PRAMANA
— journal of
physics

Vol. 58, Nos 5 & 6
May & June 2002
pp. 855–859

Spectral properties of doped bilayer cuprates at finite temperatures

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Abstract. Recently, angle-resolved photoemission spectroscopy measurements on $Bi_2Sr_2CaCu_2O_{8+\delta}$, which possesses two CuO_2 layers in the same unit cell, have yielded very interesting results. For the overdoped samples, these results show a splitting of electronic states near $k = (\pi, 0)$ point of Brillioun zone. On the other hand, no splitting is observed in the underdoped samples. In view of this, the detailed studies including the doping and temperature dependence of the spectral properties become desirable. In this paper, we consider cuprates possessing two CuO_2 layers per unit cell. Each layer in the system is described by the t–t'–J model and the two layers are coupled via an intrabilayer hopping term ($t_\perp$) and an intrabilayer exchange coupling ($J_\perp$). A self-consistent perturbation approach is used to calculate the electronic spectral function for different values of hole density, hole momentum and temperature. We find that the imaginary part of the self energy is strongly momentum dependent which contradicts the suggestion that the Fermi surface of cuprates may be described by marginal Fermi liquid theory. We have calculated the spectral function for various values of intrabilayer parameters $t_\perp$ and $J_\perp$. For larger values of intrabilayer interactions we observe the splitting in the quasi-particle peak at $k = (\pi, 0)$ which is in agreement with the recent observations. The splitting is also found to be sensitive to the hole concentration as well as the temperature of the system. We have also discussed the reasons why the splitting is absent in underdoped bilayer cuprates at low temperature.

Keywords. Doped bilayer cuprates; spectral properties; self-consistent perturbation approach.

PACS Nos 74.62.-h; 74.80.-g

1. Introduction

With recent advancement in the energy and momentum resolution, the angle-resolved photoemission spectroscopy (ARPES) has uncovered several new features in the hole spectrum of cuprates. The spectral function has been obtained for various cuprates including the single layer (e.g. La-214, Bi-2201) [1], the bilayer (e.g. Bi-2212 and Y-123) [2–4] and the trilayer (Bi-2223) [5] compounds. An interesting feature obtained for bilayer compound Bi-2212 is the splitting of electronic states in the overdoped regime [2,3]. The splitting is seen to increase along the (0, 0) to $(\pi, 0)$ direction with a maximum at $(\pi, 0)$ point of the Brillioun zone and vanishes along the direction of high symmetry, i.e., (0, 0) to (π, π)

[2,3]. Such splitting has not been observed in underdoped Bi-2212 [4] as well as in the single layer compounds [1–3]. This is a clear pointer, as earlier predicted by the LDA calculations [6], towards the importance of the coupling between the two CuO_2 planes in the same unit cell.

In this paper, we evaluate the spectral function $A(\mathbf{k},\ \omega)$ for various values of hole densities and temperature for bilayer cuprates and show that the intrabilayer coupling indeed leads towards the splitting of electronic states at $(\pi,\ 0)$ point of Brillioun zone in the optimal and overdoped regimes. Our detailed numerical analysis suggests that the splitting may also be observed in the underdoped samples provided the temperature and the intrabilayer coupling is high enough. We also describe the situations suitable for obtaining the bilayer splitting in these systems.

2. Results and discussion

The detailed theoretical formulation is given elsewhere [7]. We start by considering a system composed of two CuO_2 layers, each characterized by t–t'–J model Hamiltonian, in the same unit cell. We then introduce the coupling between these layers (i.e. the intrabilayer interactions) via hopping of holes between the two layers (i.e. intrabilayer hopping $t_\perp$) and an intrabilayer exchange coupling strength ($J_\perp$) between the spins in the two layers. To the Néel ordered ground state with four sublattices A, B, C and D as shown in figure 1 of [7], we first perform 180° rotation to the 'down' spins at sublattices B in layer 1 and C in layer 2, so that the resulting state is ferromagnetic with spins 'up' only at all the four sublattices. We then transform the correlated hole operators and the spin operators respectively into the spinless fermions and the pseudo-spin operator form and write the model Hamiltonian in k-representation, which reads [7]

$$\begin{aligned} H = & \sum_{lkq} \left\{ t(k-q) f_{lk-q} f^{+}_{lk} s^{+}_{lq} + t(k) f_{lk+q} f^{+}_{lk} s^{-}_{lq} \right\} \\ & + \sum_{ll'kq} \left\{ t_\perp(k-q) f_{lk-q} f^{+}_{l'k} s^{+}_{l'q} + t_\perp(k) f_{lk+q} f^{+}_{l'k} s^{-}_{lq} \right\} \\ & + \sum_{lq} J_\parallel(q) \left\{ s^{+}_{lq} s^{+}_{l-q} + s^{-}_{lq} s^{-}_{l-q} \right\} + \sum_{l \neq l' q} \tilde{J}_\perp \left\{ s^{+}_{lq} s^{+}_{l'-q} + s^{-}_{lq} s^{-}_{l'-q} \right\} \\ & - \sum_{lq} 2 z_{ab} \tilde{J}_\parallel \left\{ s^{Z}_{lq} s^{Z}_{l-q} \right\} - \sum_{l \neq l' q} 2 \tilde{J}_\perp \left\{ s^{Z}_{lq} s^{Z}_{l'-q} \right\} \end{aligned} \tag{1}$$

where

$$\begin{aligned} t(k) &= -2st_\parallel(\cos\ k_x + \cos\ k_y) - 4t'\ \cos\ k_x \cos\ k_y \\ J_\parallel(q) &= 2sz_{ab}\tilde{J}_\parallel(\cos\ q_x + \cos\ q_y) \\ t_\perp(k) &= t_\perp(\cos\ k_x - \cos\ k_y)^2 \end{aligned} \tag{2}$$

and

$$\tilde{J}_\parallel = J_\parallel(1-\delta)^2, \quad \tilde{J}_\perp = J_\perp(1-\delta)^2\ ,$$

where $l(l')$ are the layer indices, k, q are respectively the hole and magnon momenta, $t_\parallel$, t' are the nearest and next nearest neighbor bare hole hopping in the planes, $t_\perp$ is the hopping between the two planes in the same unit cell and $J_\parallel(J_\perp)$ is the exchange between the Cu spins in (between) the two planes, $z_{ab}(=4)$ is the coordination number, $s = 1/2$ is the spin, $f(f^+)$ are the spinless hole annihilation (creation) operators, $s^{\pm,z}$ are the pseudo-spin operators and δ describes the hole density.

We apply the Green's function method and obtain the equations of motion for Green's function $G_\parallel(\mathbf{k},\ \omega)$. The self-energy contributions due to the interaction of holes with the spin excitations are obtained by restricting ourselves only to the first Born approximation. In this manner, we obtain

$$G_\parallel(\mathbf{k},\ \omega) = 1/[\omega - \Sigma(\mathbf{k},\ \omega)] \tag{3}$$

where $\Sigma(\mathbf{k},\ \omega)$ is the contribution due to the self energy. Our numerical calculations suggest that the imaginary part of the self energy shows strong momentum dependence. This indicates that the description of cuprates in terms of marginal Fermi liquid may be inappropriate [7].

With the knowledge of the Green's function $G_\parallel(\mathbf{k},\ \omega)$ we obtain the spectral function $A(\mathbf{k},\ \omega)$ as

$$A(\mathbf{k}, \omega) = -\text{Im}\ G_\parallel(\mathbf{k},\ \omega). \tag{4}$$

We now present the results for the spectral function with $t_\parallel = 0.4$ eV, $t' = 0.25t_\parallel$ and $J_\parallel = 0.3t_\parallel$ for various values of hole density (δ). The effects of intrabilayer interactions are manifested through the anisotropy of the system (r). We define

$$r = J_\parallel/J_\perp = t_\parallel^2/t_\perp^2\,. \tag{5}$$

As shown in figure 1, we have obtained the spectral function $A(\mathbf{k}, \omega)$ at $(\pi, 0)$ point of the Brillioun zone for various values of hole density (δ), temperature (T) and anisotropy (r). In figure 1a, the behavior of the spectral function at $(\pi, 0)$ point is shown for $T = 0.025t_\parallel$ and $\delta = 0.10$ for the anisotropy $r = 6.7$ and 10.0. It is clear that the broad quasiparticle peak (marked as p) at $r = 10.0$ splits into two peaks (marked as p_1 and p_2) for $r = 6.7$. According to eq. (5), a low value of r implies high value of $t_\perp$. Thus, on lowering r, the intrabilayer coupling increases and produces a splitting in the electronic state.

In figure 1b, we analyze the effects of doping on the spectral function at $(\pi, 0)$ point for $t = 0.025t_\parallel$ and $r = 6.7$. We observe that the broad peak present at $\delta = 0.07$ splits into two peaks (marked as p_1 and p_2) for $\delta > 0.10$. In addition, the peak p_1 becomes more and more separated from p_2 on increasing the doping. The reason for the peak splitting lies in the fact that on increasing doping the coupling between the two CuO_2 layers is effectively enhanced. In fact, this a peculiar feature of the t–J model where t scales with δ.

We next present the doping dependence of the spectral peaks in $A(\mathbf{k}, \omega)$ for higher temperature ($T = 0.15t_\parallel$) at $(\pi,\ 0)$ point in figure 1c. With increased temperature the higher energy states are also occupied and effectively enhance the intrabilayer coupling. We, therefore expect peak splitting at even lower values of r for higher values of T. From figure 1c, it is clear that at high T and high δ values, the peak in fact splits even for $r = 10.0$.

These features of spectral function at $(\pi,\ 0)$ point as obtained in figures 1a and 1b are consistent with the recent ARPES measurements performed on underdoped as well as overdoped bilayer system Bi-2212 [2,3]. However, the results predicted in figure 1c are yet to be verified as there exist no experimental observation of spectral function at elevated temperatures.

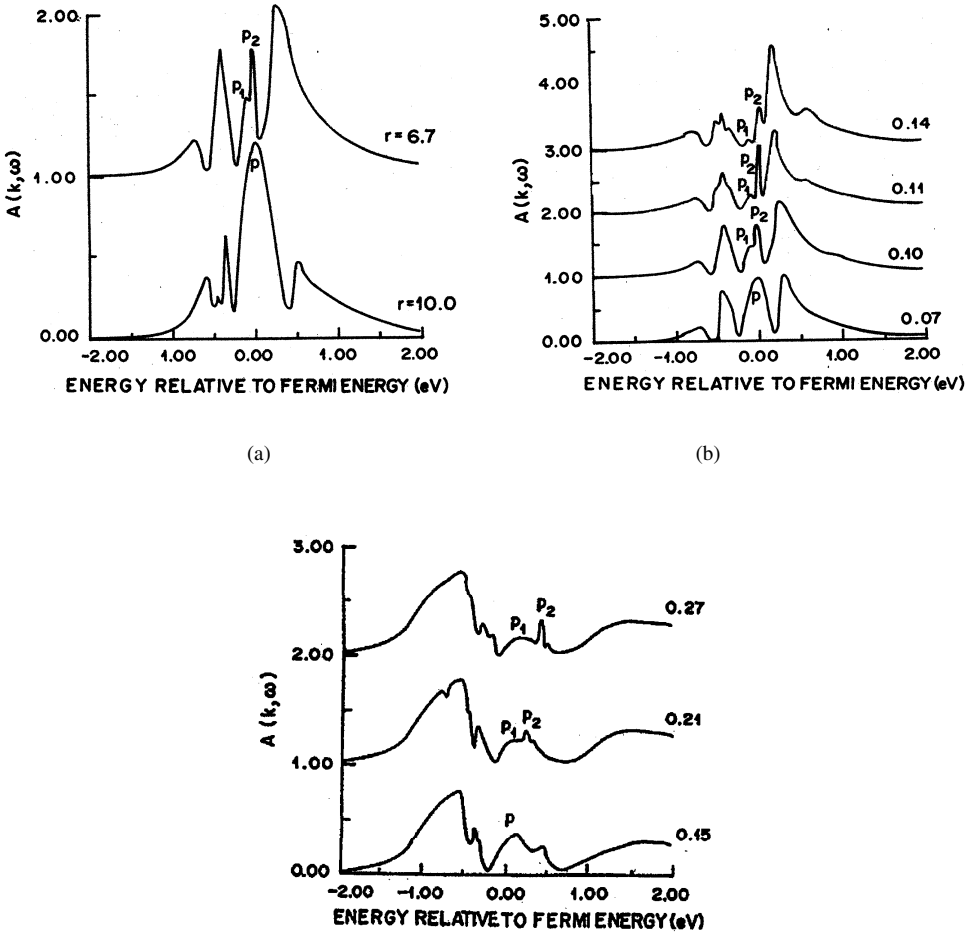

Figure 1. (**a**) Effects of anisotropy (r) on the spectral function $A(\mathbf{k}, \omega)$ at momentum $(\pi, 0)$ for $T = 0.025t_{\|}$ and $\delta = 0.10$. (**b**) Dependence of $A(\mathbf{k}, \omega)$ on δ for $T = 0.025t_{\|}$ and $r = 6.7$ at momentum $(\pi, 0)$. The value next to the curve is the corresponding hole concentration. p marks the broad quasi-particle peak while p_1 and p_2 represent the two split parts of the peak. (**c**) Doping dependence of $A(\mathbf{k}, \omega)$ at momentum $(\pi, 0)$ for $T = 0.15t_{\|}$ and $r = 10.0$. The value next to the curve is the corresponding hole concentration. p marks the broad quasi-particle peak while p_1 and p_2 represent the two split parts of the peak.

3. Conclusion

In conclusion, we have performed a detailed evaluation of temperature and doping dependence of the spectral function at $(\pi,\ 0)$ point of the Brillioun zone for bilayer cuprates. We

notice that the intrabilayer coupling significantly affects the behavior of hole dynamics in the system. In particular, we obtain the splitting of electronic states for overdoped systems at $(\pi,\ 0)$ point of the Brillioun zone. We speculate that the splitting may also be observed in the underdoped cuprates having large intrabilayer coupling at higher temperatures.

Acknowledgements

This work is financially supported by the Department of Science and Technology (DST), Government of India via Grant No. SP/S2/M-32/99. One of us, Govind is thankful to the Council for Scientific and Industrial Research (CSIR), Government of India, for financial support via Grant No. 31/1/(180)/2000EMR-I.

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