ORBITAL-LATTICE QUASIPARTICLES IN FERROMAGNETIC LaMnO$_3$*

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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.

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To explain the colossal magnetoresistance [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,

$$H = H_t + H_\Delta + H_J + H_{IT} + E_t + H_{ph},$$  \hspace{1cm} (1)

which includes the kinetic energy of a hole ($H_t$), the polarization of orbitals around a hole ($H_\Delta$) [5], superexchange interaction between the Mn$^{3+}$--Mn$^{3+}$

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(839)
ions due to charge excitations ($H_J$) [6], the Jahn-Teller (JT) interaction ($H_{JT}$) with the distorted lattice energy ($E_l$) [7], and the oxygen ion oscillations around their distorted positions ($H_{ph}$). The alternating orbital ordering is defined by two orbital sublattices with the occupied $e_g$ orbitals,

$$|q\rangle = \cos \left( \frac{\pi}{3} - \phi \right) |iz\rangle \pm \sin \left( \frac{\pi}{3} - \phi \right) |ix\rangle,$$

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 $\phi$ 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-orbital problem in momentum space [3],

$$H_{LPOW} = \sum_{\mathbf{k}} \varepsilon_k \hat{h}_k \hat{h}_k + \sum_{\mathbf{q}} \left( \sum_{\xi = 1, 2} \Omega_{\mathbf{q}}^{(\xi)} \beta_{\mathbf{q}, \xi} \beta_{\mathbf{q}, \xi} + \omega_0 \sum_{\xi = 1, 3} B_{\mathbf{q}, \xi} \beta_{\mathbf{q}, \xi} \right)$$

$$+ \sum_{\mathbf{k}, \mathbf{q}} \left\{ \hat{h}_{\mathbf{k}-\mathbf{q}} \hat{h}_k \left[ \sum_{\xi = 1, 3} M_{0, \mathbf{q}, \xi} \beta_{\mathbf{q}, \xi} + \sum_{\xi = 1, 2} \left( M_{0, \mathbf{q}, \xi} \beta_{\mathbf{q}, \xi} + N_{0, \mathbf{q}, \xi} \beta_{\mathbf{q}, \xi} \right) \right] + H.c. \right\},$$

with the free hole dispersion, $\varepsilon_k = t \left[ 1 - 2 \sin(2\phi) \right] \gamma_k$, and the nesting vector $Q = (\pi, \pi)$. $M_{0, \mathbf{q}, \xi}$ and $\{ M_{0, \mathbf{q}, \xi}, N_{0, \mathbf{q}, \xi} \}$ are the structureless hole-phonon and mixed orbital-phonon vertices, respectively, while $B_{\mathbf{q}, \xi}$ and $\beta_{\mathbf{q}, \xi}$ 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, $G(k, \omega) = (\omega - \varepsilon_k - \Sigma(k, \omega))^{-1}$, is determined in the self-consistent Born approximation [10] by the hole self-energy obtained from the dressed Green’s function,

$$\Sigma(k, \omega) = \sum_{\mathbf{q}} \sum_{\xi = 1, 2} \left\{ (M_{0, \mathbf{q}, \xi})^2 G[k - \mathbf{q}, \omega - \Omega_{\mathbf{q}}^{(\xi)}] \right\}$$

$$+ (N_{0, \mathbf{q}, \xi})^2 G[k - \mathbf{q}, \omega - \Omega_{\mathbf{q}+\mathbf{Q}}^{(\xi)}] \} + 3M_0^2 \sum_{\mathbf{q}} G[k - \mathbf{q}, \omega - \omega_0],$$

leading to the hole spectral functions, $A(k, \omega) = -\frac{1}{\pi} \text{Im} G(k, \omega + i0^+)$. Here, we have concentrated on three representative alternating orbital orderings: $|x^2 - y^2\rangle, |x| \pm |y\rangle, |(x^2 + y^2)/2 - z^2\rangle, |(x^2 + y^2)/2 + z^2\rangle$, realized for $\phi = \pi/12, 0, \text{and } -\pi/12$, respectively. At finite momenta the spectra consist of quasiparticle (QP) peaks at low energies and the incoherent background at higher energies, whereas at $k \simeq (0, 0)$ one finds a completely
Fig. 1. The hole spectral functions $A(k, \omega)$ calculated on a grid with $20 \times 20$ $q$-points, as obtained along the $(0,0)-(\pi,\pi)$ direction for the staggered $(|x| - |z|)/(|x| + |z|)$ 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 $k \rightarrow (\pi,\pi)$ is accompanied by a broad ($\Delta \omega \sim t$) structure above, which represents a sideband 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 $k \rightarrow (0,0)$ 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 $A(k, \omega)$ as in Fig. 1, but for the staggered directional $|3x^2 - r^2|/|3y^2 - r^2|$ orbital ordering ($\phi = -\pi/12$).
TABLE I

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

<table>
<thead>
<tr>
<th>$\Delta/\tilde{t}$</th>
<th>$\phi = -\pi/12$</th>
<th>$\phi = 0$</th>
<th>$\phi = \pi/12$</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>$Z_k$</td>
<td>$E_b/\tilde{t}$</td>
<td>$Z_k$</td>
</tr>
<tr>
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<td>0.375</td>
<td>0.900</td>
<td>0.274</td>
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<td>0.25</td>
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<td>0.970</td>
<td>0.232</td>
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<tr>
<td>0.50</td>
<td>0.341</td>
<td>1.095</td>
<td>0.157</td>
</tr>
<tr>
<td>0.75</td>
<td>0.315</td>
<td>1.275</td>
<td>0.084</td>
</tr>
<tr>
<td>1.0</td>
<td>0.285</td>
<td>1.510</td>
<td>0.048</td>
</tr>
</tbody>
</table>

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 $[x^2 - z^2]/[y^2 - z^2]$ ($\phi = \pi/12$) orbital ordering (Table I).

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REFERENCES