ORBITAL-LATTICE QUASIPARTICLES IN FERROMAGNETIC $LaMnO_3$*

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(Received July 10, 2002)

We investigate the combined influence of electron-phonon and orbital polarization interactions on hole propagation in a ferromagnetic plane of orbitally ordered $LaMnO_3$. The quasiparticle band found at the bottom of the hole spectrum is accompanied by broad structures representing vibrational side-bands resulting from the hole-lattice coupling.

PACS numbers: 75.47.Lx, 75.30.Et, 73.20.Mf, 79.60.–i

To explain the colossal magnetoresistence [1] and metal-insulator transition observed in manganese oxides beyond the simple double-exchange model one has to understand a complex interplay between magnetic, charge, and structural order as well as the mobility of itinerant strongly correlated e_g carriers in undoped $LaMnO_3$ with A-type antiferromagnetic order. Considering the hole motion within ferromagnetic (a,b) planes one can constrain the effective model to the hole scattering on orbital [2] and phononic [3] excitations only. Both kinds of the excitations have been observed recently using Raman scattering measurements [4]. The propagation of a single hole is considered using the lattice-orbital-hole model,

$$H = H_t + H_\Delta + H_J + H_{\rm JT} + E_l + H_{\rm ph}, \tag{1}$$

which includes the kinetic energy of a hole (H_t), the polarization of orbitals around a hole (H_Δ) [5], superexchange interaction between the Mn^{3+}–Mn^{3+}

* Presented at the International Conference on Strongly Correlated Electron Systems, (SCES 02), Cracow, Poland, July 10–13, 2002.

ions due to charge excitations (H_J) [6], the Jahn–Teller (JT) interaction ($H_{\rm JT}$) with the distorted lattice energy (E_l) [7], and the oxygen ion oscillations around their distorted positions ($H_{\rm ph}$). The alternating orbital ordering is defined by two orbital sublattices with the occupied e_g orbitals,

$$|i\mu\rangle = \cos\left(\tfrac{\pi}{4}-\phi\right)|iz\rangle \pm \sin\left(\tfrac{\pi}{4}-\phi\right)|ix\rangle, \tag{2}$$

where + (−) refers to $i \in A$ ($i \in B$) orbital sublattice, and $|ix\rangle$ ($|iz\rangle$) stands for the orbital $|x^2-y^2\rangle$ ($|3z^2-r^2\rangle$) at site i, respectively. The angle ϕ describes the type of orbital ordering and depends on external pressure [8].

In the linear phonon-orbital-wave (LPOW) theory the effective Hamiltonian (1) represents a coupled hole-phonon-orbiton problem in momentum space [3],

$$H_{\rm LPOW} = \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} h^\dagger_{\boldsymbol{k}} h_{\boldsymbol{k}} + \sum_{\boldsymbol{q}} \left(\sum_{\xi=1,2} \Omega^{(\xi)}_{\boldsymbol{q}} \beta^\dagger_{\boldsymbol{q},\xi}\beta_{\boldsymbol{q},\xi} + \omega_0 \sum_{\xi=1,3} B^\dagger_{\boldsymbol{q},\xi} B_{\boldsymbol{q},\xi} \right)$$
$$+ \sum_{\boldsymbol{k},\boldsymbol{q}} \left\{ h^\dagger_{\boldsymbol{k}-\boldsymbol{q}} h_{\boldsymbol{k}} \left[\sum_{\xi=1,3} M^{(\xi)}_0 B^\dagger_{\boldsymbol{q},\xi} + \sum_{\xi=1,2} \left(M^{(\xi)}_{\boldsymbol{k},\boldsymbol{q}} \beta^\dagger_{\boldsymbol{q},\xi} + N^{(\xi)}_{\boldsymbol{k},\boldsymbol{q}} \beta^\dagger_{\boldsymbol{q}+\boldsymbol{Q},\xi} \right) \right] + \text{H.c.} \right\}, \tag{3}$$

with the free hole dispersion, $\varepsilon_{\boldsymbol{k}} = t\left[1-2\sin(2\phi)\right]\gamma_{\boldsymbol{k}}$, and the nesting vector $\boldsymbol{Q} = (\pi,\pi)$. $M^{(\xi)}_0$ and $\{M^{(\xi)}_{\boldsymbol{k},\boldsymbol{q}},\, N^{(\xi)}_{\boldsymbol{k},\boldsymbol{q}}\}$ are the structureless hole-phonon and mixed orbiton-phonon vertices, respectively, while $B_{\boldsymbol{q},\xi}$ and $\beta_{\boldsymbol{q},\xi}$ are bosonic operators for the phonon and mixed excitations [9], respectively, which depend on the JT coupling $\propto \lambda$ and on the polarization interactions $\propto \Delta$. The Green's function, $G(\boldsymbol{k},\omega) = \left[\omega - \varepsilon_{\boldsymbol{k}} - \Sigma(\boldsymbol{k},\omega)\right]^{-1}$, is determined in the self-consistent Born approximation [10] by the hole self-energy obtained from the dressed Green's function,

$$\Sigma(\boldsymbol{k},\omega) = \sum_{\boldsymbol{q}} \sum_{\xi=1,2} \Big\{ (M^{(\xi)}_{\boldsymbol{k},\boldsymbol{q}})^2 G[\boldsymbol{k}-\boldsymbol{q}, \omega - \Omega^{(\xi)}_{\boldsymbol{q}}]$$
$$+ \; (N^{(\xi)}_{\boldsymbol{k},\boldsymbol{q}})^2 G[\boldsymbol{k}-\boldsymbol{q}, \omega - \Omega^{(\xi)}_{\boldsymbol{q}+\boldsymbol{Q}}] \Big\} + 3M_0^2 \sum_{\boldsymbol{q}} G[\boldsymbol{k}-\boldsymbol{q}, \omega-\omega_0], \tag{4}$$

leading to the hole spectral functions, $A(\boldsymbol{k},\omega) = -\frac{1}{\pi}{\rm Im}G(\boldsymbol{k},\omega+i0^+)$.

Here, we have concentrated on three representative alternating orbital orderings: $|x^2-z^2\rangle/|y^2-z^2\rangle$, $(|x\rangle+|z\rangle)/(|x\rangle-|z\rangle)$, and $|3x^2-r^2\rangle/|3y^2-r^2\rangle$, realized for $\phi = \pi/12$, 0, and $-\pi/12$, respectively. At finite momenta the spectra consist of quasiparticle (QP) peaks at low energies and the incoherent background at higher energies, whereas at $\boldsymbol{k} \simeq (0,0)$ one finds a completely

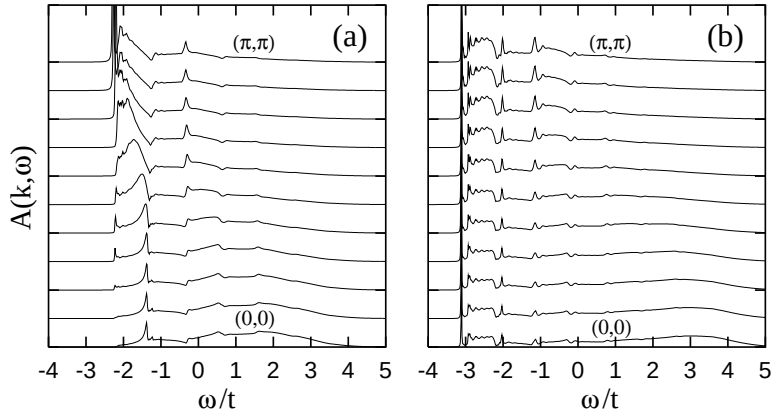

Fig. 1. The hole spectral functions $A(\boldsymbol{k},\omega)$ calculated on a grid with 20×20 $\boldsymbol{q}$-points, as obtained along the $(0,0)$-(π,π) direction for the staggered $(|x\rangle - |z\rangle)/(|x\rangle + |z\rangle)$ orbital ordering ($\phi = 0$) for $\lambda/t = 7$ with: (a) $\Delta = 0$ and (b) $\Delta = t$. Other parameters as in Ref. [3].

incoherent spectrum. As presented in Figs. 1 and 2, the QP at $\boldsymbol{k} \to (\pi,\pi)$ is accompanied by a broad ($\Delta\omega \sim t$) structure above, which represents a side-band effect for the anti-JT distortions predicted by Allen and Perebeinos for $LaMnO_3$ [11]. Increasing the in-plane hopping by changing the orbital ordering to $\phi = -\pi/12$, we find a band-like structure at $\boldsymbol{k} \to (0,0)$ and $\omega \simeq 3t$ which gets broader as a result of the JT interaction [see Fig. 2(a) and (b)].

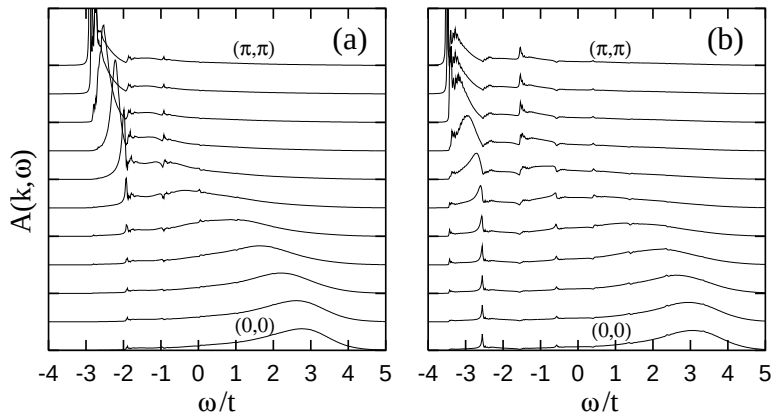

Fig. 2. The hole spectral functions $A(\boldsymbol{k},\omega)$ as in Fig. 1, but for the staggered directional $|3x^2 - r^2\rangle/|3y^2 - r^2\rangle$ orbital ordering ($\phi = -\pi/12$).

TABLE I

The QP spectral weight ($Z_{\boldsymbol{k}}$) and the QP binding energy (E_b) found at the bottom of the QP band [$\boldsymbol{k} = (\pi, \pi)$] as a function of Δ/t, obtained for the orbital orderings given by $\phi = 0$ and $\pm\pi/12$, respectively.

	$\phi = -\pi/12$		$\phi = 0$		$\phi = \pi/12$	
Δ/t	$Z_{\boldsymbol{k}}$	E_b/t	$Z_{\boldsymbol{k}}$	E_b/t	$Z_{\boldsymbol{k}}$	E_b/t
0.0	0.375	0.900	0.274	1.280	0.110	1.685
0.25	0.362	0.970	0.232	1.295	0.047	1.705
0.50	0.341	1.095	0.157	1.430	0.027	1.940
0.75	0.315	1.275	0.084	1.710	0.024	2.215
1.0	0.285	1.510	0.048	2.105	0.003	2.550

The orbital polarization does not influence the orbital excitation energy, but contributes instead new vertices $\propto \Delta$ (see [12]) to the hole-orbiton scattering. These local processes around a hole drastically decrease the width of the QP band, increasing simultaneously the polaron binding energy [see Figs. 1(b) and 2(b)]. The binding energy originates in this case from the local hole hopping within the orbital polaron leading to the localization of a hole and its large effective mass. This process is also accompanied by a decrease of the QP spectral weight which is particularly striking for the $|x^2 - z^2\rangle/|y^2 - z^2\rangle$ ($\phi = \pi/12$) orbital ordering (Table I).

This work was supported by the Polish State Committee for Scientific Research (KBN), Project No. 5 P03B 055 20.

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