Available online at www.sciencedirect.com
SCIENCE DIRECT®
Physica B 359–361 (2005) 702–704
PHYSICA B
www.elsevier.com/locate/physb

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

Alexander Weiße[a], Holger Fehske[b], Dieter Ihle[c,*]

[a]School of Physics, The University of New South Wales, Sydney NSW 2052, Australia
[b]Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, 17487 Greifswald, Germany
[c]Institut für Theoretische Physik, Universität Leipzig, Augustusplatz 10-11, 04109 Leipzig, Germany

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.

PACS: 02.70.Ss; 71.10.−w; 75.47.Ck

Keywords: Colossal magneto-resistance manganites; Double-exchange; Polaron formation; Cluster Monte Carlo

Over the last decade the magnetic and transport properties of CMR manganites ($La_{1-x}[Ca,Sr]_xMnO_3$ 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. Our starting point is the Holstein-DE model

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

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

*Corresponding author. Tel.: +49 341 97 32433; fax: +49 341 97 32548.
E-mail address: dieter.ihle@itp.uni-leipzig.de (D. Ihle).

0921-4526/$ - see front matter © 2005 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2005.01.199

amplitude

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

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.

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 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 [2], but so far this approach was combined only with standard Metropolis single-spin updates [3]. 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 [4]. 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.

As an alternative, we propose a combination of kernel polynomial expansion and cluster MC (CMC) [5], which is known to be the fastest approach to non-frustrated classical models. Averaging the first part of (1) over the fermionic hopping we can define an approximate classical spin Hamiltonian

$$H_{\text{eff}} = -J_{\text{eff}} \sum_{\langle ij \rangle} \sqrt{1 + \boldsymbol{S}_i \cdot \boldsymbol{S}_j} \qquad (2)$$

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) all spins of the system are altered by multiple cluster flips, where preferably J_{eff} is random with $\langle J_{\text{eff}} \rangle = x(1-x)/\sqrt{2}$, (ii) the fermionic energy is evaluated using the kernel polynomial method, and (iii) the new spin configuration is accepted with probability

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

Here $W(a)$, $W(b)$ are the Boltzmann weights of the spin configurations a, b, and $A(a \to b)$, $A(b \to a)$ are the accumulated a priori probabilities of the cluster flips connecting a and b [5]. Of course, the MC update is no longer rejection-free, but since H_{eff} yields very good estimates for H, $\tilde{P}(a \to b)$ is sufficiently high for a reliable and fast simulation of reasonably large clusters. This allows for a confirmation and possible future extension of previous results for the DE model [4].

Encouraged by the above findings we can now rely entirely on the effective spin model H_{eff} and include lattice polaron effects on a variational level. Applying the modified variational Lang–Firsov transformation [7], from (1) and (2) we

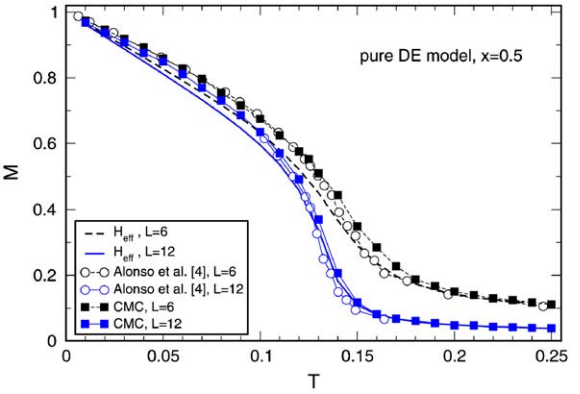

Fig. 1. Comparison of magnetisation data for the pure DE model at $x = 0.5$, obtained with the effective model (2), the hybrid MC approach [4], and the new CMC method. Here and in the following all energies are measured in units of t.

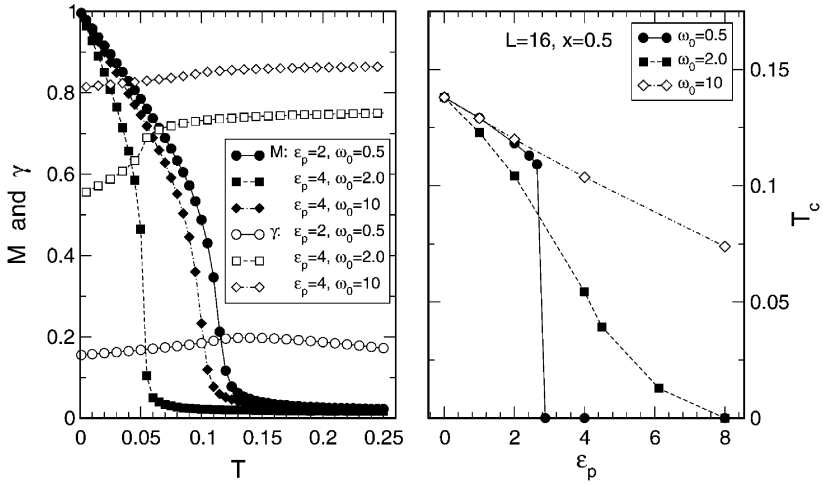

Fig. 2. Left: Magnetisation data (filled symbols) and polaron parameter γ (open symbols) for typical values of ε_p and ω_0. Right: Dependence of the critical temperature on the electron–phonon interaction strength.

obtain the effective polaron-DE model,

$$H_p = -J_{\text{eff}}\, e^{-(\gamma^2\varepsilon_p/\omega_0)\coth[\beta\omega_0/2]} \sum_{\langle ij\rangle} \sqrt{1+\boldsymbol{S}_i\cdot\boldsymbol{S}_j} + \frac{N\omega_0}{e^{\beta\omega_0}-1} + N\varepsilon_p x[(1-\gamma)^2(1-x)-1], \quad (3)$$

where γ is a variational parameter which measures the importance of the polaron effect ($0\leqslant\gamma\leqslant 1$). 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 (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. Fig. 2 shows the magnetisation as well as γ for a few typical parameter sets. Clearly the polaronic effect (larger γ) is most pronounced near and above the critical temperature. As expected, the electron–phonon interaction reduces the critical temperature, and for small phonon frequencies (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

[1] A.J. Millis, P.B. Littlewood, B.I. Shraiman, Phys. Rev. Lett. 74 (1995) 5144.
[2] R.N. Silver, H. Röder, A.F. Voter, D.J. Kress, J. Comp. Phys. 124 (1996) 115.
[3] Y. Motome, N. Furukawa, J. Phys. Soc. Japan 68 (1999) 3853;
Y. Motome, N. Furukawa, J. Phys. Soc. Japan 69 (2000) 3785.
[4] J.L. Alonso, L.A. Fernández, F. Guinea, V. Laliena, V. Martín-Mayor, Nucl. Phys. B 596 (2001) 587.
[5] W. Janke, Math. Comput. Simul. 47 (1998) 329
W. Krauth, cond-mat/0311623.
[6] U. Wolff, Phys. Rev. Lett. 62 (1989) 361.
[7] H. Fehske, H. Röder, G. Wellein, A. Mistiotis, Phys. Rev. B 51 (1995) 16582.
[8] A. Weiße, H. Fehske, Eur. Phys. J. B 30 (2002) 487;
A. Weiße, H. Fehske, New J. Phys. 6 (2004) 158.
[9] D. Ihle, Z. Phys. B 58 (1985) 91.