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# Zhang-Rice Localization and Quasiparticles in CuO$_2$ Planes

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**We solve the spin-fermion model for CuO$_2$ planes and find that the hole spectral density consists of a narrow band of the singlet quasiparticles which coexists with damped oxygen states at larger energies.**

It is well known that the commonly performed band structure calculations based on the local spin density approximation (LSDA) do not explain the large gaps observed in the angle-resolved inverse photoemission (ARIPES) experiments in transition metal oxides, and cannot reproduce the antiferromagnetic (AF) long-range order in La$_2$CuO$_4$ and YBa$_2$Cu$_3$O$_6$ [1]. In these systems strong electron correlation dominate and have to be treated explicitly. We have shown recently that an effective spin-fermion model derived for NiO(100) reproduces the experimental observations [2]. Here we present a similar spin-fermion model for CuO$_2$ planes.

We start from the four-band model for a CuO$_2$ plane which includes Cu($3d_{x^2-y^2}$), Cu($3d_{3z^2-1}$), and O($2p_\sigma$) orbitals and assume weak $d$-$p$ hybridization. The O$2p$ bands lie in between the Cu$3d^9$ upper (UH) and $3d^8$ lower (LH) Hubbard bands. The UH band has $^2E_2(e_g)$ character, while the LH band is split into one high-spin ($^3A_2$) and two low-spin ($^1A_2$, $^1E_1$) subbands. After integrating out the transitions to these excited states one finds in second order the effective spin-fermion model. The undoped system is described by the Heisenberg model with the AF superexchange between the Cu$3d^9$ ions. Doped holes occupy the O($2p_\sigma$) orbitals and interact with Cu spins $\vec{S}_i$ by the Kondo interaction,

$$H_{h-s} = \sum_{imn} J_K \vec{S}_i \cdot \vec{s}_{mn}, \qquad (1)$$

where $\vec{s}_{mn,e}$ are nonlocal spin operators, and $J_K = 4[J_K(\Delta) + J_K(^1E_1)] + 2[J_K(^1A_2) - J_K(^3A_2)]$. The free hole propagation ($H_h^0$), given by direct oxygen-oxygen hoppings $t_{pp}$ and $t'_{pp}$, is renormalized by the effective three-site hopping terms ($H_h^J$), $\sim T_{ee} = \frac{1}{4}[2J_K(\Delta) - 3J_K(^3A_2) - 2J_K(^1E_1) - J_K(^1A_2)]$. The derived total spin-fermion Hamiltonian has in the linear spin wave (LSW) approximation [3] the following form,

$$\begin{aligned} H_{LSW} = {} & \sum_{\vec{k},\mu\sigma} \varepsilon_\mu(\vec{k}) a^\dagger_{\vec{k},\mu\sigma} a_{\vec{k},\mu\sigma} + \sum_{\vec{q}} \omega_{\vec{q}} \beta^\dagger_{\vec{q}} \beta_{\vec{q}} \\ & + \sum_{\vec{k}\vec{q},\mu\nu\sigma} M_{\mu\nu} (\beta^\dagger_{\vec{q}} + \beta_{-\vec{q}}) a^\dagger_{\vec{k}-\vec{q},\mu\sigma} a_{\vec{k}\nu,-\sigma}, \end{aligned} \qquad (2)$$

where $\omega_q = 4J(1-\gamma_{\vec{q}}^2)^{1/2}$ is the magnon dispersion in the unfolded Brillouin zone (BZ), with $\gamma_{\vec{q}} = \frac{1}{2}(\cos 2q_x + \cos 2q_y)$. The hole bands $\varepsilon_\mu(\vec{k})$ are derived from the diagonalization of $H_h^0 + H_h^J$ in the reciprocal space. The hole-magnon bare vertex, $M_{\mu\nu} = M_{\mu\nu}(\vec{k},\vec{q})$, depends on the geometrical factors which follow from the Bogoliubov transformation. As a result, we have obtained the single hole spectral functions,

$$A_{\mu\mu}(\vec{k},\omega) = \pi^{-1} Im G_{\mu\mu}(\vec{k},\omega), \qquad (3)$$

by iterating selfconsistently the hole selfenergy,

$$\Sigma_{\mu\nu}(\vec{k},\omega) = \sum_{\alpha\beta,\vec{q}} M_{\mu\alpha} M_{\beta\nu} G_{\alpha\beta}(\vec{k}-\vec{q},\omega-\omega_{\vec{q}}), \qquad (4)$$

with $G^{-1}_{\mu\nu}(\vec{k},\omega) = \omega - \varepsilon_\mu(\vec{k})\delta_{\mu\nu} - \Sigma_{\mu\nu}(\vec{k},\omega)$ on a $16\times16$ lattice with torroidal boundary conditions.

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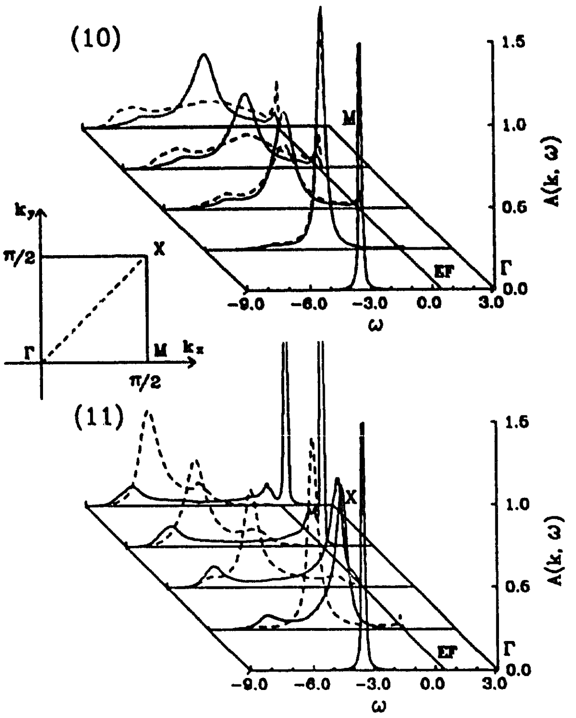

Figure 1. Spectral functions $A_{\mu\mu}(\vec{k},\omega)$ along the main directions (inset): $\vec{k} = (\frac{n\pi}{8}, 0)$ (top) and for $\vec{k} = (\frac{n\pi}{8}, \frac{n\pi}{8})$ (bottom), $n = 0, 1, 2, 3, 4$ . Doping by ~ 7% holes gives the Fermi energy $E_F$.

We have used the realistic parameters, as extracted from the LSDA calculations [4, 5]: $t_{pp} = 0.65$, $t'_{pp} = 0.4$, $t_x = 1.3$, $t_z = t_x/\sqrt{3}$, $\Delta = \varepsilon_x - \varepsilon_p = 3.5$, $\varepsilon_x - \varepsilon_z = 0.6$, $U(^3A_2) = 5.3$, $U(^1E_1) = 7.3$, and $U(^1A_2) = 8.3$ (all in eV). The oxygen spectral functions $A_{\mu\mu}(\vec{k},\omega)$ (3) depend strongly on the momentum $\vec{k}$ (see Fig. 1). As in NiO(100) plane [2], the hole-magnon coupling vanishes at the Γ point and is at maximum at the $X$ point. Along Γ-$M$ direction the coupling is much weaker than along Γ-$X$, but in both cases one finds sharp quasiparticle (QP) states due to the formation of Zhang-Rice (ZR) bound states [6] close to the Fermi level $E_F$. Going towards $X$ point these QP states cross $E_F$ and a rather small dispersion ~ 0.4 eV is found. Even on the quantitative level the agreement with the experiment [7, 8] is astonishing (Fig. 2). We have identified a nondispersive band around the $M$ point, as observed in ARUPS [8]. It agrees with the singlet pole found in the three-band model [9].

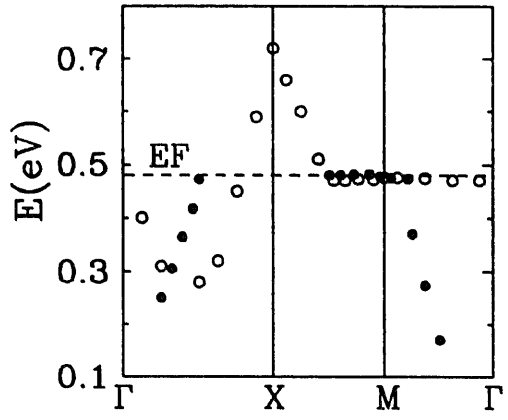

Figure 2. The calculated ZR states (empty circles) and the maxima measured in ARUPS experiments [8]. The Fermi energy as in Fig. 1.

The preliminary results obtained in the more general model which includes the states of $t_{2g}$ symmetry confirms the above picture, but the ZR states became less distinct, in particular in the Γ-$M$ direction. Thus, the essential features observed in the photoemission for $p$-type cuprates may be understood in terms of a strongly correlated spin-fermion model. The spectra are dominated by the incoherent processes at high energy, accompanied by the the local singlet bound states.

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