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Spin excitations in ferromagnetic manganites

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Abstract

An effective one-band Hamiltonian for colossal-magnetoresistance (CMR) manganites is constructed and the spin excitations are determined. Fitting the experimental data by the derived spin–wave dispersion gives an e_g-electron hopping amplitude of about 0.2 eV in agreement with LDA band calculations. © 1999 Elsevier Science B.V. All rights reserved.

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The theoretical description of the striking magnetic and transport phenomena in CMR manganites is far from being satisfactory. There exist inconsistencies even in the calculations based on the widely used purely electronic double exchange (DE) and ferromagnetic (FM) Kondo lattice (KL) models. Indeed, Millis et al. [1] estimated the Curie temperature T_c from the spin-dependent hopping amplitude of the DE model and obtained a much higher value than the observed one; they ascribed this disagreement to the neglect of the electron–phonon coupling. On the other hand, Müller–Hartmann and Dagotto [2] reexamined the large Hund's rule coupling (J_H) limit of the KL model and found a nontrivial total bond-spin dependent sign in the effective hopping, arguing that this discrepancy to the DE model may be the source of the overestimation of T_c.

The purpose of this contribution is to analyse the spin excitation spectrum of FM manganites ($[La, A]MnO_3$) on the basis of an effective one-band model. Adapting the approach [3] to the Mn^{3+}–Mn^{4+} system, the matrix elements related to the hopping of an itinerant e_g-electron can be determined in the space of spin functions with the Mn^{3+} spin functions restricted to the $S = 2$ subspace ($J_H \to \infty$).[1] Then, focusing on the metallic FM phase and applying the spin–wave approximation, the relevant part of the effective hopping Hamiltonian is

$$\mathscr{H}_{\text{eff}} = -t \sum_{\langle i,j \rangle} (C^{\dagger}_{j_{\frac{1}{2}}} C_{i_{\frac{1}{2}}} + C^{\dagger}_{j-\frac{1}{2}} C_{i-\frac{1}{2}}), \tag{1}$$

$$C_{i_{\frac{1}{2}}} = |i\tfrac{3}{2}\rangle\langle i\,2| + \tfrac{\sqrt{3}}{2}\,|i\tfrac{1}{2}\rangle\langle i1|, \tag{2}$$

$$C_{i-\frac{1}{2}} = \tfrac{1}{2}\,|i\tfrac{3}{2}\rangle\langle i\,1| + \tfrac{\sqrt{2}}{2}\,|i\tfrac{1}{2}\rangle\langle i0|. \tag{3}$$

Here the indices i,j indicate the positions of Mn^{4+} and Mn^{3+} ions with spin projections $[\frac{1}{2}, \frac{3}{2}]$ and $[0, 1, 2]$, respectively. Based on Eq. (1), the effective transport Hamiltonian in second quantized form may be derived analogically to Ref. [3]. However, owing to the strong electronic correlations, the equivalent "hole representation" introduced by Kubo and Ohata [4] seems to be more suited for the lightly doped manganites. In this picture, the moving hole with spin $s = 1/2$ is strongly antiferromagnetically coupled to the Mn^{3+} spin background. Consequently, we use the Schwinger-boson representation for the $S = 2$ spin functions, and express the basis vectors of the $S' = 3/2$ spin space in terms of fermionic hole operators.

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[1] We proved that these matrix elements agree with those following from Eqs. (6), (8) given in Ref. [2].

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As a result we get an effective Hamiltonian for holes interacting with magnons, where the "free" hole part becomes

$$\mathscr{H}_t^{(0)} = \sum_k \varepsilon_{k\downarrow}^{(0)} h_{k\downarrow}^\dagger h_{k\downarrow} \tag{4}$$

with $\varepsilon_{k\downarrow}^{(0)} = -2t_h(\cos k_x + \cos k_y + \cos k_z)$ and $t_h = [2S/(2S+1)]\,t$. The interaction terms lead to the spin-dependent hole self-energies

$$\Sigma_\downarrow(\boldsymbol{k},\omega) = \frac{1}{4N}\sum_q \left[(\varepsilon_{k-q\downarrow}^{(0)} - 2\,\varepsilon_{k\downarrow}^{(0)})\, n_q + (\varepsilon_{k\downarrow}^{(0)})^2 \frac{n_q + 1 - n_{k-q\uparrow}}{\omega - \omega_q - \varepsilon_{k-q\uparrow} + \mu} \right], \tag{5}$$

$$\Sigma_\uparrow(\boldsymbol{k},\omega) = \frac{1}{4N}\sum_q \left[\varepsilon_{k+q\downarrow}^{(0)} n_q + (\varepsilon_{k+q\downarrow}^{(0)})^2 \frac{n_q + n_{k+q\downarrow}}{\omega + \omega_q - \varepsilon_{k+q\downarrow} + \mu} \right] \tag{6}$$

with $n_q = [\exp(\beta\omega_q) - 1]^{-1}$, $n_{k\sigma} = \langle h_{k\sigma}^\dagger h_{k\sigma} \rangle$, and

$$\varepsilon_{k\sigma} - \varepsilon_{k\sigma}^{(0)} = \Re\mathrm{e}[\Sigma_\sigma(\boldsymbol{k}, \varepsilon_{k\sigma} - \mu)]. \tag{7}$$

The spectrum of elementary spin excitations is determined by

$$\omega_q = \frac{1}{4N}\sum_k \left[(\varepsilon_{k-q\downarrow}^{(0)} - 2\varepsilon_{k\downarrow}^{(0)}) n_{k\downarrow} + \varepsilon_{k+q\downarrow}^{(0)} n_{k\uparrow} + (\varepsilon_{k\downarrow}^{(0)})^2 \frac{n_{k\downarrow} - n_{k-q\uparrow}}{\varepsilon_{k\downarrow} - \varepsilon_{k-q\uparrow} - \omega_q} \right]. \tag{8}$$

The full solution of the coupled integral Eqs. (5)–(8) lies outside the scope of the present treatment; we estimate the spin–wave dispersion at $T = 0$ assuming $n_{k\uparrow} \simeq 0$, $\varepsilon_{k\uparrow} \simeq 0$ and $\varepsilon_{k\downarrow} \simeq \varepsilon_{k\downarrow}^{(0)}$. The latter approximations, justified for small hole concentrations $x \ll 1$, are expected to give reasonable estimates also for higher doping level, provided that the minority spin-up subband remains unimportant with respect to the majority spin-down subband owing to their different spectral weights.

As a direct test of the theory developed so far, in Fig. 1 the calculated ω_q has been compared with recent neutron scattering results for the spin–wave dispersion in FM $La_{0.7}Pb_{0.3}MnO_3$ at 10 K. Obviously, the dispersion relation (8) is entirely sufficient to account for the measured behaviour throughout the whole Brillouin zone. For $x = 0.3$ the best least squares fit to the experimental data fixes the only free parameter of the theory: $t = 0.188$ eV. Note that this value is in excellent agreement with the result obtained from LDA band structure

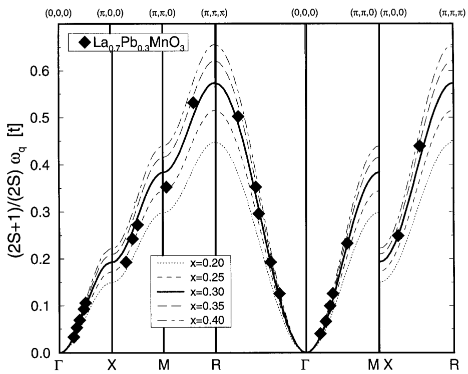

Fig. 1. Spin–wave dispersion ω_q along all major symmetry directions of the Brillouin zone compared with the experimental data taken from Ref. [6], whereby a small constant anisotropy gap $\Delta \simeq 2$ meV has been subtracted.

calculations [6]. Also the consistency of the measured magnon bandwidth and T_c was stressed in Ref. [5].

According to the above estimate of t, no polaron band-narrowing is apparent at low temperatures. On the other hand, the observed anomalously large oxygen isotope effect on T_c shows the relevance of the lattice dynamics near T_c, i.e., in the vicinity of the metal–insulator transition [7]. To comprise the possible role of polarons, the effective Hamiltonian may be easily generalized taking into account the Holstein-type interaction of holes with the lattice degrees of freedom. However, in order to discuss the effects near T_c one has to go beyond the spin–wave approximation.

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References

[1] A.J. Millis, P.B. Littlewood, B.I. Shraiman, Phys. Rev. Lett. 74 (1995) 5144.
[2] E. Müller-Hartmann, E. Dagotto, Phys. Rev. B 54 (1996) R6819.
[3] J. Loos, H. Fehske, Phys. Rev. B 56 (1997) 3544.
[4] K. Kubo, N. Ohata, J. Phys. Soc. Japan 33 (1972) 21.
[5] T.G. Perring et al., Phys. Rev. Lett. 77 (1996) 711.
[6] S. Satpathy, Z.S. Popović, F.R. Vukajlovicć, Phys. Rev. Lett. 76 (1996) 960.
[7] G. Zhao, K. Conder, H. Keller, K.A. Müller, Nature 381 (1996) 676.