Spin-lattice coupling effects in CMR manganites - 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.

Introduction

Over the last decade the magnetic and transport properties of CMR manganites ($La_{1-x}[Ca,Sr]_xMnO_3$ 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) [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.

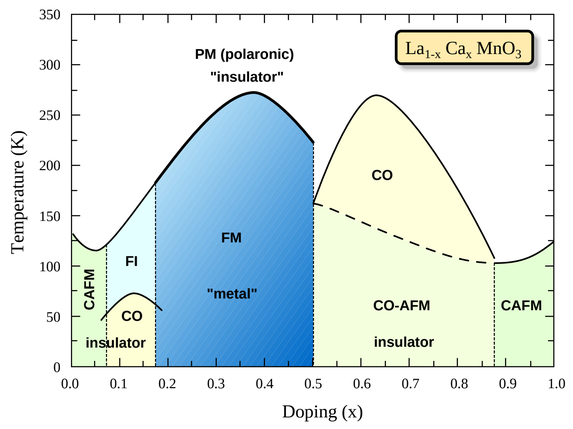

Fig. 1: Schematic experimental phase diagram for $La_{1-x}Ca_xMnO_3$ after [2].

Model

Our starting point is the Holstein-DE model

$$H = -\sum_{\langle i,j\rangle} t_{ij} c_i^\dagger c_j - \sqrt{\varepsilon_p \omega_0} \sum_i (b_i^\dagger + b_i) c_i^\dagger c_i + \omega_0 \sum_i b_i^\dagger b_i \,, \tag{1}$$

where the first term describes the well known DE interaction, characterised by the transfer amplitude

$$t_{ij} = \cos\tfrac{\theta_i-\theta_j}{2}\cos\tfrac{\phi_i-\phi_j}{2} + i\cos\tfrac{\theta_i+\theta_j}{2}\sin\tfrac{\phi_i-\phi_j}{2} \tag{2}$$

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 ω_0, and the last term refers to the dynamics of the harmonic lattice.

From (1) an effective polaron model may be derived by the modified variational Lang-Firsov transformation [3] $H_p = e^S H e^{-S} = H_0 + H_1$, where

$$H_1 = -\sum_{\langle i,j\rangle} t_{ij} \Phi_{ij} c_i^\dagger c_j \,, \tag{3}$$

$$\Phi_{ij} = \exp\{-\gamma\sqrt{\varepsilon/\omega_0}(b_i^\dagger - b_i - b_j^\dagger + b_j)\} \,, \tag{4}$$

and γ is a variational parameter which measures the importance of the polaron effect ($0 \le \gamma \le 1$). Averaging Φ_{ij} over the phonon vacuum we obtain the polaronic band narrowing factor

$$\langle \Phi_{ij} \rangle_0 = \exp\{-S_0 \coth\left[\tfrac{\beta\omega_0}{2}\right]\} \tag{5}$$

with $S_0 = \gamma^2 \varepsilon_p / \omega_0$.

Numerical technique

As a first step let us neglect the coupling to the phonons and 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 evaluate the fermionic trace as fast and as seldom as possible. The first requirement can be matched by using Chebyshev expansion and kernel polynomial methods [4], but so far this approach was combined only with standard Metropolis single-spin updates [5]. For the second requirement a hybrid MC involving classical time evolution of an effective spin model and an approximate diagonalisation of the fermionic problem was suggested [6]. However, both approaches have a few drawbacks, the first suffers from the frequent evaluation of the fermionic trace, the latter is rather complicated since it involves a molecular dynamics type simulation of the classical degrees of freedom.

Kernel Polynomial Method

Idea: Avoid full diagonalisation of the fermionic Hamiltonian (time $\sim N^3$) by using Chebyshev expansion together with KPM (time $\sim N^2$ or less) [4]!

The energy of the system then reads

$$E_{\{S_i\}} = \int \rho_{\{S_i\}}(\varepsilon)/(e^{\beta(\varepsilon-\mu)}+1)\, d\varepsilon \,, \tag{6}$$

and $\rho_{\{S_i\}}(\varepsilon)$ is approximated by

$$\begin{aligned} \rho_{\{S_i\}}(\varepsilon) &\approx \frac{g_0\mu_0 + 2\sum_{m=1}^{M-1} g_m \mu_m\, T_m[(\varepsilon-b)/a]}{\pi\sqrt{a^2-(\varepsilon-b)^2}} \,, \\ T_m(x) &= \cos(m\ \mathrm{acos}(x)) \,, \\ \mu_m &= \frac{1}{N}\mathrm{Tr}\{T_m[(H_{\{S_i\}}-b)/a]\} \,, \end{aligned} \tag{7}$$

where g_m account for the Jackson kernel and a, b for scaling of the spectrum to the domain of the polynomials T_m, $[-1,1]$. The expansion coefficients μ_m are obtained by iteratively evaluating the above trace.

New Cluster Monte Carlo approach

Idea: Combine KPM with Cluster Monte Carlo [7,8]!

In general, the MC transition probability from state a to state b can be separated into the probabilities of *considering*, $A(a\to b)$, and of *accepting*, $\tilde{P}(a\to b)$, the move $a\to b$,

$$P(a\to b) = A(a\to b)\tilde{P}(a\to b) \,. \tag{8}$$

Given the Boltzmann weights $W(a)$ and $W(b)$, detailed balance requires

$$W(a)P(a\to b) = W(b)P(b\to a) \,, \tag{9}$$

or equivalently

$$\tilde{P}(a\to b) = \min\left(1, \frac{W(b)A(b\to a)}{W(a)A(a\to b)}\right) \,. \tag{10}$$

Within CMC we choose an algorithm, such that the *a priori* probabilities $A(a\to b)$ and $A(b\to a)$ "soak up" most of the difference in the weights $W(a)$ and $W(b)$, and the acceptance probability $\tilde{P}(a\to b)$ remains reasonably large.

Strategy:

1. Update all spins with classical, rejection free CMC [9] for the effective Hamiltonian

$$H_{\text{eff}} = -J_{\text{eff}} \sum_{\langle kl\rangle} \sqrt{1+\vec{S}_k\cdot\vec{S}_l} \,, \tag{11}$$

   derived from the full double-exchange model by averaging over fermionic degrees of freedom. J_{eff} is chosen randomly with $\langle J_{\text{eff}}\rangle = x(1-x)/\sqrt{2}$.
2. Calculate new energy $E_{\{S_i\}}$ with KPM and accept move according to Eq. (10).
3. Continue with step 1 until sufficient data collected.

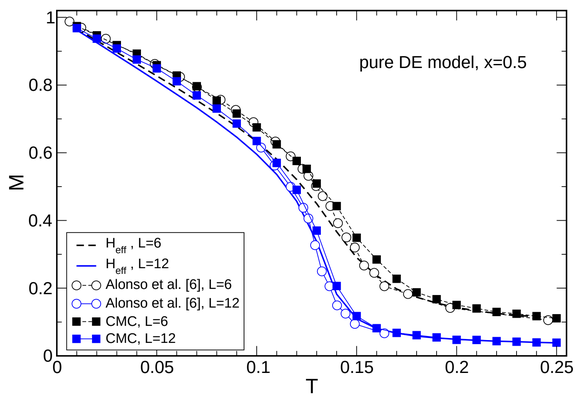

Fig.2: Magnetisation of the double-exchange model based on CMC, hybrid MC [6], and the effective model (11).

The data obtained with the new approach reproduces previous Hybrid MC results [6] and shows that interestingly the effective model (11) is a very good approximation to the full double-exchange model.

Magnetisation data

Encouraged by the above findings we can now rely entirely on the effective spin model H_{eff} and include lattice polaron effects on the variational level outlined above. From (1), (3), (5) and (11) we obtain an effective polaronic DE model:

$$\begin{aligned} H_p &= -J_{\text{eff}}\langle\Phi_{ij}\rangle_0 \sum_{\langle ij\rangle}\sqrt{1+\vec{S}_i\cdot\vec{S}_j} \\ &\quad + \tfrac{N\omega_0}{e^{\beta\omega_0}-1} + N\varepsilon_p x\left[(1-\gamma)^2(1-x)-1\right] . \end{aligned} \tag{12}$$

The above model is treated by single cluster MC, where the optimal γ is adjusted after each cluster flip. Note that the spin-lattice part of (12) 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. The left panel of Fig. 3 shows the magnetisation for a few typical parameter sets. The polaronic reduction of the magnetisation with increasing ε_p increases with temperature, which is ascribed to the decrease of the effective spin coupling proportional to $\langle\Phi_{ij}\rangle_0$ and to the increase of γ (cf. Fig. 4, left panel) with increasing temperature. As a result the electron-phonon interaction reduces the critical temperature, and for small phonon frequencies (adiabatic case) the ferromagnetic phase may cease to exist completely.

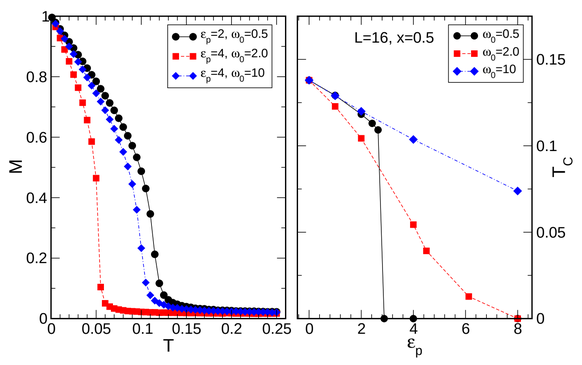

Fig.3: Magnetisation & critical temperature of the effective double-exchange Holstein model.

Conductivity

The small-polaron dc hopping conductivity can be calculated along the lines of Ref. [10]. Starting point is the Kubo formula

$$\mathrm{Re}\sigma^{\nu\nu}(\omega) = \frac{\tanh(\beta\omega/2)}{2\Omega\omega}\int_{-\infty}^{\infty} dt e^{i\omega t}\langle[J^\nu, J^\nu(t)]_+\rangle \tag{13}$$

with the polaron current operator

$$\vec{J} = ie\sum_{\langle i,j\rangle}(\vec{R}_i - \vec{R}_j)\, t_{ij}\Phi_{ij} c_i^\dagger c_j \,. \tag{14}$$

In the current correlator of (13),

$$\begin{aligned} \langle J^\nu J^\nu(t)\rangle &= e^2 \sum_{\langle i,j\rangle}(R_i^\nu - R_j^\nu)^2 \langle t_{ij}^2\rangle \langle c_i^\dagger c_j c_j^\dagger(t) c_i(t)\rangle \\ &\quad \times \{(\langle\Phi_{ij}\Phi_{ji}(t)\rangle_0 - \langle\Phi_{ij}\rangle_0\langle\Phi_{ji}\rangle_0) + \langle\Phi_{ij}\rangle_0\langle\Phi_{ji}\rangle_0\} \,, \end{aligned} \tag{15}$$

we have replaced t_{ij}^2 by its average over the classical spin variables $\langle t_{ij}^2\rangle$ and separated the polaron hopping conductivity σ_h ($\propto$ red terms) and the polaron band conductivity σ_b ($\propto$ blue term). $\sigma_h(\omega)$ is related to transitions with multiphonon absorptions and emissions, whereas $\sigma_b(\omega)$ is due to transitions without change of phonon occupation numbers.

Evaluating the dynamic phonon correlator

$$\langle\Phi_{ij}\Phi_{ji}(t)\rangle_0 = \langle\Phi_{ij}\rangle^2 \mathrm{e}^{2S_0\sinh^{-1}\left[\frac{\beta\omega_0}{2}\right]\cos\omega_0\left[t-\frac{i\beta}{2}\right]} \tag{16}$$

the dc hopping conductivity is obtained for

$$T > T_0 = \omega_0\{2\ln[2S_0 + (1+4S_0^2)^{1/2}]\}^{-1} \tag{17}$$

as

$$\sigma_h = \sigma_0\langle t^2\rangle x(1-x)\beta\tau\,\mathrm{e}^{-2S_0\tanh\left[\frac{\beta\omega_0}{4}\right]} \,, \tag{18}$$

where $\tau = (1/2\omega_0)[\sinh(\beta\omega_0/2)/S_0]^{1/2}$,
and $\sigma_0 = za^2\sqrt{\pi}e^2N/\Omega$.

The temperature dependence of the related resistivity is shown in Fig. 4 (right panel). We observe an abrupt increase of $\rho/\rho_{\max}$ in the vicinity of the CMR transition.

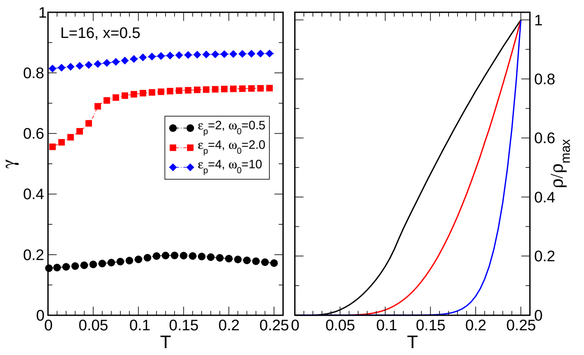

Fig.4: Polaron variational parameter γ (left panel) and resistivity (right panel) versus temperature.

Outlook

Potential future extensions of the present work could include Jahn-Teller modes [11]. In addition, the formation of magnetic polarons in the DE model should be accessible within the proposed CMC approach.

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