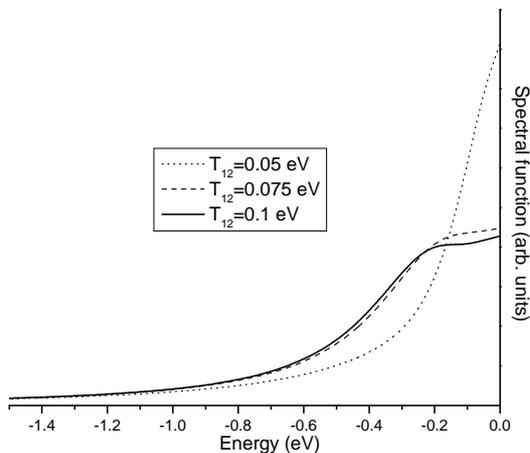


Figure 3. Spectral function versus energy at $(\pi, 0)$ point of the Brillouin zone keeping $t = 0.4$ eV, $t_{\perp} = 0.1$ eV, $U = 0.0$ eV, $n = 0.2$, $\Gamma = 0.25$ eV, and $\varepsilon_0 = 0.05$ eV.

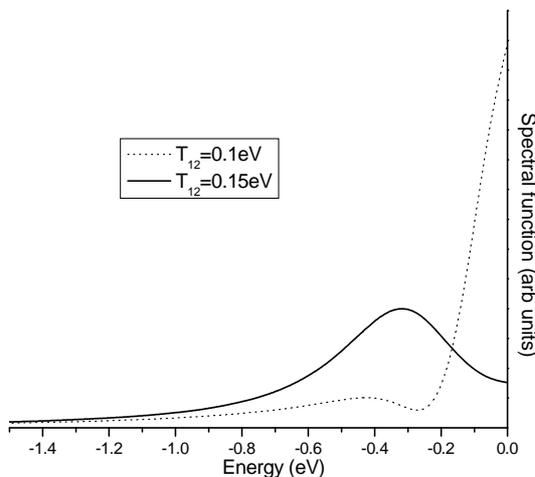


Figure 4. Spectral function versus energy at $(\pi, 0)$ point of the Brillouin zone keeping $t = 0.4$ eV, $t_{\perp} = 0.2$ eV, $U = 0.0$ eV, $n = 0.2$, $\Gamma = 0.25$ eV, and $\varepsilon_0 = 0.05$ eV.

tion Equation (18). In **Figure 5**, the spectral function versus energy for different values of inter cell resonant tunneling term ($T_{12} = 0.1$ eV to 0.25 eV) in the presence of Coulomb correlation (*i.e.* $U = 3$ eV) have been plotted. It is pointed out from the **Figure 5** that in the presence of both the electronic correlations, and inter cell resonant tunneling (T_{12}) the broadening in spectra [1-4] is more as compare to the absence of Coulomb correlations (**Figures 3 and 4**).

Finally, it is concluded that the intra unit cell coupling is responsible for bilayer splitting of electronic spectra, while the inter unit cell resonant tunneling leads to broadening in the spectral features especially at $(\pi, 0)$ point of optimally doped bilayer (Bi-2212) cuprates and in good correspondence with recent ARPES measurements [12]. The electron correlations also play an important role in determining the shape of spectral function. As the antinodal region of hole doped cuprates is so called hot spot, in which the electron-electron correlation broaden the spectral function. Besides, there may be another source to broaden the spectral function like as randomness in the CuO_2 planes alongwith inter cell incoherent resonant tunneling and carrier concentration. Therefore, the presence of finite electron correlations, the inter unit cell resonant tunneling (T_{12}) suppresses the bilayer splitting in the spectral function due to broadening in the spectral features close to Fermi level in optimal doped bilayer cuprates.

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5. References

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