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MIXED VALENCE QUASIPARTICLES IN CuO_2 PLANES

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The motion of a single hole doped to a CuO_2 plane of a high temperature superconductor is described by a spin-fermion model which treats explicitly the hybridization with the upper Hubbard band. One finds that sectors of Zhang–Rice bound states coexist with reasonably damped oxygen and copper-like quasiparticles, with a considerable transfer of the spectral weight to the upper Hubbard band. The oxygen states have small dispersions and can be identified in the angle-resolved photoemission experiments for $Bi_2Sr_2CaCu_2O_8$.

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It is well known that large gaps observed in the angle-resolved inverse photoemission (ARPES) experiments in transition metal oxides cannot be explained using band structure calculations based on the local spin density approximation (LSDA) which also fail to reproduce the antiferromagnetic (AF) long-range order observed in the parent compounds of high temperature superconductors (HTS), like La_2CuO_4 and $YBa_2Cu_3O_6$ [1]. In such systems strong electron correlations are of crucial importance and have to be treated explicitly. One way is to construct a spin-fermion model (SFM), where the doped oxygen holes interact with the localized Cu spins by Kondo-like AF interactions [2]. This approach has been successful in reproducing the quasiparticle (QP) bands in NiO [3] and the weakly dispersive states near the Fermi level (FL) in HTS [4]. The covalent character of the localized $3d^9$ states [5,6] motivated us to consider an extension of a strongly correlated SFM to a CuO_2 plane which implements explicitly the mixed valence (MV) behaviour of the p and d-holes.

We consider the four-band model for a CuO_2 plane including $Cu(3d_{x^2-y^2})$ (x), $Cu(3d_{3z^2-1})$ (z), and $O(2p_\sigma)$ orbitals, and assume the weak Cu–O hybridization as compared with the Coulomb repulsion at Cu sites ($|t_{xp}| \ll U$). Thus, we have integrated out the transitions to the lower Hubbard band (LHB) $(3d^8)$ [2] [which is split into one high-spin ($^3A_2$) and two low-spin ($^1A_2$, $^1E_1$) multiplets], while the upper Hubbard band (UHB) $(3d^9)$, described by the projected operators, $\widetilde{d}_{i\sigma} = d_{i\sigma}(1 - n_{i,-\sigma})$, still hybridizes with $2p$ holes. The effective Hamiltonian is

$$H_{\rm MV} = \Delta_x \sum_{i\sigma} \tilde{d}^\dagger_{i\sigma}\tilde{d}_{i\sigma} + \sum_{\langle jj'\rangle,\sigma} t_{jj'} a^\dagger_{j\sigma} a_{j'\sigma} + \sum_{\langle ij\rangle,\sigma} t_{ij}(\tilde{d}^\dagger_{i\sigma} a_{j\sigma} + {\rm h.c.})$$

$$+T_k \sum_{\langle ijj'\rangle,\sigma} (a^\dagger_{j\sigma} a_{j'\sigma} + {\rm h.c.}) + J_k \sum_{\langle ijj'\rangle} \boldsymbol{S}_i \boldsymbol{s}_{jj'} + J \sum_{\langle ii'\rangle} \boldsymbol{S}_i \boldsymbol{S}_{i'}, \qquad (1)$$

with *nonlocal* oxygen spin operators, $s^\dagger_{jj',\xi} = a^\dagger_{j,\xi\uparrow} a_{j',\xi\downarrow}$ and $s^z_{jj',\xi} = \frac{1}{2}(a^\dagger_{j,\xi\uparrow} a_{j',\xi\uparrow} - a^\dagger_{m,\xi\downarrow} a_{n,\xi\downarrow})$, with $\xi = p_x, p_y$, and i (j, j') labels Cu (O) sites. $\Delta_x = \varepsilon_x - \varepsilon_p$ is the charge transfer (CT) energy between electron O($2p$) and Cu($3d$) states. $J_{\rm K} = \left[2J_k(^1E_1) + J_k(^1A_2) - J_k(^3A_2)\right]$ and $T_k = \left[2J_k(^1E_1) + 3J_k(^3A_2) + J_k(^1A_2)\right]/4$ are the three-site Kondo elements, with $J_k(^3A_2) = t_z^2/\left[U(^3A_2) - \Delta_z\right]$, $J_k(^1A_2) = t_z^2/\left[U(^1A_2) - \Delta_z\right]$, and $J_k(^1E_1) = t_x^2/\left[U(^1E_1) - \Delta_x\right]$.

We derived the hole–magnon coupling by rotating the spins on one (B) sublattice by 180 degrees which changes the AF order into the ferromagnetic one [7]. We treat the excitations of the spin system within the linear spin-wave (LSW) theory and calculate the d and p spectral functions in the self-consistent Born approximation (SCBA) [8]. This approximation includes the leading hole–magnon interactions and turned out to be surprisingly accurate for the t–J model [7], and for systems with $S = 1$ [3, 9]. After Fourier and Bogolyubov transformations one finds the following Hamiltonian in the LSW approximation:

$$H_{\rm LSW} = \sum_{\boldsymbol{k},\mu\sigma} \varepsilon_\mu(\boldsymbol{k}) a^\dagger_{\boldsymbol{k},\mu\sigma} a_{\boldsymbol{k},\mu\sigma} + \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}} \beta^\dagger_{\boldsymbol{q}} \beta_{\boldsymbol{q}}$$

$$+ \sum_{\boldsymbol{k}\boldsymbol{q},\mu\nu\sigma} \left[M^{pp}_{\mu\nu} a^\dagger_{\boldsymbol{k}-\boldsymbol{q},\mu\sigma} a_{\boldsymbol{k},\nu-\sigma} (\beta^\dagger_{\boldsymbol{q}} + \beta_{-\boldsymbol{q}}) + M^{pd}_{\mu\nu} \left(a^\dagger_{\boldsymbol{k}-\boldsymbol{q},\mu\sigma} a_{\boldsymbol{k},\nu\sigma} \beta^\dagger_{\boldsymbol{q}} + {\rm h.c.} \right) \right], \qquad (2)$$

where $\varepsilon_\mu(\boldsymbol{k})$ stands for the oxygen subbands $(\mu = 1, 2)$ and for the copper UHB $(\mu = 3)$ obtained from the first four terms in Eq. (1). $M^{pp}_{\mu\nu}$ is the hole–magnon vertex obtained from the Kondo interactions while $M^{pd}_{\mu\nu}$ describes the direct d–p hoppings and has a similar structure as the one found in the t–J model [7] making the Cu spins mobile. Both hole–magnon bare vertices, found in the LSW–SCBA, depend on the coefficients of the Bogolyubov transformation for bosons, $\{u_{\boldsymbol{q}}, v_{\boldsymbol{q}}\}$, and for fermions, $\{V^\xi_{\mu,\boldsymbol{k}}\}$. As in the case of NiO [3], the Green function has been iterated self-consistently in SCBA,

$$G^{-1}_{\mu\nu}(\boldsymbol{k},\omega) =$$

$$\omega - \delta_{\mu\nu}\varepsilon_\mu(\boldsymbol{k}) - \sum_{\boldsymbol{q},\alpha\beta} \left[M^{pp}_{\mu\alpha} M^{pp}_{\beta\nu} + M^{pd}_{\mu\alpha} M^{pd}_{\beta\nu} \right] G_{\alpha\beta}(\boldsymbol{k}-\boldsymbol{q}, \omega-\omega_{\boldsymbol{q}}). \qquad (3)$$

There is no diagram $\sim M^{pp}_{\mu\alpha} M^{pd}_{\beta\nu}$ as it would correspond to coupling two different spin processes: $\sigma \rightarrow -\sigma$ and $\sigma \rightarrow \sigma$. All the numerical calculations were performed on a 16×16 lattice with toroidal boundary conditions. We describe the dynamics of a doped hole by single hole spectral functions, $A_\mu(\boldsymbol{k},\omega) = -\frac{1}{\pi}{\rm Im} G_{\mu\mu}(\boldsymbol{k},\omega)$.

Here we present the results for the realistic parameters of CuO_2 planes in HTS, as extracted from the LSDA calculations and experiments [5]: $t_{pp} = 0.65$, $t_{xp} = 1.3$, $t_{zp} = t_{xp}/\sqrt{3}$, $\Delta_x = \varepsilon_x - \varepsilon_p = 3.5$, $\Delta_z = \varepsilon_z - \varepsilon_p = 2.9$, $U(^3A_2) = 5.3$,

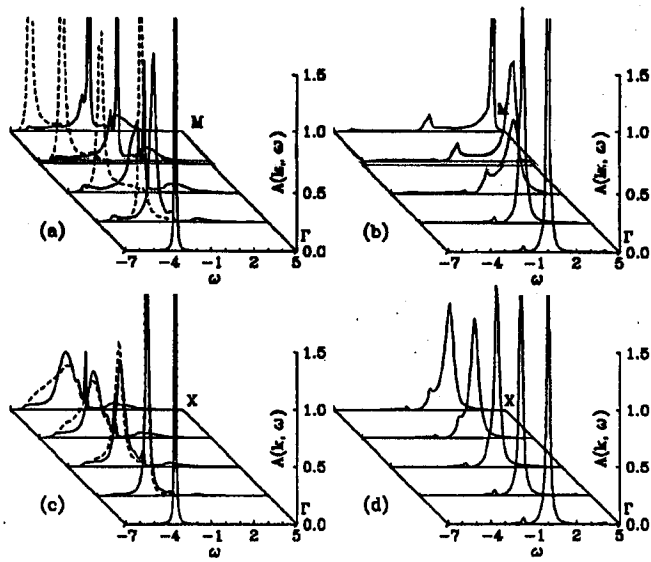

Fig. 1. Spectral functions $A(\boldsymbol{k},\omega)$ for $\boldsymbol{k} = (\frac{n\pi}{8}, 0)$ in Γ–M and for $\boldsymbol{k} = (\frac{n\pi}{8}, \frac{n\pi}{8})$ in Γ–X direction ($n = 0, 1, 2, 3, 4$) for CuO_2 plane for $2p$ [(a), (c)] and $3d$ [(b), (d)] states.

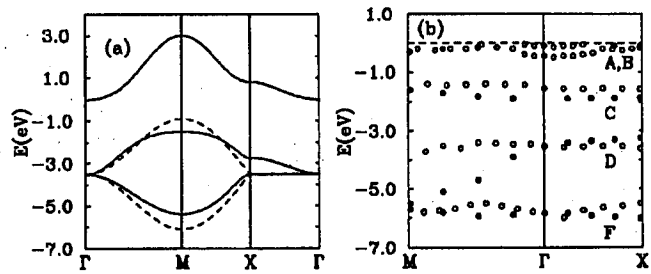

Fig. 2. (a) Free electron bands, $\varepsilon_\mu(\boldsymbol{k})$ (full lines), and unhybridized oxygen bands at $t_{xp} = 0$ (dashed lines). (b) The calculated QP states in the MV SFM (full circles) and the maxima measured in ARPES experiments of Ref. [12] (empty circles).

$U(^1E_1) = 7.3$, and $U(^1A_2) = 8.3$ (all in eV). The spin waves $\omega_{\boldsymbol{q}}$ were calculated for the superexchange interaction $J = 0.15$ eV [10]. One finds that the oxygen spectral functions $A_\mu(\boldsymbol{k},\omega)$ ($\mu = 1, 2$) strongly depend on the momentum $\boldsymbol{k}$ (Fig. 1). The oxygen Zhang–Rice (ZR) states [11] are less bound ($\omega \approx -2$ eV), and absorb less spectral weight than in the localized SFMs [3,4], but retain their nondispersive character. The copper states ($\mu = 3$) are coherent only around the M point, with the bound state at $\omega \approx 4$ [eV] and antibound one near the Fermi level (FL) (see Fig. 1b). As $M^{pd}_{\mu\nu}$ *does not* vanish at the Γ point, one can see a weak antibound state below the δ-like Cu peak (Fig. 1b,d). Moreover, some of the oxygen spectral weight is transferred to the UHB (Fig. 1a,c) and as a consequence the FL is located in the UHB at $\omega \approx 0$.

Unlike in the previous SFMs [3,4], one finds the d-like antibound states at the FL, and rather flat oxygen bands at lower energies. Comparing Fig. 2a with 2b below the FL, one can see that the two free oxygen bands (Fig. 2a) split into four well visible features in the spectrum due to the fermion–magnon interactions. These features fit quite well the ARPES experimental data for $Bi_2Sr_2CaCu_2O_8$ (Fig. 2b). We consider this remarkably successful, as the only visible discrepancy occurs along the Γ–M direction for the "D" feature. Moreover, the total dispersion of the oxygen spectrum increases (decreases) with increasing (decreasing) Δ_x, while the position of the ZR QPs remains almost unchanged.

In summary, we have found that the essential features observed in the photoemission of hole-doped cuprates in broad energy range are well described within the SFM which implements explicitly the MV character of the QPs at the FL.

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