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POSSIBLE SCENARIOS FOR THE QUASIPARTICLE BEHAVIOR IN THE UNDOPED $LaMnO_3$*

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We show that the spectral functions in the ferromagnetic planes of orbitally ordered $LaMnO_3$ strongly depend on the Jahn–Teller interaction and on the polarization of orbitals around the hole. Using realistic parameters and available experimental information we suggest that the incoherent spectral weight and the mass enhancement in $LaMnO_3$ might be quite large.

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It is evident that the orbital degrees of freedom play a major role in the colossal magneto-resistence [1] effect and transport properties observed in doped manganites. In the undoped $LaMnO_3$ the charge fluctuations are suppressed by large on-site Coulomb interactions $\propto U$, while the motion of a doped hole along the c axis is hindered by the double exchange [2]. Therefore, one can constrain the effective model to the hole scattering on orbital excitations [3] in the ferromagnetic (a,b) planes. Such excitations have been observed recently using Raman scattering measurements [4]. The propagation of a single hole is considered using the orbital–hole model,

$$H = H_t + H_{\Delta} + H_J + H_{\rm JT} + E_{\rm l}, \qquad (1)$$

which includes the kinetic energy of a hole (H_t), the polarization of orbitals around a hole (H_{Δ}) which induces the energy splitting $\propto \Delta$ between the e_g orbitals next to the hole [5], superexchange interaction between the Mn^{3+}–Mn^{3+} ions due to charge excitations (H_J) [6], the Jahn–Teller (JT) interaction $\propto \lambda$ ($H_{\rm JT}$), and the distorted lattice energy ($E_{\rm l}$) [7].

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We consider the orbital order in the (a, b) planes stabilized by the superexchange $\propto J \simeq 44$ meV [6,8], with alternating occupied e_g orbitals

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

where $+$ $(-)$ refers to $i \in A$ $(i \in B)$ orbital sublattice, and $|ix\rangle$ $(|iz\rangle)$ stands for the local basis orbital $|x^2 - y^2\rangle$ $(|3z^2 - r^2\rangle)$ at site i, respectively. The angle ϕ depends on external pressure [9] and plays here a role of an external parameter. The effect of lattice distortion is described by three independent parameters: δ_x (δ_z) — uniform deformation along the a and b (c) cubic directions, respectively, and u — oxygen displacement along the Mn–O–Mn bond in the (a, b) plane. All distortions are dimensionless in the units of the Mn–Mn distance $(d = 1)$ of the ideal cubic perovskite [7].

The JT interaction describes the coupling between the occupied orbital at a particular Mn^{3+} ion and the distortions of the surrounding oxygen ions [7]. This interaction acts at both sublattices as the staggered fields [9]

$$H_{\rm JT} = -2\lambda\left[(\delta_x - \delta_z)\sin 2\phi - 2\sqrt{3}u\cos 2\phi\right]\left(\sum_{i\in A}\tilde{T}_i^z - \sum_{i\in B}\tilde{T}_i^z\right), \qquad (3)$$

with the pseudospin operators $\tilde{T}_i^z$ referring to the rotated states (2).

In the Linear Orbital Wave (LOW) theory the effective Hamiltonian (1) represents a coupled hole–orbiton problem in momentum space,

$$\begin{aligned} H_{\rm LOW} \;=\; & \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}}(\phi) h_{\boldsymbol{k}}^\dagger h_{\boldsymbol{k}} + \sum_{\boldsymbol{q}} \omega_{\boldsymbol{q}}(\phi)\alpha_{\boldsymbol{q}}^\dagger \alpha_{\boldsymbol{q}} \\ & + \tfrac{1}{\sqrt{N}} \sum_{\boldsymbol{k},\boldsymbol{q}} \left\{ h_{\boldsymbol{k}-\boldsymbol{q}}^\dagger h_{\boldsymbol{k}} \left[M_{\boldsymbol{k},\boldsymbol{q}} \alpha_{\boldsymbol{q}}^\dagger + N_{\boldsymbol{k},\boldsymbol{q}} \alpha_{\boldsymbol{q}+\boldsymbol{Q}}^\dagger \right] + \text{H.c.} \right\}, \end{aligned} \qquad (4)$$

with the free hole dispersion, $\varepsilon_{\boldsymbol{k}}(\phi) = t\,[1 - 2\sin(2\phi)]\,\gamma_{\boldsymbol{k}}$, the dispersion of the orbital excitation, $\omega_{\boldsymbol{q}}(\phi) = 3J\sqrt{A(\lambda)[A(\lambda) + \frac{1}{3}(2\cos 4\phi - 1)\gamma_{\boldsymbol{q}}]}$, the nesting vector $\boldsymbol{Q} = (\pi, \pi)$, and two different hole–orbiton vertices:

$$\begin{aligned} M_{\boldsymbol{k},\boldsymbol{q}} \;&=\; 2t\cos(2\phi)\,(u_{\boldsymbol{q}}\gamma_{\boldsymbol{k}-\boldsymbol{q}} + v_{\boldsymbol{q}}\gamma_{\boldsymbol{k}}) + \Delta\cos(2\phi)\,(\gamma_{\boldsymbol{q}} - 1)\,(u_{\boldsymbol{q}} + v_{\boldsymbol{q}})\,, & (5)\\ N_{\boldsymbol{k},\boldsymbol{q}} \;&=\; -\sqrt{3}t\,(u_{\boldsymbol{q}+\boldsymbol{Q}}\eta_{\boldsymbol{k}-\boldsymbol{q}} + v_{\boldsymbol{q}+\boldsymbol{Q}}\eta_{\boldsymbol{k}}) - \sqrt{3}\Delta\sin(2\phi)\eta_{\boldsymbol{q}}\,(u_{\boldsymbol{q}+\boldsymbol{Q}} + v_{\boldsymbol{q}+\boldsymbol{Q}})\,. & (6) \end{aligned}$$

Here $\gamma_{\boldsymbol{q}} = \frac{1}{2}(\cos q_x + \cos q_y)$, $\eta_{\boldsymbol{q}} = \frac{1}{2}(\cos q_x - \cos q_y)$, $A(\lambda) = 1 + 2\lambda^2/(JK)$, with K being the nearest-neighbor Mn–O spring constant, and $\{u_{\boldsymbol{q}},\ v_{\boldsymbol{q}}\}$

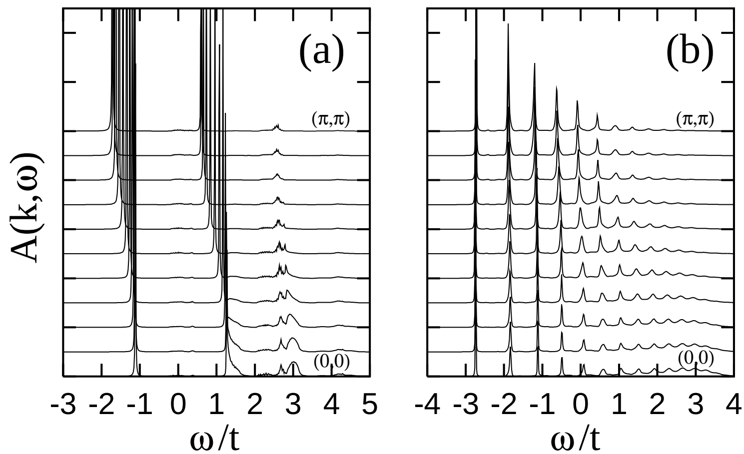

Fig. 1. The hole spectral functions calculated on a grid using 22×22 $\boldsymbol{q}$-points as obtained along the $(0,0)$–(π,π) direction with $\phi = 0$, $K = 500\,t$, and $J = 0.1\,t$, for: (a) $\lambda = 10\,t$, $\Delta = 0.75\,t$, and (b) $\lambda = 0$, $\Delta = t$. The energy unit is $t = 0.4\,$eV.

follow from the respective Bogoliubov transformation for the orbital waves. The Green's function, $G(\boldsymbol{k},\omega) = [\omega - \varepsilon_{\boldsymbol{k}}(\phi) - \Sigma(\boldsymbol{k},\omega)]^{-1}$, is determined in the self-consistent Born approximation [10] by the hole self-energy,

$$\Sigma(\boldsymbol{k},\omega) = \sum_{\boldsymbol{q}} \left\{ M^2_{\boldsymbol{k},\boldsymbol{q}} G[\boldsymbol{k}-\boldsymbol{q}, \omega - \omega_{\boldsymbol{q}}(\phi)] + N^2_{\boldsymbol{k},\boldsymbol{q}} G[\boldsymbol{k}-\boldsymbol{q}, \omega - \omega_{\boldsymbol{q}+\boldsymbol{Q}}(\phi)] \right\}, \tag{7}$$

to obtain the spectral functions, $A(\boldsymbol{k},\omega) = -1/\pi\, \mathrm{Im}\, G(\boldsymbol{k},\omega + i0^+)$.

The spectra consist of Quasi-Particle (QP) peaks at low energies and the incoherent background at higher energies, with a large incoherent spectral weight found close to $\boldsymbol{k} = 0$ momentum [3]. As an example, we consider the $(|x\rangle + |z\rangle)/(|x\rangle - |z\rangle)$ orbital ordering ($\phi = 0$). The spectral weight distribution is controlled by the coupling constant $\propto t$ and the orbiton energy $\omega_{\boldsymbol{q}}(\phi)$. Therefore, when λ increases, $\omega_{\boldsymbol{q}}(\phi)$ increases [9], and the incoherent part is suppressed at $\lambda = 10\,t$ (see Fig. 1(a)). The one-particle excitations are here dominated by a large gap between the first QP peak with dispersion $\sim 0.7\,t$, separated by $\sim 2\,t$ from the next QP peak. In contrast, the entire spectrum becomes incoherent and resembles that derived for the one hole problem in the t–J^z model [10] when the JT coupling is absent, but the orbitals around a hole are polarized at $\Delta = t$ (Fig. 1(b)).

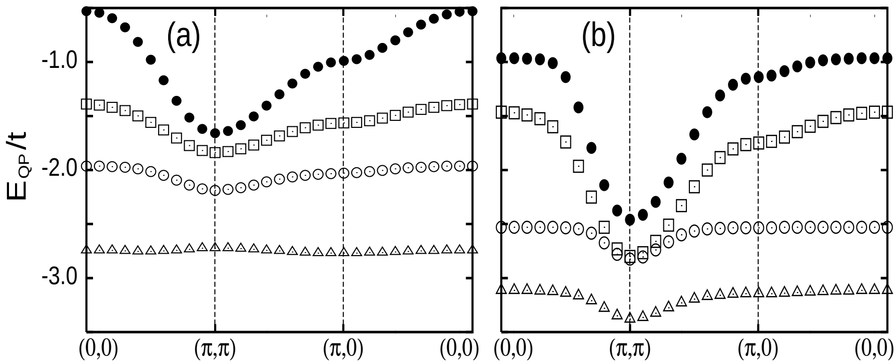

Fig. 2. Dispersion relation of the QP band calculated for: (a) $\phi = 0$, and (b) $\phi = -\pi/12$, with $\Delta = \lambda = 0$ (∘), $\Delta = 0$, $\lambda = 10\,t$ (•), $\Delta = t$, $\lambda = 0$ (▵), and $\Delta = t$, $\lambda = 10\,t$ (▫). Other parameters as in Fig. 1.

The shape and the position of the QP band (Fig. 2) strongly depend on both polarization of orbitals $\propto \Delta$, and on the JT coupling $\propto \lambda$. With polarized e_g orbitals around a hole at $\Delta = t$, for $\phi = 0$ and no JT interaction ($\lambda = 0$) (Fig. 2(a)), the QP band is narrowed by a factor of 50 in comparison with the free hole dispersion $\varepsilon_{\boldsymbol{k}}(\phi)$ and moves to *much lower* energies. Increasing slightly the admixture of $|x\rangle$ orbitals we find a larger QP dispersion and somewhat reduced mass enhancement at $\phi = -\pi/12$ (Fig. 2(b)). The increasing JT interaction leads in both cases to a rigid orbital ordering, and to the coherent hole motion on the energy scale $\sim t$, and almost no scattering off orbital waves.

In summary, the JT coupling λ enhances the coherent spectral weight and leads to a smaller mass enhancement. Recent experiments [4] detected the orbiton energy of ~ 150 meV, being only somewhat larger than $3J$. This result is puzzling and suggests that the JT coupling *might be smaller* than originally expected. This would imply that, independently of the realized orbital order, the incoherent spectral weight and the mass enhancement in $LaMnO_3$ are quite *large* — due to the relatively *small* orbiton energy.

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