Spin-lattice coupling effects in the Holstein double-exchange model

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Abstract

Based on the Holstein double-exchange model and a highly efficient single cluster Monte Carlo approach we study the interplay of double-exchange and polaron effects in doped colossal magneto-resistance (CMR) manganites. The CMR transition is shown to be appreciably influenced by lattice polaron formation.

Key words: colossal magneto-resistance manganites, double-exchange, polaron formation, cluster Monte Carlo

Over the last decade the magnetic and transport properties of CMR manganites (La\(_{1-x}\)[Ca, Sr]\(_x\)MnO\(_3\) with 0.2 \(\lesssim x \lesssim 0.5\)) have attracted a considerable amount of research activity, and in particular polaronic features near the transition from the ferromagnetic to the paramagnetic phase remain to be an intensely studied subject. A realistic description of the observed \(T_c\) and of the electrical resistivity data is complicated by the requirement of incorporating strong electron-phonon interactions in addition to the magnetic double-exchange (DE) \cite{1}. In the present study we aim at developing realistic effective models for the spin lattice interaction and appropriate Monte Carlo (MC) techniques for their simulation. Our starting point is the Holstein-DE model

\[
H = - \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j - \sqrt{\varepsilon_p \omega_0} \sum_i (b_i^\dagger + b_i) c_i^\dagger c_i + \omega_0 \sum_i b_i^\dagger b_i + \frac{\varepsilon_0}{2} \sum_i (\cos \theta_i - \sin \phi_i) \cos \frac{\delta_i}{2} + \frac{i}{2} \sin \frac{\delta_i}{2} \sin \frac{\delta_i}{2}
\]

where the first term describes the well known DE interaction, characterised by the transfer amplitude \(t_{ij} = \cos \theta_i - \sin \phi_i \cos \frac{\delta_i}{2} + \frac{i}{2} \sin \frac{\delta_i}{2} \sin \frac{\delta_i}{2}\) which depends on the classical spin variables \(\{\theta_i, \phi_i\}\). The second term accounts for a local coupling \((\propto \varepsilon_p)\) of doped carriers to a dispersionless optical phonon mode with frequency \(\omega_0\), and the last term refers to the dynamics of the harmonic lattice.

As a first step let us focus on the numerical solution of the DE part, which is characterised by non-interacting fermions coupled to classical spin degrees of freedom. In a MC simulation of such types of models the calculation of the fermionic energy contribution, which depends on the classical degrees of freedom, is usually the most time consuming part, and an efficient MC algorithm should therefore eva

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proximate classical spin Hamiltonian
\[ H_{\text{eff}} = -J_{\text{eff}} \sum_{\langle ij \rangle} \sqrt{1 + \mathbf{S}_i \cdot \mathbf{S}_j}, \]
which can be easily simulated with a rejection-free Wolff [6] single cluster type approach. Setting \( J_{\text{eff}} = x(1 - x)/\sqrt{2} \), where \( x \) is the hole concentration, the magnetisation data and critical temperatures of this approximate model agree surprisingly well with the full DE system (cf. Fig. 1). Thus, the latter can efficiently be simulated by the new hybrid approach: (i) the optimal \( \mathbf{S}_j \) are obtained from the effective DE model \( H_{\text{eff}} \) for the DE model \([4]\). Encouraged by the above findings we can now rely entirely on the effective spin model \( H_{\text{eff}} \) and include lattice polaron effects on a variational level. Applying the modified variational Lang-Firsov transformation \([7]\)

\[ \beta \omega_{\text{eff}} \begin{bmatrix} \alpha_{\text{eff}} \\ \beta_{\text{eff}} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \alpha_{\text{eff}} \\ \beta_{\text{eff}} \end{bmatrix} + N_\epsilon \omega_{\text{eff}} \left( (1 - \gamma)^2 (1 - x) - 1 \right) , \]

where \( \gamma \) is a variational parameter which measures the importance of the polaron effect \( (0 \leq \gamma \leq 1) \). The above model is treated by single cluster MC, where the optimal \( \gamma \) is adjusted after each cluster flip. Note that the spin-lattice part of (3) is symmetric with respect to \( x = 0.5 \), i.e., to explain the asymmetry of the manganite phase diagram additional Jahn-Teller type lattice interactions need to be included. Figure 2 shows the magnetisation as well as \( \gamma \) for a few typical parameter sets. Clearly the polaronic effect \( (\text{larger} \gamma) \) is most pronounced near and above the critical temperature. As expected, the electron-phonon interaction reduces the critical temperature, and for small phonon frequencies \( \omega \) \((\text{adiabatic case})\) the ferromagnetic phase may cease to exist completely. Potential future extensions of the present work could include Jahn-Teller modes \([8]\) and studies of the conductivity, e.g., along the lines of Ref. [9]. In addition, the formation of magnetic polarons in the DE model should be accessible within the proposed CMC approach.

References
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