Zhang-Rice Localization and Quasiparticles in CuO₂ Planes

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We solve the spin-fermion model for CuO₂ 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 La₂CuO₄ and YBa₂Cu₃O₆ [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 CuO₂ planes.

We start from the four-band model for a CuO₂ plane which includes Cu(3dₓ²₋ᵧ²), Cu(3dₓ²₋ᵧ), and O(2p) orbitals and assume weak d-p hybridization. The O2p bands lie in between the Cu3d upper (U₁) and 3d lower (L₁) Hubbard bands. The U₁ band has 2E₂(ε₉) character, while the L₁ band is split into one high-spin (₃A₂) and two low-spin (₁A₂, ₁E₁) subbands. After integrating out the transitions to these excited states one finds in second order the effective spin-fermion Hamiltonian. The undoped system is described by the Heisenberg model with the AF superexchange between the Cu3d ions. Doped holes occupy the O(2p) orbitals and interact with Cu spins \( S_i \) by the Kondo interaction,

\[
H_{h-s} = \sum_{i,m} J_K S_i \cdot S_m,
\]

where \( S_{mn} \) are nonlocal spin operators, and

\[
J_K = 4[J_K(Δ) + J_K(₁E₁)] + 2[J_K(₁A₂) - J_K(₃A₂)].
\]

The free hole propagation (\( H₈ \)), given by direct oxygen-oxygen hoppings \( t_{pp} \) and \( t'_{pp} \), is renormalized by the effective three-site hopping terms (\( H₈' \)), ~ \( T_{ss} = \frac{1}{4}[2J_K(Δ) - J_K(₃A₂) - 2J_K(₁E₁) - J_K(₁A₂)] \). The derived total spin-fermion Hamiltonian has in the linear spin wave (LSW) approximation [3] the following form,

\[
H_{LSW} = \sum_{k,μτ} \varepsilon_k(\tilde{k}) a_{k,μσ}^π a_{k,μσ} + \sum_{q} \varepsilon_q \beta_q^π \beta_q^π + \sum_{k,q,μνσ} M_{μν}(\beta_q^π + \beta_{-q}^π) a_{k,q,μσ}^π a_{k,q,νσ}^π,
\]

where \( \varepsilon_q = 4J(1 - \gamma_q^2)^{1/2} \) is the magnon dispersion in the unfolded Brillouin zone (BZ), with \( \gamma_q = \frac{1}{2}(\cos 2q_x + \cos 2q_y) \). The hole bands \( \varepsilon_k(\tilde{k}) \) are derived from the diagonalization of \( H_h^π + H₈ \) in the reciprocal space. The hole-magnon bare vertex, \( M_{μν} = M_{μν}(\tilde{k}, \tilde{q}) \), depends on the geometrical factors which follow from the Bogoliubov transformation. As a result, we have obtained the single hole spectral functions,

\[
A_{μν}(\tilde{k}, ω) = π^{-1} Im G_{μν}(\tilde{k}, ω),
\]

by iterating selfconsistently the hole selfenergy,

\[
Σ_{μν}(\tilde{k}, ω) = \sum_{αβ, q} M_{μα} M_{νβ} G_{αβ}(\tilde{k} - q, ω - ω_q),
\]

with \( G_{μν}^{-1}(\tilde{k}, ω) = ω - \varepsilon_k(\tilde{k}) δ_{μν} - Σ_{μν}(\tilde{k}, ω) \) on a 16x16 lattice with toroidal boundary conditions.
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 \( A_{\mu \nu}(\tilde{k}, \omega) \) (3) depend strongly on the momentum \( \tilde{k} \) (see Fig. 1). As in NiO(100) plane [2], the hole-magnon coupling vanishes at the \( \Gamma \) point and is at maximum at the \( X \) point. Along \( \Gamma - M \) direction the coupling is much weaker than along \( \Gamma - X \), 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 \( \sim 0.4 \) 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].

**REFERENCES**