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Quasiparticle bands in plane-chain coupled cuprates

X.-J. Fan[1,2,a], W.-G. Yin[2], X.-G. Li[1], and C.-D. Gong[2]

[1] Structure Research Laboratory, Department of Materials Science & Engineering, University of Science and Technology of China, Hefei, Anhui 230026, P.R. China
[2] Department of Physics, Nanjing University, Nanjing 210093, P.R. China

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Abstract. The dispersion spectrum of single hole in a bilayer composed of plane and chain, each described by t–J model, coupled by $t_\perp$–$J_\perp$ interactions between them, is calculated in terms of self-consistent Born approximation. It was found that for a weak interlayer coupling the two different quasiparticle bands, plane-like and chain-like bands, show a minimum at $(\pi/2,\ \pi/2)$ and a maximum at (0, 0) or $(\pi,\ \pi)$. In plane-like dispersion we can find an anomalous "flat" region near Fermi surface along the antiferromagnetic Brillouin zone boundary, which favors the formation of the van-Hove singularities. With increasing interlayer coupling, a large modification of the dispersions is carried out, the minimum deviates from $(\pi/2,\ \pi/2)$ and the energy gap of the two bands decreases and finally disappears when the vertical coupling is larger enough. The shapes of the QP bands are sensitive to the vertical hopping $t_\perp$ rather than the vertical exchange energy $J_\perp$. As the interlayer coupling increases, the shapes of the two QP bands suggest that the chain-like band approaches to that of quasi-one dimensional model, and the plane-like band undergoes the one layer $t-t'$–J models' band.

PACS. 71.27.+a Strongly correlated electron systems; heavy fermions – 75.50.Ee Antiferromagnetics – 74.20.-z Theories and models of superconducting state

1 Introduction

The investigation of hole QP (quasiparticles) dispersion is of significant importance for the searching of the generic features of the high-temperature superconductors. Recent angle-resolved photoemission experiments (ARPES) for $Bi_2Sr_2CaCu_2O_8$ (Bi2212) and Y–Ba–Cu–O near optimal doping showed a very anomalous flat region of their energy dispersion around $(\pi, 0)$ which is absent in the measurement on the insulating copper oxide $Sr_2CuO_2Cl_2$ [1]. In addition, the observed small bandwidth ($\sim 2J$) suggests that the strong correlation is crucial for a proper description of carriers in the cuprates. Consequently, the theoretical calculations [2,3] in the framework of t–J-like model with single or more CuO_2 planes agree with experimental results. It is well established that almost degenerate dispersion along the magnetic Brillouin zone (MBZ) boundary $[(\pi, 0)-(0, \pi)$ line] is an intrinsic property of the pure t–J model, and it can be modulated by any small additional interlayer coupling, such as $t_\perp$ between two planes or hopping integral, or the next-nearest-neighbor hopping t'.

An increasing interest in studying the structure of CuO_3 chains in cuprates is set up recently. The theoretical investigations of the multiband Hamiltonian [4–6] describing the CuO_3 chains of $YBa_2Cu_3O_{7-\delta}$ (YBCO) have shown a good agreement with experimental observations. The electronic structure of the one-dimensional CuO_3 subsystem in YBCO can determine the doping of the superconducting CuO_2 planes which are sometimes described by simple 2D tight binding bands with first and second nearest neighbor hopping. A stack of CuO_2 planes weakly coupled through a transverse hopping $t_\perp$ can be taken as a simple model. In $Bi_2Sr_2CaCu_2O_8$ [7] $t_\perp$ is small in the order of 10^{-1} meV. But in the optimum doped YBCO it is much large with the order of a few tens of meV that is almost in the same order of magnitude as the in-plane hopping integral, which indicates that this material may be fairly three dimensional. The CuO chains coupled to the planes in YBCO participate significantly in the superconductivity [8–10]. In order to examine the important influence of chains on the superconductivity, we can simply limit ourselves here to a model of two layers, one is a plane layer with tetragonal symmetry, while the other is a chain layer with orthorhombic symmetry [11]. In this paper we propose a model which consists of plane and chain layers with an antiferromagnetic (AF) spin interaction between the two layers. It was found that with strongly increasing the interlayer coupling $t_\perp$–$J_\perp$, the quasiparticle dispersions change much more as expected.

The paper is organized as following: in Section 2 we generalize a bilayer model, one layer is square lattice plane,

[a] e-mail: xjfan@ustc.edu.cn

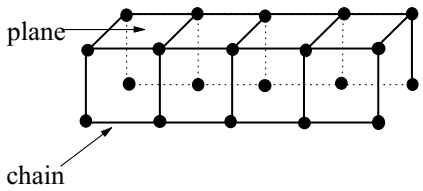

Fig. 1. Schematic illustration of the model on a plane-chain coupled bilayer with intralayer coupling t–J and interlayer coupling $t_\perp$–$J_\perp$.

and the other is chain, which are described by the two–dimension and one-dimension t–J model respectively, and coupled by $t_\perp$ and $J_\perp$ between the two layers. In Section 3 we analysis the Green's functions of the model in self-consistent Born approximation. Numerical results for self-energies and spectral functions are summarized in Section 4. This section also contains the quasiparticle dispersion, spectral weight, bandwidth and discussion of the properties of this model.

2 Plane-chain coupled t–J model

The Hamiltonian of the t–J model considered here for plane-chain bilayer cuprate oxide shown in Figure 1 is expressed as

$$H = -\sum_{\langle ij\rangle,\sigma} t_\alpha(\tilde{c}^{(\alpha)+}_{i\sigma}\tilde{c}^{(\alpha)}_{j\sigma} + H.c.) + \sum_{\langle ij\rangle,\alpha} J_\alpha S^\alpha_i S^\alpha_j - t_\perp \sum_i (\tilde{c}^{(1)+}_{i\sigma}\tilde{c}^{(2)}_{i\sigma} + H.c.) + J_\perp \sum_i S^{(1)}_i S^{(2)}_i. \quad (1)$$

Here $\alpha = 1, 2$ labels plane and chain respectively, i labels sites in each layer, and i and j are nearest neighbors in the same plane. $\tilde{c}^{(\alpha)}_{i\sigma} = c^{(\alpha)}_{i\sigma}(1 - n_{i,-\sigma})$ are hole creation operator with the constraint of no double occupancy. We set an antiferromagnetic interlayer spin coupling $J_\perp$ between the two layers. The kinetic part has a vertical link $t_\perp$. The single hole motion is studied in a two-dimensional Heisenberg antiferromagnet [2,12,13], and the numerical solution by self-consistent method within the Born approximation is in good quantitative agreement with previous numerical diagonalization studies. Hence this method may provide a valuable scheme for further work on spectral properties, quasi-particle dispersion, etc. Here for long-range AF order the spin dynamics is treated in linear spin-wave theory and the hole is described as well-known spinless hole, with polaronlike coupling between holes and spin waves. According to the approach proposed by Schmitt-Rink *et al.* [13], the Hamiltonian of equation (1) becomes

$$H = H_t + H_J,$$
$$H_J = \sum_q \left(\omega_+(q)\alpha^+_q\alpha_q + \omega_-(q)\beta^+_q\beta_q\right), \quad (2)$$

$$H_t = \sum_{kqi}\Big[h^{(i)+}_k h^{(i)}_{k-q}\left[g_{\alpha1}(k,q)\alpha_q + g_{\alpha2}(k,q)\beta_q\right] + H.c.\Big] + \sum h^{(1)+}_k h^{(2)}_{k-q}\Big[g_{121}(k,q)\alpha_q + g_{122}(k,q)\beta_q + g_{211}(k,q)\alpha^+_{-q} + g_{212}(k,q)\beta^+_{-q}\Big] \quad (3)$$

with spin wave energy $\omega^2_i(q) = 2\left(A^2 \pm \sqrt{A^4 - 4B^2}\right)$, $i = 1, 2$, and

$$A^2 = a^2 + b^2 - c^2 - d^2 - 2e^2, \quad (4)$$
$$B^2 = a^2b^2 - a^2d^2 - b^2c^2 - 2abe^2 + (cd - e^2)^2, \quad (5)$$

here $a = J_1 + \dfrac{J_\perp}{4}$, $b = \dfrac{J_2}{2} + \dfrac{J_\perp}{4}$, $c = J_1\gamma_q$, $d = \dfrac{1}{2}J_2\xi_q$, $e = \dfrac{J_\perp}{4}$, $\gamma_k = \dfrac{1}{2}(\cos k_x + \cos k_y)$, and $\xi_k = \cos k_x$. The Bogoliubov transformation factors are

$$u_{ij}(q) = x_{ij}y_1, \quad (i,j = 1,2),$$
$$u_{ij}(q) = x_{ij}y_2, \quad (i = 1,2, \;\; j = 3,4),$$

$$x_{i1} = e\left[\left(\omega_i(q) + a\right)\left(\omega_i(q) - b\right) - cd + e^2\right], \quad (6a)$$
$$x_{i2} = e\left[bc + ad - d\omega_i(q) - c\omega_i(q)\right], \quad (6b)$$
$$x_{i3} = d\left[\omega^2_i(q) - a^2 + c^2\right] - ce^2, \quad (6c)$$
$$x_{i4} = \omega^3_i(q) - b\omega^2_i(q) + (c^2 + e^2 - a^2)\omega_i(q) + a^2b - bc^2 - ae^2, \quad (6d)$$

and

$$y_1 = \sqrt{\frac{x_{13}x_{24} - x_{14}x_{23}}{\mathrm{Det}}}, \quad y_2 = \sqrt{\frac{x_{12}x_{21} - x_{11}x_{22}}{\mathrm{Det}}},$$

where $\mathrm{Det} = (x^2_{11} - x^2_{12})(x_{13}x_{24} - x_{14}x_{23}) - (x^2_{13} - x^2_{14})(x_{11}x_{22} - x_{12}x_{21})$. The hole-magnon vertex factors are

$$g_{111}(k,q) = \frac{4t_1}{\sqrt{N}}\left[\gamma_{k-q}u_{11}(q) + \gamma_k u_{12}(q)\right],$$
$$g_{112}(k,q) = \frac{4t_1}{\sqrt{N}}\left[\gamma_{k-q}u_{13}(q) + \gamma_k u_{14}(q)\right],$$
$$g_{221}(k,q) = \frac{2t_2}{\sqrt{N}}\left[\xi_{k-q}u_{21}(q) + \xi_k u_{22}(q)\right],$$
$$g_{222}(k,q) = \frac{2t_2}{\sqrt{N}}\left[\xi_{k-q}u_{23}(q) + \xi_k u_{24}(q)\right],$$
$$g_{121}(k,q) = \frac{t_\perp}{\sqrt{N}}\left[u_{11}(q) + u_{22}(q)\right],$$
$$g_{122}(k,q) = \frac{t_\perp}{\sqrt{N}}\left[u_{13}(q) + u_{24}(q)\right],$$
$$g_{211}(k,q) = \frac{t_\perp}{\sqrt{N}}\left[u_{12}(q) + u_{21}(q)\right],$$
$$g_{212}(k,q) = \frac{t_\perp}{\sqrt{N}}\left[u_{14}(q) + u_{23}(q)\right]. \quad (7)$$

We mention the similarity of the Hamiltonian with that of the classical polaron problem [14,15]. Here the spin waves play the role of the phonons. For copper-oxides $t > J$, the Hamiltonian defined by equations (2, 3) poses a strong-coupling problem.

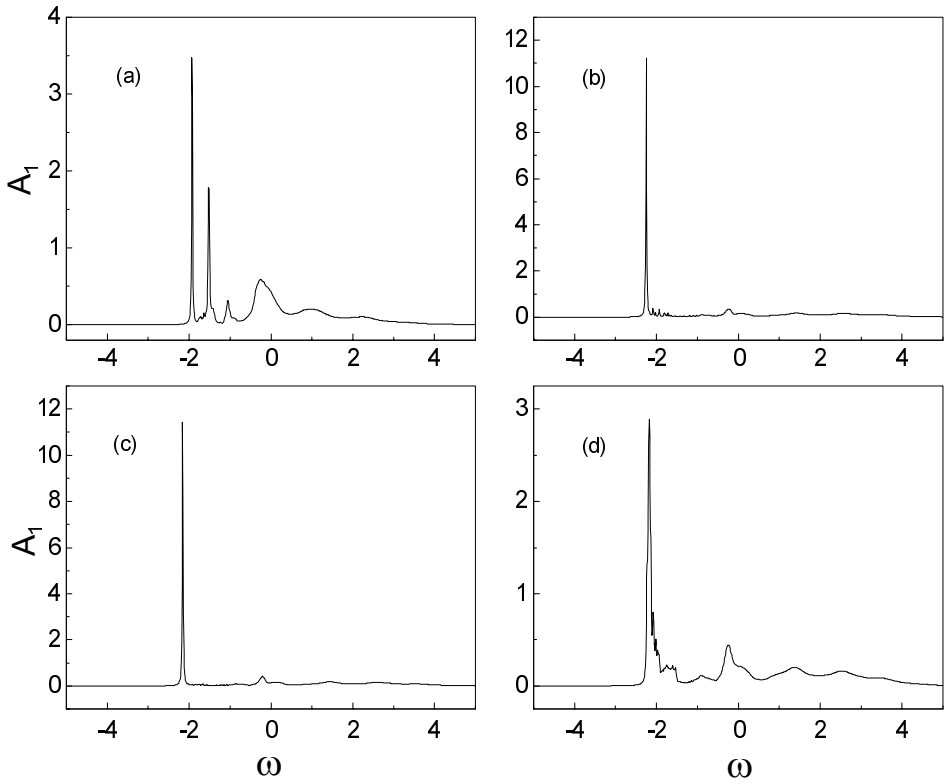

Fig. 2. Spectral functions $A_1(\mathbf{k},\omega)$: (a) $\mathbf{k}=(0,0)$, (b) $\mathbf{k}=(\pi/2,\pi/2)$, (c) $\mathbf{k}=(\pi,0)$, (d) density of states (DOS), for $J=0.4$, $t_\perp=0.7$, $J_\perp=0.2$.

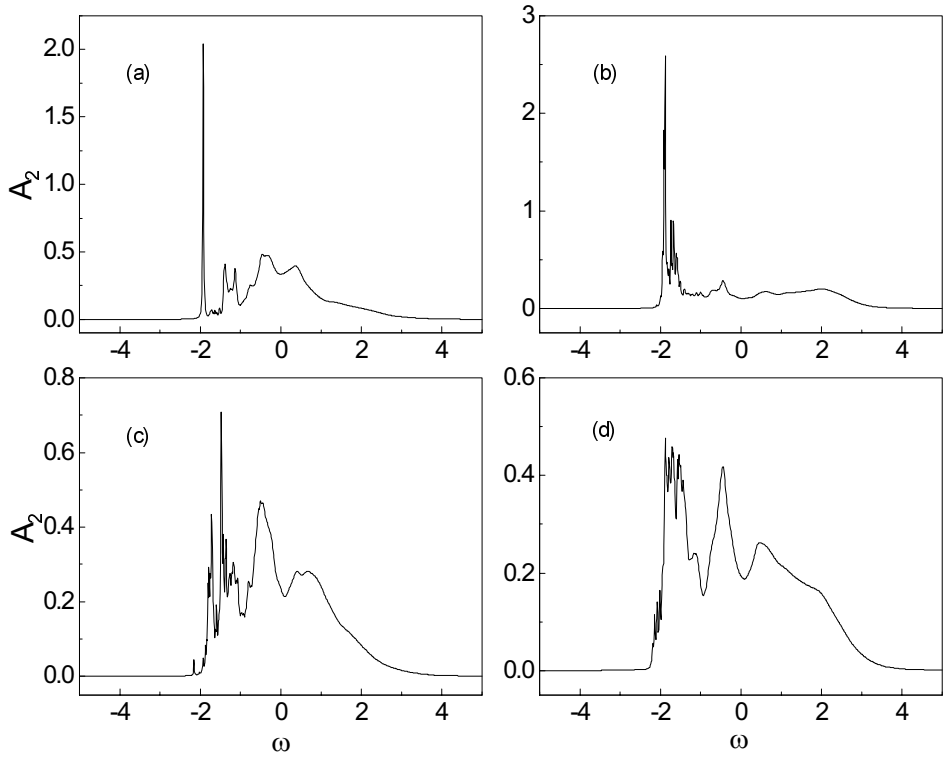

Fig. 3. Spectral functions $A_2(\mathbf{k},\omega)$: (a) $\mathbf{k}=(0,0)$, (b) $\mathbf{k}=(\pi/2,\pi/2)$, (c) $\mathbf{k}=(\pi,0)$, (d) density of states(DOS), for $J=0.4$, $t_\perp=0.7$, $J_\perp=0.2$.

Table 1. Different quantities associated to the quasiparticle spectrum calculated using a 16×16 lattice as function of $t_\perp$ and $J_\perp$. Energies of QP states E_+ and E_- at $\mathbf{k} = (\pi/2, \pi/2)$, bandwidths ΔE_+ and ΔE_-, relative spectral weights a_+ and a_- at the same $\mathbf{k}$ point. Energy parameters are in units of t.

$t_\perp$	$J_\perp$	$E_+(\pi/2,\pi/2)$	$E_-(\pi/2,\pi/2)$	a_+	a_-	ΔE_+	ΔE_-
0.1	0.01	−2.211	−1.670	0.345	0.285	0.783	0.416
0.2	0.04	−2.198	−1.658	0.348	0.228	0.747	0.438
0.3	0.09	−2.196	−1.653	0.350	0.292	0.728	0.473
0.4	0.16	−2.20	−1.644	0.348	0.397	0.718	0.454
0.5	0.25	−2.21	−1.737	0.351	0.076	0.340	0.567
0.6	0.36	−2.22	−1.844	0.347	0.191	0.332	0.664
0.7	0.4	−2.25	−1.913	0.343	0.107	0.341	0.733
0.8	0.4	−2.29	−1.986	0.348	0.115	0.301	0.537
1.0	0.4	−2.36	−2.079	0.345	0.144	0.241	0.481

3 Self-consistent Green's-function approach

From the Hamiltonian of the t–$t_\perp$–J–$J_\perp$ model in equations (2, 3), describing holons (spinless fermions) strongly coupled to spin-wave excitations, we calculate the holon Green's function as follows:

$$G_{\mu\nu} = G^0_{\mu\nu}\delta_{\mu\nu} + \sum_{\rho\lambda} G^0_{\mu\rho}\Sigma_{\rho\lambda}G_{\lambda\nu}, \tag{8}$$

with the self-energy

$$\Sigma_{\mu\nu} = \sum_{\rho\lambda\alpha} g_{\mu\rho\alpha}G_{\rho\lambda\alpha}g_{\nu\lambda\alpha}. \tag{9}$$

In order to simplify the calculations we set hopping constants $t_1 = t_2 = t$, and coupling constants $J_1 = J_2 = J$, and choose the realistic values of parameters: $t = 0.4$ eV, $J/t = 0.2 \sim 0.4$ to study the behaviors of the QP states *versus* various $t_\perp$ and $J_\perp$ from 0 to 1 (we will refer all quantities in units of t from now). The iteration steps are carried out on the 16×16 sites, and ω mesh was set 1 000 points from -5 to 5.

Figures 2 and 3 show the spectral function $A_\alpha = -1/\pi \mathrm{Im} G_{\alpha\alpha}(k,\omega)$, $(\alpha = 1, 2)$, at different momentum for $J = 0.4$, $t_\perp = 0.7$, $J_\perp = 0.2$. In Figure 2, the quasiparticle peak carriers a substantial percentage of the spectral weight in agreement with the calculations for a single layer, and it is stronger for the momentum to the bottom of the band. It can be seen that after considering the AF interaction between plane and chain layers, the shape of $A_1(k,\omega)$ describing the plane-like branch is different from that in reference [3]. The spectral function $A_1(\mathbf{k},\omega)$ at $\mathbf{k} = (0, 0)$ described by an extra peak located at the second-lowest energy which is not found in the identical plane bilayer model is probably due to chain's effect in this chain-plane bilayer model. The main influence of chains is that the spectral weight is largely reduced at $(\pi/2, \pi/2)$ by raising the hole energy at that point. The hole energy at $(\pi, 0)$ is slightly enhanced as comparison with that at $(\pi/2, \pi/2)$. In Figure 3 one can see that the spectral function $A_2(\mathbf{k},\omega)$ has some extra small peaks at the low-energy side of the spectrum which is probably set up by the plane influence. The quasiparticle dispersion relations $E_\pm(\mathbf{k})$ (plane band $E_+(\mathbf{k})$ and chain band $E_-(\mathbf{k})$) are displayed in Figure 4 for $J = 0.4$, $t_\perp = 0.7$, $J_\perp = 0.4$, and for non-coupling situation $t_\perp = J_\perp = 0^+$ as a comparison. It is noted that the plane-like band has a "flat" region around the wave vectors $\mathbf{k} = (\pi, 0)$, which is a remarkable feature of cuprates observed in photoemission experiments. The anomalous flatness is closely near the minimum at $(\pi/2, \pi/2)$, which has been used to explain the spin gap in the normal state of cuprates, the hole pockets forming large Fermi surface, and the superconductivity for the low hole density case [2,3,16]. With the increase of vertical coupling between the two layers, the width of plane-like band decreases, and the peak around $(\pi, 0)$ becomes sharp, which is just like the t–t'–J model [17]. Furthermore, the increase of width of chain-like band is in agreement with a quasi-one dimension model. Table 1 gives the minimum data, the spectral weight of the QP, as well as the two bandwidths for various vertical coupling constants (we choose $J_\perp/t = (t_\perp/t)^2$). The plane-like and chain-like bandwidths decrease rapidly at $t_\perp = 0.5$ and $t_\perp = 0.8$, respectively. The spectral weight at $\mathbf{k} = (\pi/2, \pi/2)$ are different in the two branches. As the vertical coupling increases, the spectral weight is approximately constant for plane-like, but decreases for chain-like band. In Figure 5a, the overall dispersion shape is not very sensitive to the exchange coupling $J_\perp$, but it changes drastically with the hopping $t_\perp$ as shown in Figure 5b. We find that the minimum of the plane-like band deviates from the point $(\pi/2, \pi/2)$ if the vertical coupling $t_\perp$ is large enough $(t_\perp/t = 1.5)$, which can be explained that the orthorhombic character in chains affects the plane-like spectral upon a strong vertical link between plane and chain layers. The energy gap between plane-chain bands disappears at momentum point $(\pi/2, \pi/2)$ and around $(\pi, 0)$ as $t_\perp/t = 1.5$.

The variations of the two dispersions with $t_\perp = 0.3$ and $J_\perp = 0.09$ can be fit by the following trigonometric functions, namely (see Fig. 6)

$$E_+ = -2.162 + 0.158(\cos k_x + \cos k_y)^2 + 0.034(\cos 2k_x + \cos 2k_y) \tag{10a}$$

$$E_- = -1.651 + 0.532\cos^2 k_x. \tag{10b}$$

Equation (10) includes hopping processes to first- and second-nearest neighbors on the same sublattice, which

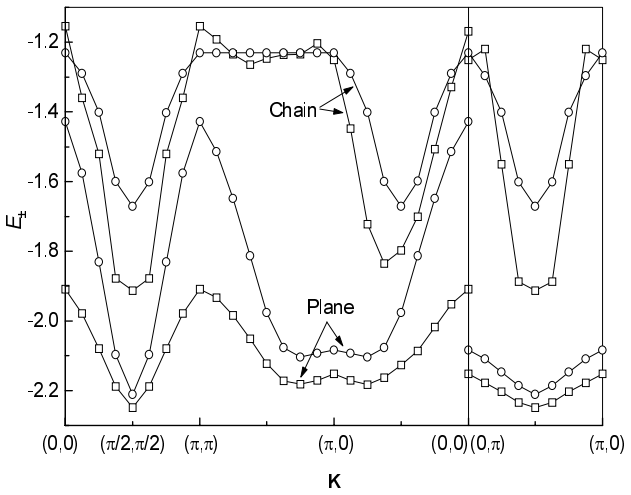

Fig. 4. Dispersion relations of the quasiparticle bands $E_\pm(\mathbf{k})$ (chain-like $E_-(\mathbf{k})$ and plane-like $E_+(\mathbf{k})$), along symmetry lines in the Brillouin zone for $J = 0.4$, $t_\perp = 0.7$, $J_\perp = 0.4$ on a 16×16 sites (open square), and for non-vertical coupling $t_\perp = J_\perp = 0^+$ (open circle).

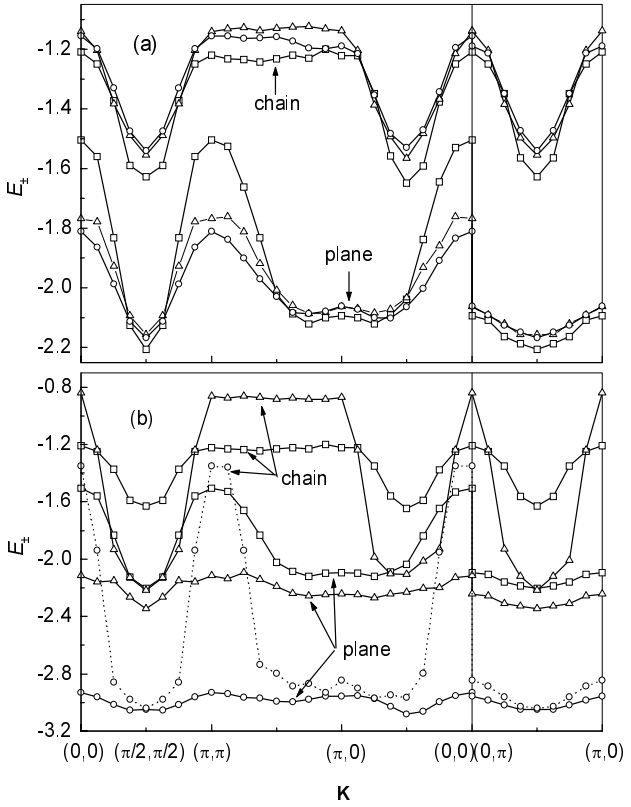

Fig. 5. Dispersion relations for (a) $J = 0.4$, $t_\perp = 0.3$, $J_\perp = 0.1$ (square), 0.4 (uptriangle), 0.7 (circle), and (b) $J = 0.4$, $J_\perp = 0.1$, $t_\perp = 0.3$ (square), 0.7 (uptriangle), 1.5 (circle). The dispersion shape changes drastically with the coupling $t_\perp$, but it is not very sensitive to the exchange coupling $J_\perp$.

is suggested by several works on a single-plane [2,16,17]. The imbalance coefficient x_3 in equation (10) distinguishes between a dispersion where the minimum energy for holes

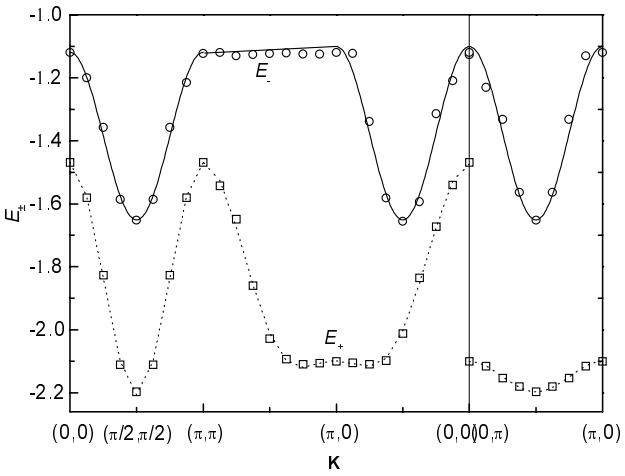

Fig. 6. One hole dispersion for parameters $J = 0.4$, $t_\perp = 0.3$, $J_\perp = 0.09$. Open squares belong to the plane-like branch E_+, while open circles correspond to branch E_-. The dotted (solid) line is a fit using trigonometric functions for plane-like (chain-like) branch.

is on Fermi surface for noninteracting electrons ($x_3 = 0$) and a case characterizing hole pockets $x_3 > 0$ [18]. Here, the hole pockets result from the quantum fluctuations in the ground state rather than a consequence of high-order processes in t [18,19].

4 Summary

From the study on the motion of a single hole in a quantum antiferromagnetic model of plane-chain coupled bilayer within self-consistent Born approximation, we found two split energy bands, plane-like and chain-like bands. The anomalous flatness region along AF Brillouin zone boundary occurs in the plane-like band. With increasing interlayer coupling, the dispersion shape changes apparently, and the gap decreases and finally disappears when the vertical coupling is larger than the magnitude of in-plane coupling. The quasiparticle energy spectrum depends on both structures of plane and chain layers. More evolution of spectrum arises from the vertical hopping $t_\perp$ rather than vertical exchange energy $J_\perp$. The main contribution to the QP dispersion relations $E_\pm(\mathbf{k})$ comes from hole hopping processes on the same sublattice, to avoid distorting the antiferromagnetic background. The extended van-Hove singularities can occur in plane and chain bilayer model. With varying vertical coupling constants it suggests that plane-like and chain-like bands display a transition to one layer t–t'–J model and quasi-one dimension model respectively. As a whole, the vertical coupling between plane and chain layers plays a crucial role to the spectral energy of cuprates.

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