

**Effect of bilayer coupling on tunneling conductance of double-layer high- $T_c$  cuprates**

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Physical effects of bilayer coupling on the tunneling spectroscopy of high- $T_c$  cuprates are investigated. The bilayer coupling separates the bonding and antibonding bands and leads to a splitting of the coherence peaks in the tunneling differential conductance. However, the coherence peak of the bonding band is strongly suppressed and broadened by the particle-hole asymmetry in the density of states and finite quasiparticle lifetime, and is difficult to resolve by experiments. This gives a qualitative account why the bilayer splitting of the coherence peaks was not clearly observed in tunneling measurements of double-layer high- $T_c$  oxides.

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The interlayer coupling of electrons in high- $T_c$  cuprates was predicted to depend strongly on the in-plane momentum and vanish along the zone diagonals of the two-dimensional (2D) Brillouin zone.<sup>1-3</sup> This would lead to an anisotropic splitting of the energy bands in bilayer compounds. This bilayer splitting was first observed by Feng *et al.* in the angle-resolved photoemission spectroscopy (ARPES) of heavily overdoped (OD)  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$  (Bi2212) compounds.<sup>4</sup> The maximum splitting occurs near the antinodal points  $(\pm\pi, 0)$  and  $(0, \pm\pi)$  and varies from 20 meV in the superconducting state to 88 meV in the normal state. Chuang *et al.* also observed this splitting in OD Bi2212 samples in the normal state, but with a larger splitting energy 110 meV.<sup>5</sup> Furthermore, by analyzing the energy dependence of ARPES spectra, Kordyuk *et al.* concluded that the peak-dip-hump lineshape observed in ARPES are stemmed from the bilayer splitting.<sup>6</sup>

Tunneling spectroscopy is an important tool for exploring low-energy properties of high- $T_c$  superconductors (HTSC), as the tunneling conductance is proportional to the density of states (DOS) of electrons. The tunneling measurements reveal important features of  $d$ -wave superconductors, such as the superconducting coherence peak at the gap edges and the V-shape low-energy spectrum associated with the linear DOS.<sup>7-13</sup> In addition to these  $d$ -wave features, an asymmetric tunneling conductance background with a negative slope has also been observed.<sup>7-9</sup> In contrast to the ARPES, the bilayer coupling effect in tunneling experiments has not been reported.

In this paper we investigate the effect of the bilayer coupling on tunneling measurements. The bilayer coupling splits the energy bands into the bonding and antibonding ones and leads to a separation of the superconducting coherence peaks. This property can be used to probe the bilayer effect from tunneling measurements. Furthermore, it is shown that the DOS contributed from the bonding and antibonding bands behave differently in presence of the particle-hole asymmetry. With a negative slope in the normal density of states, the particle-hole asymmetry tends to reduce the DOS of the bonding band, but enhance that of the antibonding band. This will enhance one coherence peak but reduce the other one, and eventually cause the disappearance of two-coherence-peak structure.

Our model involves the anisotropic  $c$ -axis coupling between two  $\text{CuO}_2$  planes and is defined by the following Hamiltonian:

$$H = \sum_{l, \mathbf{k}\sigma} \varepsilon(\mathbf{k}) c_{l, \mathbf{k}\sigma}^\dagger c_{l, \mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} t_\perp(\mathbf{k}) (c_{1, \mathbf{k}\sigma}^\dagger c_{2, \mathbf{k}\sigma} + \text{H.c.}) - \sum_{l, \mathbf{k}} \Delta(\mathbf{k}) (c_{l, \mathbf{k}\uparrow}^\dagger c_{l, -\mathbf{k}\downarrow}^\dagger + c_{l, -\mathbf{k}\downarrow} c_{l, \mathbf{k}\uparrow}), \quad (1)$$

where  $c_{l, \mathbf{k}\sigma}^\dagger$  ( $l=1,2$ ) creates electrons in the  $l$ th  $\text{CuO}_2$  plane with momentum  $\mathbf{k}$  and spin  $\sigma$ . The kinetic energy  $\varepsilon(\mathbf{k})$  includes the chemical potential and thus the Fermi energy  $\varepsilon_F = 0$ . The superconducting energy gap is assumed to have  $d_{x^2-y^2}$  symmetry and  $\Delta(\mathbf{k}) = \Delta_0(\cos k_x - \cos k_y)/2$ . In a tetragonal high- $T_c$  cuprate, the  $c$ -axis electron hopping integral is anisotropic:<sup>1-3</sup>

$$t_\perp(\mathbf{k}) = -\frac{t_z}{4} (\cos k_x - \cos k_y)^2.$$

This anisotropy results from the hybridization between the bonding O  $2p$  and unoccupied Cu  $4s$  orbitals. If  $\Delta(\mathbf{k}) = 0$  in one of the double planes, Eq. (1) is the model that was widely used for studying the proximity effect in YBCO materials.<sup>14,15</sup>

Defining the operators  $d_{1, \mathbf{k}\sigma} = (c_{1, \mathbf{k}\sigma} + c_{2, \mathbf{k}\sigma})/\sqrt{2}$  and  $d_{2, \mathbf{k}\sigma} = (c_{1, \mathbf{k}\sigma} - c_{2, \mathbf{k}\sigma})/\sqrt{2}$ , we can decouple the above Hamiltonian into two independent parts

$$H = H_1 + H_2, \quad (2)$$

$$H_i = \sum_{\mathbf{k}\sigma} \varepsilon_i(\mathbf{k}) d_{i, \mathbf{k}\sigma}^\dagger d_{i, \mathbf{k}\sigma} - \sum_{\mathbf{k}} \Delta(\mathbf{k}) (d_{i, \mathbf{k}\uparrow}^\dagger d_{i, -\mathbf{k}\downarrow}^\dagger + \text{H.c.}), \quad (3)$$

with  $\varepsilon_{1,2}(\mathbf{k}) = \varepsilon(\mathbf{k}) \pm t_\perp(\mathbf{k})$ .  $H_{1,2}$  are the BCS Hamiltonians for the bonding and antibonding bands, respectively. From the decoupled Hamiltonian, we can readily obtain the energy spectra of the Bogoliubov quasiparticles

$$H_i = \sum_{\mathbf{k}} E_i(\mathbf{k}) (\gamma_{i, \mathbf{k}\uparrow}^\dagger \gamma_{i, \mathbf{k}\uparrow} + \gamma_{i, -\mathbf{k}\downarrow}^\dagger \gamma_{i, -\mathbf{k}\downarrow}),$$

where  $E_{1,2}(\mathbf{k}) = \sqrt{\Delta^2(\mathbf{k}) + [\varepsilon(\mathbf{k}) \pm t_{\perp}(\mathbf{k})]^2}$  and the Bogoliubov quasiparticle operators are defined by

$$\gamma_{i,\mathbf{k}\uparrow} = u_{i,\mathbf{k}} d_{i,\mathbf{k}\uparrow} - v_{i,\mathbf{k}} d_{i,-\mathbf{k}\downarrow}^{\dagger}, \quad (4)$$

$$\gamma_{i,-\mathbf{k}\downarrow}^{\dagger} = v_{i,\mathbf{k}} d_{i,\mathbf{k}\uparrow} + u_{i,\mathbf{k}} d_{i,-\mathbf{k}\downarrow}^{\dagger}, \quad (5)$$

and

$$u_{i,\mathbf{k}}^2 = \frac{1}{2} \left( 1 + \frac{\varepsilon_i(\mathbf{k})}{E_i(\mathbf{k})} \right), \quad (6)$$

$$v_{i,\mathbf{k}}^2 = \frac{1}{2} \left( 1 - \frac{\varepsilon_i(\mathbf{k})}{E_i(\mathbf{k})} \right). \quad (7)$$

The energy spectra of the two quasiparticle bands demonstrate the bilayer splitting as observed in ARPES.<sup>4,5</sup> Because of the anisotropy of  $t_{\perp}(\mathbf{k})$ , the largest splitting occurs at the Fermi surface in the vicinity of  $(\pm\pi, 0), (0, \pm\pi)$ .

The density of states of electrons  $\rho(\omega)$  is defined by the imaginary part of the retarded Green function  $G_{i,\sigma}^R(\mathbf{k}, \omega)$  of fermions  $\{d_{i,\mathbf{k}\sigma}^{\dagger}, d_{i,\mathbf{k}\sigma}\}$ ,

$$\rho(\omega) = -\frac{1}{\pi N} \sum_{i\mathbf{k}\sigma} \text{Im} G_{i,\sigma}^R(\mathbf{k}, \omega), \quad (8)$$

where  $N$  is the total number of  $\mathbf{k}$  vectors in the first Brillouin zone. For the  $i$ th band, the density of states is given by

$$\rho_i(\omega) = -\frac{2}{N\pi} \sum_{\mathbf{k}} \text{Im} \left( \frac{u_{i,\mathbf{k}}^2}{\omega - E_i(\mathbf{k}) + i\Gamma} + \frac{v_{i,\mathbf{k}}^2}{\omega + E_i(\mathbf{k}) + i\Gamma} \right).$$

$\Gamma$  is the quasiparticle scattering rate which originates from the lifetime effects, stoichiometry variations, noise smearing, etc.<sup>16,17</sup> It can be also taken as a free parameter associated with the energy resolution in the tunneling experiment if the scattering rate is smaller than the experimental resolution.

Since the low-energy physics is governed by excitations near the Fermi energy, we assume that the kinetic energy depends only on the absolute value of the momentum, i.e.,  $\varepsilon(\mathbf{k}) = \varepsilon(k)$ . The anisotropic  $d$ -wave gap function and  $c$ -axis coupling  $t_{\perp}(\mathbf{k})$  can also be simplified as  $\Delta_i(\mathbf{k}) = \Delta_{i,0} \cos(2\phi)$  and  $t_{\perp}(\mathbf{k}) = -t_z \cos^2(2\phi)$  in the vicinity of the Fermi surface.

Near the Fermi energy, the normal density of states can be written as

$$\rho_N(\varepsilon) \approx \rho_N(0) + \rho'_N(0)\varepsilon \quad (9)$$

up to the leading order approximation in  $\varepsilon$ , where  $\rho_N(0)$  is the normal DOS at the Fermi energy.  $\rho'_N(0)$  is the linear coefficient of the DOS.  $\rho'_N(0)$  is finite if particle-hole symmetry is broken. A number of ARPES experiments have shown that there is a flat band at about 200 meV below the Fermi energy in deeply underdoped cuprates.<sup>18,19</sup> The presence of this flat band is an indication of Van Hove singularity and suggests that the variation of the DOS around the Fermi surface can no longer be neglected as in conventional metals. Moreover, as revealed by the tunneling measurements, the tunneling conductance varies almost linearly with the applied

bias around the Fermi energy in the normal state.<sup>7-9</sup> It suggests that particle-hole symmetry is broken in high- $T_c$  cuprates. Thus, it is important to include the particle-hole asymmetric term in the analysis of tunneling measurement data. The linear approximation of DOS, defined by Eq. (9), is valid if the energy of the Van Hove singularity is close to the Fermi energy but still much lower than the energy range we are interested in.

With the above equations, it is straightforward to show that

$$\rho_i(\omega) \approx \rho_N(0) I_{i,1}(\omega) + \rho'_N(0) \text{sgn}(\omega) I_{i,2}(\omega) \pm t_z \rho'_N(0) I_{i,3}(\omega), \quad (10)$$

where  $I_{i,l}(\omega)$  are

$$I_{i,1}(\omega) = \frac{1}{2\pi^2} \int d\phi \int d\varepsilon \frac{\Gamma}{(|\omega| - \Omega_i)^2 + \Gamma^2}, \quad (11)$$

$$I_{i,2}(\omega) = \frac{1}{2\pi^2} \int d\phi \int d\varepsilon \frac{\varepsilon^2}{\Omega_i} \frac{\Gamma}{(|\omega| - \Omega_i)^2 + \Gamma^2}, \quad (12)$$

$$I_{i,3}(\omega) = \frac{1}{2\pi^2} \int d\phi \int d\varepsilon \frac{\cos^2(2\phi)\Gamma}{(|\omega| - \Omega_i)^2 + \Gamma^2}, \quad (13)$$

and  $\Omega_i \equiv \sqrt{\Delta_{i,0}^2 \cos^2(2\phi) + \varepsilon^2}$ . The first term at the right-hand side of Eq. (10) has the largest contribution to the DOS. The superconducting coherence peaks are located at the gap edge, namely, at  $\omega_i = \pm \Delta_{i,0}$ . In the limit  $\Gamma \rightarrow 0^+$ ,  $I_{i,1}(\omega) \propto |\omega|$  near the Fermi energy, thus the low energy DOS of quasiparticles is linear  $\rho_i(\omega) \approx \rho_N(0)|\omega|/\Delta_{i,0}$ . These special  $d$ -wave characters have already been observed in the tunneling measurements.<sup>7-13</sup>

Particle-hole symmetry is broken by the second term in Eq. (10). The asymmetric DOS induced by this term has been observed in STM or other tunneling spectra.<sup>7-9</sup> Since  $I_{i,2}(\omega)$  is positive, a negative  $\rho'_N(0)$  will enhance the DOS below the Fermi energy, but reduce that above the Fermi energy.

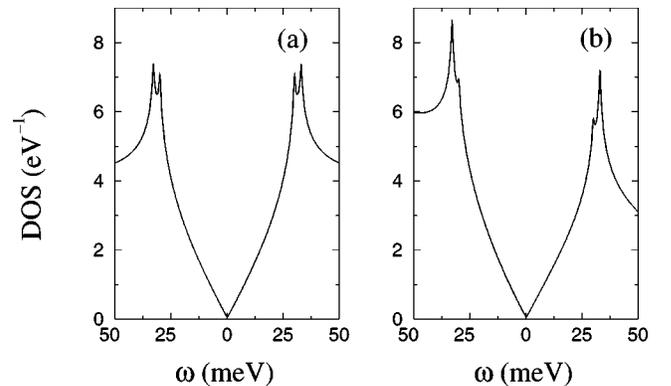


FIG. 1. Density of states in a bilayer compound. The parameters used are  $\Delta_{1,0} = 30$  meV,  $\Delta_{2,0} = 33$  meV,  $t_z = 50$  meV,  $\Gamma = 0.25$  meV,  $\rho_N(0) = 1$  eV<sup>-1</sup>, (a)  $\rho'_N(0) = 0$ , (b)  $\rho'_N(0) = -8$  eV<sup>-2</sup>.

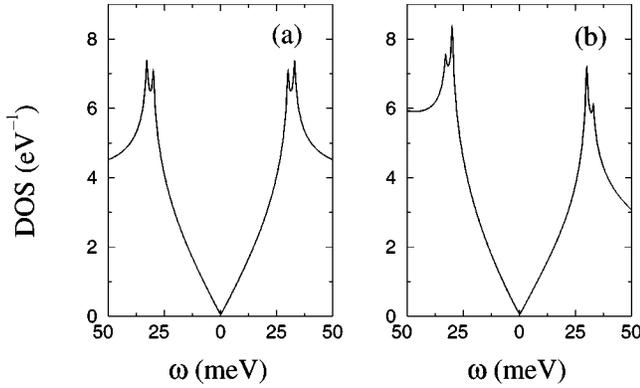


FIG. 2. Same as for Fig. 1 but with  $\Delta_{1,0}=33$  meV,  $\Delta_{2,0}=30$  meV.

The bilayer coupling appears in the third term of Eq. (10). It leads to the difference in the DOS of the bonding and antibonding bands. This difference is proportional to both the  $c$ -axis hopping integral  $t_z$  and  $\rho'_N(0)$ . For a system with  $\rho'_N(0) < 0$ , the bonding band DOS  $\rho_1(\omega)$  is reduced and the antibonding band DOS  $\rho_2(\omega)$  is enhanced.

Because of the  $c$ -axis coupling, the coherence peaks of the bonding and antibonding bands are separated. The maxima of the energy gap for both bonding and antibonding bands are located near the four points  $(\pm\pi, 0), (0, \pm\pi)$ . Therefore, the largest difference in the energy gap,  $\delta_s \equiv |\Delta_{1,0} - \Delta_{2,0}|$ , also occurs near these positions, where  $\Delta_{i,0} \approx \Delta(\mathbf{k}_{i,F})$  is the gap maximum of the  $i$ th band at the Fermi momentum  $\mathbf{k}_i$  along the antinodal direction. From the ARPES data in Ref. 4, we estimate the difference between the antinodal Fermi momentum to be  $|\mathbf{k}_{1,F} - \mathbf{k}_{2,F}| \approx 0.12\pi$  and the difference of the largest energy gaps to be  $\delta_s \approx 0.1\Delta_0$ . In OD Bi2212 compounds,  $\Delta_0 \approx 30$  meV, thus  $\delta_s \approx 3$  meV.

Figure 1 shows the DOS for a system with  $\Delta_{1,0} = 30$  meV,  $\Delta_{2,0} = 33$  meV, and  $\rho_N(0) = 1$  eV $^{-1}$ . The results for both  $\rho'_N(0) = 0$  and  $\rho'_N(0) = -8$  eV $^{-2}$  are shown. In the case  $\rho'_N(0) = 0$ , two coherence peaks appear due to the bilayer splitting. These two peaks, at 30 and 33 meV, come from the bonding and antibonding bands, respectively. When  $\rho'_N(0) = -8$  eV $^{-2}$ , the DOS becomes nonsymmetric, as expected. This asymmetric feature exists in both the normal and superconducting states, consistent with the reported data.<sup>12,13</sup> However, the peak of the bonding band is strongly suppressed.

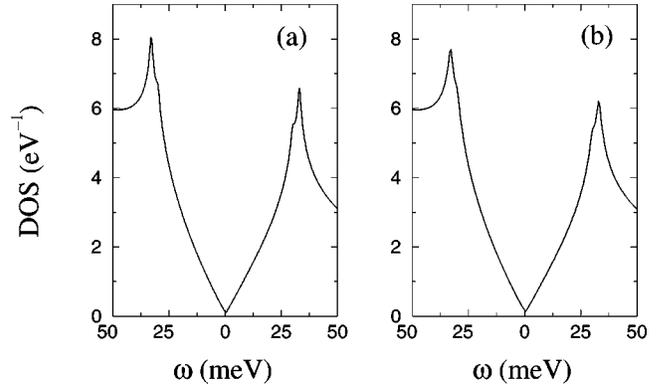


FIG. 3. Density of states with (a)  $\Gamma=0.5$  meV, (b)  $\Gamma=0.75$  meV. Other parameters used are the same as for Fig. 1(b).

For comparison, Fig. 2 shows the DOS for a system with  $\Delta_{1,0} = 33$  meV and  $\Delta_{2,0} = 30$  meV. The asymmetric behavior shown in Fig. 2(b) is similar to the case for Fig. 1(b), but the higher coherence peak is located at lower energy.

Compared with the case  $\rho'_N(0) = 0$ , the particle-hole asymmetry suppresses strongly the lower coherence peak. If the quasiparticle scattering rate  $\Gamma$  is large or the energy resolution is not high enough, it is certainly difficult to resolve this double-coherence-peak structure in the tunneling spectra. This is explicitly illustrated in Fig. 3. With increasing  $\Gamma$ , the double-peak structure disappears gradually and the lower coherence peak becomes indistinguishable from the background. Therefore, in order to observe this bilayer splitting in tunneling spectra, experimental measurements with high quality single crystal and high energy resolution are desired.

In conclusion, the superconducting coherence peaks are separated in bilayer high- $T_c$  superconductors and can be used to probe the bilayer coupling effect with tunneling measurements. The particle-hole asymmetry in the DOS enhances one of the coherence peaks, but reduces another one. If the lifetime of quasiparticles is very short or the energy resolution in tunneling measurements is not high enough, the lower coherence peak is difficult to be resolved from the conductance background. This gives a qualitative account why the bilayer splitting has not been unambiguously observed in tunneling spectra.

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