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Lattice and superexchange effects in doped CMR manganites

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Abstract

We report on the influence of the lattice degrees of freedom on charge, orbital and spin correlations in colossal magnetoresistance (CMR) manganites. For the weakly doped compounds we demonstrate that the electron–phonon coupling promotes the trapping of charge carriers, the disappearance of the orbital polaron pattern and the breakdown of ferromagnetism at the CMR transition. The role of different superexchange interactions is explored.

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Manganese oxides with perovskite structure, such as $La_{1-x}[Sr,Ca]_xMnO_3$, are examples of highly correlated electron systems near the metal–insulator transition. In these materials strong Coulomb interaction U and Hund's rule coupling J_h introduce a spin background and affect the charge mobility via double-exchange [1]. Delocalisation of the e_g valence electrons favours ferromagnetism (FM) because the kinetic energy of an itinerant carrier is minimised when all the core (t_{2g} electron) spins are aligned. A competing tendency towards localisation comes about through the electron–phonon (EP) interaction g, which stabilises a local distortion q_δ of the oxygen octahedron surrounding each manganese ion. At every Mn site two Jahn–Teller (JT) modes of E_g symmetry, q_θ and q_ε, couple to the orbital degree of freedom of the e_g electrons. In addition, a breathing-mode q_{a_1} is sensitive to the local density of doped holes. It is the novelty of the manganites that even at high densities x carriers can be trapped by self-induced lattice distortions, which provides an efficient additional mechanism for the suppression of the resistivity at the CMR transition [2].

Based on a recently derived microscopic model for doped manganites,

$$H = H_{\text{double-exchange}} + H^{\text{2nd-order}}_{\text{spin-orbital}} + H_{\text{electron-JT}} + H_{\text{hole-breathing}} + H_{\text{phonon}}, \quad (1)$$

which restricts the local electronic Hilbert space to the spin-2 orbital doublet ^5E [Mn^{3+} with $t_2^3(^4A_2)e$] and the spin-$\frac{3}{2}$ orbital singlet $^4A_2$ [Mn^{4+} with t_2^3] but includes the full quantum dynamics of charge, spin, orbital and lattice degrees of freedom (for details see Ref. [3]), we study the properties of a small manganite cluster in the physically most interesting doping regime $x = 0.25$ using exact diagonalisation techniques. In the present numerical work we focus on the role of second-order superexchange interactions $\propto t^2/U$ and compare the cases $U = 6$ eV and $U \to \infty$, where only antiferromagnetic (AFM) spin-exchange terms $\propto t^2/J_h$ survive. Taking realistic values for the hopping $t = 0.4$ eV, $t/t_\pi = 3$, the Hund's coupling $J_h = 0.7$ eV, and the phonon frequency $\omega = 70$ meV, we solve the model (1) for increasing EP interaction g.

The behaviour of selected quantities characterising the ground state properties in different electron–electron

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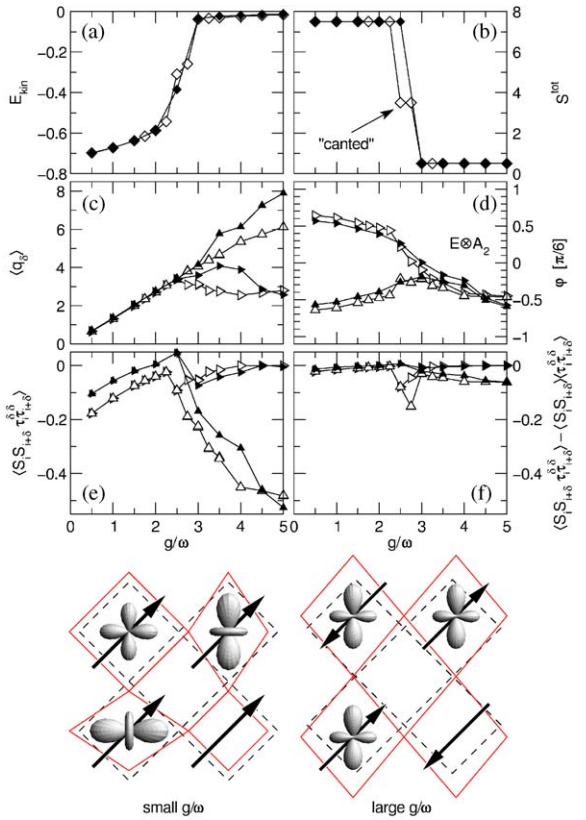

Fig. 1. Kinetic energy (a), total spin of the ground state (b), bond-length $\langle q_{x/y} \rangle$ along x and y direction (c), orbital orientation φ in the neighbourhood of a hole (d), expectation value of the spin–orbital interaction (e), and spin–orbital correlations (f) are given as a function of the rescaled EP coupling g/ω. Open (filled) symbols refer to $U = 6$ ($U = \infty$) and right (upward) triangles correspond to $\delta = x$ ($\delta = y$) in the panels (c)–(f). The lowest panel schematically visualises the lattice displacements and spin/orbital patterns at small and large EP interactions.

and EP coupling regimes are shown in Fig. 1. The main results are the following:

(i) Increasing EP interaction leads to a polaronic reduction of the kinetic energy (Fig. 1(a)) which in turn destroys the FM state (Fig. 1(b)). For finite U the system goes through a intermediate canted state, since second-order FM and AFM interactions compete.

(ii) The change from FM to AFM spin correlations is accompanied by a finite net lattice distortion $\langle q_y - q_x \rangle \neq 0$ in the x–y plane (Fig. 1(c)). The associated fluctuation $\langle q_y^2 \rangle - \langle q_y \rangle^2$ shows a kink near the FM to AFM transition point [3,4].

(iii) Orbital correlations change with increasing g: Fig. 1(d) displays the behaviour of the $E \otimes A_2$ states $(\cos\varphi|\theta\rangle_i + \sin\varphi|\varepsilon\rangle_i) \otimes |a_2\rangle_j$ on a bond $\langle ij \rangle$, where $|\theta\rangle$, $|\varepsilon\rangle$ and $|a_2\rangle$ denote the orbital doublet and singlet states, respectively. We observe the expected orbital polaron pattern, as long as the itinerant hole is mobile, and static uniform orbital order, as soon as the lattice is distorted. The orbital correlations do not depend much on the value of U.

(iv) The expectation value of the spin–orbital interaction is dominated by the orbital correlations below and above the transition (cf. Fig. 1(e)). Moreover, it is important to notice that the coupling between spin and orbital degrees of freedom, which is measured by $\langle \mathbf{S}_i \mathbf{S}_{i+\delta}\, \tau_i^\delta \tau_{i+\delta}^\delta \rangle - \langle \mathbf{S}_i \mathbf{S}_{i+\delta} \rangle \langle \tau_i^\delta \tau_{i+\delta}^\delta \rangle$ and shown in Fig. 1(f), is almost negligible except for the canted state near the FM–AFM transition point at finite U. This observation corroborates the decoupling scheme proposed by Khaliullin and Oudovenko [5] for the use with Greens function approaches.

The schematic drawing in the lowest line of Fig. 1 summarises, to some extent, the evolution of the lattice, spin and orbital correlations with increasing EP interaction. It is evident that the interplay between the double-exchange, superexchange-orbital, and electron–lattice interactions is the reason for the rich phase diagram of the manganites.

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