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Magnetic transitions in a double exchange-Holstein model with electron-phonon interactions coupled to magnetism

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In this work we study the double exchange-Holstein model with an electron-phonon interaction γ coupled to magnetism. The analysis is performed combining a mean-field approximation for the double exchange interaction and the Lang-Firsov transformation for the electron-phonon interaction. Discontinuous magnetic transitions appear when the dependence of g with m is sufficiently large, resembling those experimentally observed in manganites. We observe that the characteristic resistivity peak that arises near the critical temperature appears for broad ranges of the system parameter values, unlike what occurs in a constant-γ model.

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I. INTRODUCTION

Perovskite manganites $\mathrm{La}_{1-x}A_x\mathrm{MnO}_3$ ($A=\mathrm{Ca},\mathrm{Sr},\mathrm{Ba}$) have been studied intensively since the discovery of the spectacularly large dependence of their resistivity with the applied magnetic field: a phenomenon called colossal magnetoresistance (CMR). This unusual high response to the application of a magnetic field occurs mainly for temperatures near the critical temperature T_c of a ferromagnetic-metallic (FM) to paramagnetic-insulating (PI) transition.[1] In this range of temperatures, the curve of resistivity versus temperature exhibits a characteristic pronounced peak. It was found that the ferromagnetic-to-paramagnetic transition might be of first or second order,[2] depending on the composition of the material.

The connection between ferromagnetism and metallic behavior can be explained with the double exchange (DE) model proposed by Zener.[3] This model assumes a very large Hund's coupling between electrons and localized spins, which causes a reduction in the effective electron hopping when the ion spins are disordered.[4] Thus, the model predicts that the system is metallic in the ferromagnetic state and an insulator in the paramagnetic one. However, the magnetoresistance effect that is obtained with this theory is very poor in comparison with the experimental observations, suggesting that the double exchange mechanism alone is not enough to explain the properties of the manganites.[5] Millis *et al.*[5] proposed that a minimal model for the manganites must include a term describing a coupling between electrons and lattice degrees of freedom. The effect of such interaction was considered by Röder *et al.*[6] and by Millis *et al.*[7] In Ref. 6 the authors showed that the electron-phonon (e-ph) interaction gives a dependence of T_c with doping that is similar to the one observed experimentally. In Ref. 7, it was found that the e-ph coupling enhances the magnetoresistance effect and provides a resistivity behavior that is in qualitative agreement with the experimental observations. However, the resistivity peak near T_c is obtained with this theory only if the electron-phonon coupling γ satisfies the condition $1.08<\gamma<1.2$. A similar result was obtained by Vergés *et al.*[8] using Monte Carlo simulations. The obtained phase diagram indicates that for the case $n=0.08$, there is a FM to PI transition if $1.3<\gamma<1.6$.

In a recent paper, Dagotto and co-workers[9] studied the resistivity of the DE model including e-ph interactions using Monte Carlo computational techniques. In agreement with the previously mentioned works, it was found that the maximum of resistivity is observed in the double exchange-Holstein (DE-H) model if the coupling γ is fine tuned around some values that depend on electron density n. For instance, for $n=0.1$, the maximum resistivity appears for values of γ in the range (1.3–1.6), in agreement with the results of Ref. 8. The inclusion of disorder in the DE-H model was considered by Kumar and Majumdar in Ref. 10 and also in Ref. 9. It was found that quenched disorder favors polaronic formation and the appearance of the resistivity peaks in the curve $\rho(T)$. However, it is not clear whether the magnetoresistance effect induced by disorder reproduces the experimentally observed resistive behavior in all their aspects.

In this work we propose an alternative modification of the model. We study a DE-H with an electron-phonon coupling γ that depends on the magnetic ordering, instead of being constant as it is considered in the usual model. The variation of γ with disorder has been a long-standing problem. Both theoretical and experimental results show that γ may have important changes induced by disorder.[11–13] It is therefore of great interest to investigate how the magnetic transitions are affected by the variations in the e-ph coupling. The work is organized as follows. In Sec. II, after performing a Lang-Firsov transformation of the Hamiltonian, we construct a free energy for the system following Kubo-Ohata[14] theory. In Sec. III we discuss the dependence of the electron-phonon coupling with the magnetization. In Sec. IV we shall consider the effect of this dependence on the magnetic transitions and the resistivity. In Sec. V we summarize our results.

II. HAMILTONIAN MODEL

The Hamiltonian of the double exchange-Holstein is given by

$$H=H_Z+H_H,$$

$$H_Z = -\sum_{ij} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{H.c.}) - J_H \sum_i \sigma_i \cdot \mathbf{S}_i,$$

$$H_H = -\gamma \sum_i c^{\dagger}_{i\sigma}c_{i\sigma}(b^{\dagger}_i + b_i) + \omega \sum_i \left(b^{\dagger}_i b_i + \frac{1}{2}\right), \tag{1}$$

where t_{ij} is the electron hopping between the sites i and j, $c^{\dagger}_{i\sigma}$ is the creation operator for the itinerant electrons, J_H is the Hund's coupling, σ_i is the spin of the itinerant electrons, S_i is the spin of the Mn ions, γ is the electron-phonon coupling, and $b^{\dagger}_i$ are the phonon creation operators. Here we consider $S=3/2$, which is the total spin of the three t_{2g} electrons of the Mn^{+4} ions. To study this Hamiltonian, we assume the usually considered regime $J_H/t \to \infty$. It has been shown by various authors[4,14,15] that in this limit H_Z reduces to the DE Hamiltonian,

$$H_{\text{DE}} = -\sum_{ij} t_{ij}\sigma_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{H.c.}), \tag{2}$$

where

$$\sigma_{ij} = \left\langle \frac{S^{ij}_T + \frac{1}{2}}{2S+1} \right\rangle, \tag{3}$$

S^{ij}_T being the total spin of the subsystem formed by the ions at sites i and j and the electron, i.e., $S^{ij}_0 = |\mathbf{S}_i + \mathbf{S}_j + \sigma_i|$.[4,14,15] The value of σ_{ij} must be obtained averaging over all the states of S^{ij}_T. To calculate different averages, we follow the mean-field approach of Kubo and Ohata and introduce an effective field $\lambda = h_{\text{eff}}/T$ that tends to order the ion spins.[14,16] The magnetization is obtained from

$$m(\lambda) = z^{-1} \sum_{l=-S}^{S} (l/S)\exp(\lambda l/S), \tag{4}$$

$$z(\lambda) = \sum_{l=-S}^{S} \exp(\lambda l/S). \tag{5}$$

Since in the present model γ depends on the magnetization, it must be also a function of the field parameter λ. The value of σ_{ij} is also obtained averaging over the states of the dimer.[16] Substituting σ_{ij} by it averaged value σ, the Hamiltonian (1) becomes

$$H = -\sigma(\lambda)\sum_{ij} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{H.c.}) - \gamma(\lambda)\sum_i c^{\dagger}_{i\sigma}c_{i\sigma}(b^{\dagger}_i + b_i) + \omega \sum_i \left(b^{\dagger}_i b_i + \frac{1}{2}\right). \tag{6}$$

To treat the phonon-dependent part of Eq. (6) we use the Lang-Firsov transformation $\tilde{H} = e^S H e^{-S}$, where $S = g\sum n_i(a_i - a^{\dagger}_i)$ and $g = \gamma/\omega$. With this transformation, the Hamiltonian takes the form

$$\tilde{H} = -\sigma(\lambda)e^{-g^2}\sum_{ij} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma}e^{-g(b^{\dagger}_j - b^{\dagger}_i)}e^{g(b_j - b_i)} + \text{H.c.}) - \omega g^2 \sum_i n_i - 2\omega g^2 \sum_i n_{i\uparrow}n_{i\downarrow} + \omega \sum_i \left(b^{\dagger}_i b_i + \frac{1}{2}\right), \tag{7}$$

where $n_{i\sigma}$ are the number operators for the electrons and $n_i = n_{i\uparrow} + n_{i\downarrow}$. We approximate the wave function of the system as a tensorial product of waves function for the electrons and phonons $|\psi\rangle = |\psi\rangle_e \otimes |\psi_0\rangle_{\text{ph}}$. Considering that $|\psi_0\rangle_{\text{ph}}$ is the vacuum state and averaging over this state, the Hamiltonian takes the form

$$\tilde{H} = -\sigma(\lambda)e^{-g^2(\lambda)}\sum_{ij} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{H.c.}) - \omega g^2(\lambda)\sum_i n_i - 2\omega g^2(\lambda)\sum_i n_{i\uparrow}n_{i\downarrow}. \tag{8}$$

We note that the Lang-Firsov transformation introduces a Hubbard-type attractive interaction which can promote the formation of bipolarons.[17,18] However, we shall consider the system is in the adiabatic limit $\omega \to 0$ and thus we shall omit the last two terms of the above equation. From Eq. (8) we can obtain a free energy $F = E - TS$ for the system. The free energy of the electrons are given by

$$\Omega_e(\lambda) = -\frac{1}{2\beta}\sum_{k,\sigma} \ln[1 + e^{\beta[\mu - \epsilon_k(\lambda)]}], \tag{9}$$

where $\epsilon_k = \sigma(\lambda)e^{-g^2(\lambda)}\epsilon_{0k}$, and ϵ_{0k} stands by the energy levels of the bare band. To obtain the free energy $\mathcal{F}$ of the whole system, we follow Kubo and Ohata,[14] adding to Ω_e an entropy term corresponding to the spin ions. The free energy is thus given by

$$\mathcal{F} = \Omega_e(\lambda) - NT[\ln z(\lambda) - \lambda m(\lambda)]. \tag{10}$$

In order to determine the mean-field solutions at given temperature and doping level, we minimize $\mathcal{F}$ with respect to the variational parameter λ. We still need, however, a dependence of g with λ, or equivalently, a dependence of g with m.

III. COUPLING BETWEEN *g* AND THE MAGNETIZATION

To justify the use of an electron-phonon parameter that varies with magnetization, we examine now the calculation of the electron-phonon coupling. With this purpose, we can expand the interaction between the electron and the ions V_{ei} in the form

$$V_{\text{ei}} = \sum_{ij} V_{\text{ei}}(\mathbf{r}_j - \mathbf{R}^0_i) - \sum_{ij} \mathbf{Q}_i \nabla_j V_{\text{ei}}(\mathbf{r}_j - \mathbf{R}^0_i) + \cdots, \tag{11}$$

where $\mathbf{Q}_i$ measures the separation of the ion position $\mathbf{R}_i$ from its equilibrium value $\mathbf{R}^0_i$, i.e., $\mathbf{Q}_i = \mathbf{R}_i - \mathbf{R}^0_i$. The first term in Eq. (11) represents the potential that interacts with the electron in the absence of lattice deformation. Then, the information concerning the electron-phonon interaction is contained in the second term.[19] We can separate the interaction electron ion in the form $V_{\text{ei}} = V_{s\sigma} + V_{\text{el}}$, where $V_{s\sigma}$ corresponds to the

Hund's coupling and V_{el} includes all other possible electron-ion interactions. Supposing that the position dependence of $V_{s\sigma}$ is of the form $V_{s\sigma}=\mathcal{V}_{s\sigma}(\mathbf{r}_j-\mathbf{R}_i)(-J_H\sigma\cdot\mathbf{S}_i)$, the second term in the expansion (11) may be put as

$$V_{\mathrm{ei2}}=-\sum_{ij}\mathbf{Q}_i\nabla_j[V_{\mathrm{el}}(\mathbf{r}_j-\mathbf{R}_i^0)-J_H\sigma\cdot\mathbf{S}_i\mathcal{V}_{\sigma S}(\mathbf{r}_j-\mathbf{R}_i^0)]. \tag{12}$$

From the above expression, it becomes clear that Hund's interaction can introduce large changes in the interaction electron phonon, principally when J_H is the strong-coupling regime. To obtain a relationship involving m and g, we shall assume that the form of $V_{\mathrm{el}}(\mathbf{r}_j-\mathbf{R}_i^0)$ and $\mathcal{V}_{\sigma S}(\mathbf{r}_j-\mathbf{R}_i^0)$ are similar. In the Appendix, we show that this approximation is adequate under certain conditions. Using this simplification we can write $\mathcal{V}_{\mathrm{el}}(\mathbf{r}_j-\mathbf{R}_i^0)=\xi V_{\sigma S}(\mathbf{r}_j-\mathbf{R}_i^0)$, where ξ is a constant. Inserting this equality in Eq. (12), we obtain that

$$V_{\mathrm{ei2}}=-(1-\xi J_H\langle\sigma_i\cdot\mathbf{S}_i\rangle)\sum_{ij}[\mathbf{Q}_i\nabla_j V_{\sigma S}(\mathbf{r}_j-\mathbf{R}_i^0)], \tag{13}$$

where $J_H\langle\sigma\cdot\mathbf{S}_i\rangle$ is the spatial average of the Hund's interaction. The interaction electron phonon takes the usual form, if we except the factor $(1-\xi J_H\langle\sigma\cdot\mathbf{S}_i\rangle)$. The usual electron-phonon interaction that does not depend on the magnetization is recovered when $J_H=0$. In order to obtain the approximate dependence of g with m, we again follow the method used in Refs. 4 and 14 and consider a dimer of two ions with one itinerant electron. If we suppose that initially the electron is at the ion $i=1$, in virtue of the strong Hund's coupling the spin is aligned with the spin of this ion. When the electron jumps to the site $i=2$, it will interact with the spin $\mathbf{S}_2$. In general σ_1 and $\mathbf{S}_2$ will not be aligned. To obtain the value of $J_H\langle\sigma\cdot\mathbf{S}_i\rangle$, we average $J_H\langle\sigma_1\cdot\mathbf{S}_2\rangle$ over all the states of the total spin $\mathbf{S}_T=\sigma+\mathbf{S}_1+\mathbf{S}_2$ in the presence of the field λ. Due to the fact that σ is aligned with $\mathbf{S}_1$, these two spins can be considered as a unique spin with module $\bar{S}=S+\frac{1}{2}$. Since $S=3/2$ and $\sigma=1/2$, $\langle\sigma\cdot\mathbf{S}_2\rangle=\langle\bar{\mathbf{S}}_1\cdot\mathbf{S}_2\rangle/4$. To calculate this average, we use the identity $\bar{\mathbf{S}}_1\cdot\mathbf{S}_2=\frac{1}{2}(\mathbf{S}_T^2-\bar{\mathbf{S}}_1^2-\mathbf{S}_2^2)$. Then, the average is explicitly obtained from

$$\langle\sigma_1\cdot\mathbf{S}_2\rangle=\frac{\sum_{S_T=1/2}^{\bar{S}_1+S_2}\sum_{M=-S_T}^{S_T}\langle SM|\mathbf{S}_T^2-\bar{\mathbf{S}}_1^2-\mathbf{S}_2^2|SM\rangle e^{M\lambda}}{8\sum_{S_T=1/2}^{\bar{S}_1+S_2}\sum_{M=-S_T}^{S_T}e^{M\lambda}}, \tag{14}$$

where $\langle SM|\ \mathbf{S}_T^2-\bar{\mathbf{S}}_1^2-\mathbf{S}_2^2)|SM\rangle=[S_T(S_T+1)-\bar{S}_2(\bar{S}_2+1)-S_1(S_1+1)]$, with $\bar{S}_1=2$ and $S_2=3/2$. Since m and $\langle\sigma\cdot\mathbf{S}_i\rangle$ are functions of λ, we can obtain the relationship between these quantities. This dependence is shown in Fig. 1, and it can be accurately approximated as $\langle\sigma\cdot\mathbf{S}_i\rangle=\frac{1}{2}Sm^{1.8}$. $\langle\sigma\cdot\mathbf{S}_i\rangle$ takes its maximum value of $\frac{1}{2}S$ in the fully polarized state $m=1$, when σ and $\mathbf{S}_i$ are aligned, and becomes zero in the disordered state $m=0$. Then, from Eq. (13), the dependence of the electron-phonon coupling with m can be expressed as

$$g=g_0(1-\alpha m^{1.8}), \tag{15}$$

where α is a constant and g_0 is the value of the e-ph coupling in the absence of magnetization. From this expression, α can be expressed as $\alpha=(g_0-g_{m=1})/g_0$, i.e., is the variation of g between the paramagnetic state ($m=0$) and the fully polarized state ($m=1$) relative to g_0. We notice that in previous works,[7] the notion of an effective e-ph coupling that changes with T was already employed. However, the variations of g considered here are not only effective but real ones. As we shall show later, the real variations of g introduce important modifications in the behavior of the system.

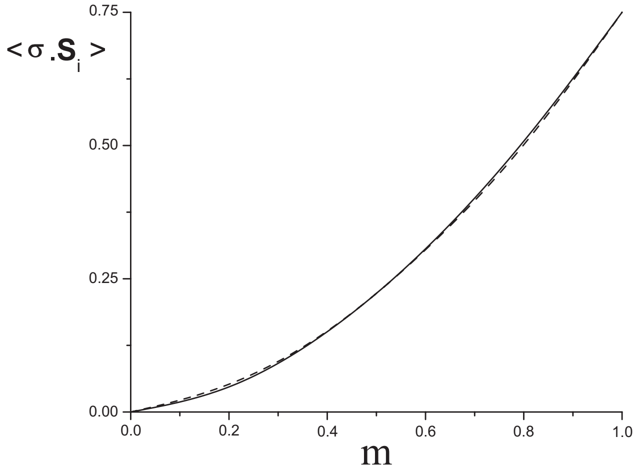

FIG. 1. Dependence of $\langle\sigma\cdot\mathbf{S}_i\rangle$ with the magnetization. The continuous line represents the values obtained with Eqs. (4) and (14). The dashed line corresponds to the approximate expression $\langle\sigma\cdot\mathbf{S}_i\rangle=3/4m^{1.8}$.

IV. NUMERICAL RESULTS

The numerical solutions are obtained minimizing the free energy $\mathcal{F}$ (18) subject to the conditions (4) and (15). In Fig. 2 we show the magnetization as a function of T for $\alpha=0.4$, a doping level $x=1-\langle n_i\rangle=0.25$, and different values of g_0. Here a square density of state (DOS) bare band of bandwidth $D=12t$ was assumed. In general, the effect of the e-ph coupling is to reduce the magnetic critical temperature for either

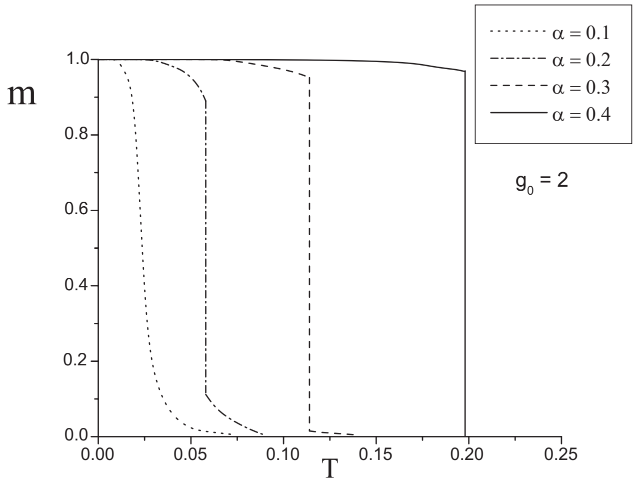

FIG. 2. Magnetization as a function of the temperature for $g_0=2$ and $\alpha=0.1,0.2,0.3,0.4$. Temperature is measured in units of t.

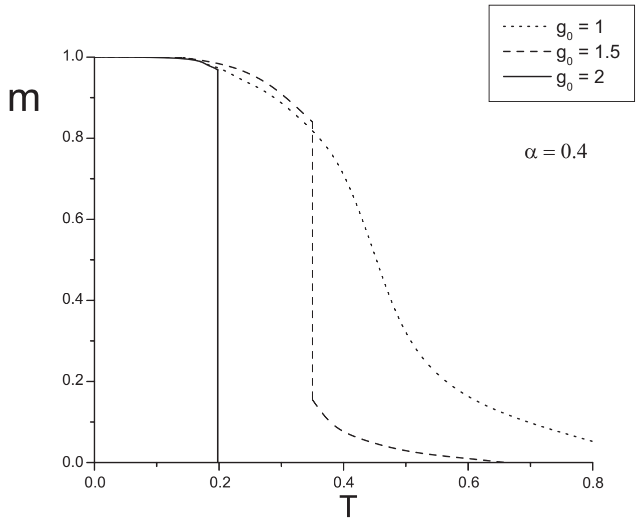

FIG. 3. Magnetization as a function of the temperature for $\alpha = 0.4$ and $g_0 = 1, 1.5, 2$.

of the cases, in which g is dependent or independent of m. This occurs due to the narrowing band effect of the electron-phonon coupling, which reduces the efficiency of the double exchange mechanism. However, when g is m dependent, the magnetic transition becomes discontinuous as long as α is above a critical value α_c that depends on the value of g_0 (see Fig. 3). We notice that as α increases, both the critical temperature and the value of m may increase. This is because larger values of α reduces the value of g in the magnetic state, increasing the bandwidth and favoring the DE mechanism. On the other hand, when the value of α is increased, the critical value of g_0 for the occurrence of discontinuous transitions decreases. The minimal value of g_0 for the occurrence of first-order transitions goes to infinity as $\alpha \to 0$, indicating that there are no discontinuous transition when $\alpha = 0$ (g independent of m) within our mean-field treatment. In Fig. 4 we show the phase diagram in the (g_0, α) space. The labeled regions correspond to (I) continuous ferromagnetic transitions, (II) discontinuous magnetic-magnetic transitions, and (III) discontinuous ferromagnetic-paramagnetic transition. The three cases are depicted in Fig. 3. Figures 2 and 3 show that the magnetic transitions obtained with an m dependent g compares well with the one obtained in experiments when $\alpha > 0$ and g_0 is strong. At this point, we remark that the detailed form of the dependence of g on m does not affect significantly the system behavior. If we employ a simple linear dependence of the form $g = g_0(1 - \alpha m)$, the phase diagram is nearly the same as those showed in Fig. 4; although there are some changes in the critical temperatures. Although we have not calculated the value of α from first principles, it is worth mentioning that the first-order transitions appear for any value of $\alpha > 0$, if g_0 is sufficiently large. Experimentally, it was found that the electron-phonon interaction may undergo variations of order 150%.[13] If we assume this level of variations, the value of α may be taken between 0 and 0.6.

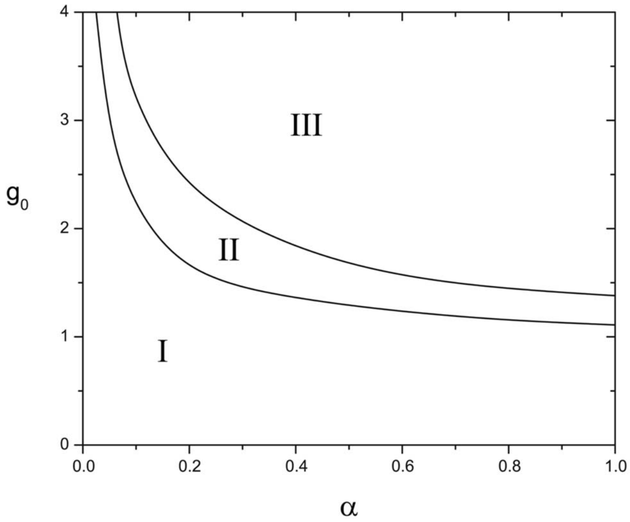

FIG. 4. Phase diagram of the DE-H model with $g = g_0(1 - \alpha m^{1.8})$. The labeled regions represent (I) continuous magnetic transitions, (II) discontinuous F-F transitions, and (III) discontinuous F-P transitions.

An important property of the manganites is the strong dependence of their resistivity with the application of a magnetic field near T_c. In order to study if this effect appears in the present model, we examine the dependence of the bandwidth with an applied field. The average physical magnetization in z direction is given by $M = g_s \mu_B N \langle S_z \rangle$, where N is the number of ions. Thus, the energy due to the magnetic interactions is given by $H_M = Nhm$, with $h = g_s \mu_B SH$. We then added the term H_M to the free energy (18) and obtained the mean-field solutions. The variations of W are shown in Fig. 5. As it can be seen, when the transitions are discontinuous ($\alpha = 0.4$), there is a strong dependence of the bandwidth with H near T_c. Since W is proportional to conductivity, this means that there is a large increment of the conductivity with application of H. This effect is relatively weak when the transition is smooth ($\alpha = 0.1$).

In many works, it has been reported that the first-order transitions in manganites are accompanied by phase separation. In order to analyze this possibility, we plotted the free

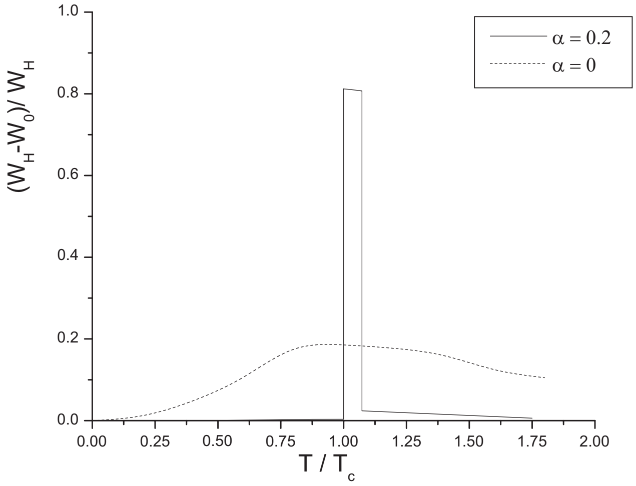

FIG. 5. Percentual variation in the bandwidth with application of magnetic field calculated as $[W(H) - W(0)]/W(H)$, for $g = 2$, $\alpha = 0, 0.2$, and $h = 0.02$. $W(H)$ and $W(0)$ denote the bandwidths with and without magnetic field.

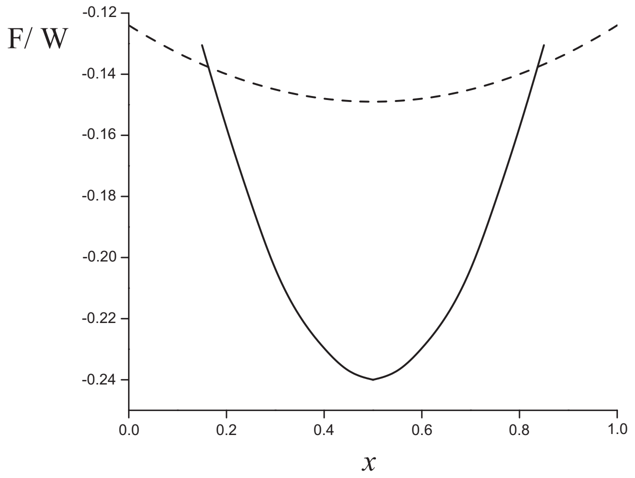

FIG. 6. Free energies per site over the bandwidth, for $g=2$, $\alpha=0.2$, and $k_BT=0.05$. The solid line corresponds to the F state and the dashed line to the P one. For these parameter values, phase separation takes place for doping value ranges $0<x<0.3$ and $0.7<x<1$.

energy of the F and P solutions as a function of doping for constant temperature. The tendency to phase separation is established when the stability condition $(\frac{\partial^2\mathcal{F}}{\partial N^2})_T\geq 0$ is not satisfied. Each solution satisfies this condition separately; but at the point at which the two free energies cross, the first transition takes place and the condition is not satisfied. We then search for biphase solutions of the form $\mathcal{F}=N_1\mathcal{F}_1(N_{e1}/N_1)+N_2\mathcal{F}_2(N_{e2}/N_2)$, where N_i are the number of sites occupied by phase i and N_{ei} are the numbers of electrons in the volume occupied by phase i. Thus, $N_1+N_2=N$ and $N_{e1}+N_{e2}=N_e$, N_e being the total number of conduction electrons. $\mathcal{F}_1$ and $\mathcal{F}_2$ are the free energies for each phase showed in Fig. 6. Defining $a_1=N_1/N$, $z_1=N_{e1}/N_e$, and $n=N_e/N$, we can express the free energy per site as

$$\mathcal{F}(T,n)/N=z_1\mathcal{F}_1(T,nz_1/a_1)+(1-z_1)\mathcal{F}_2\left(T,\frac{n(1-z_1)}{1-a_1}\right). \tag{16}$$

We then obtained the volume fraction occupied by each phase minimizing $\mathcal{F}$ with respect to z_1 and a_1, with the restriction that the density of electrons $n_i=N_{e1}/N_1$ must range between 0 and 1 in each phase. The volume fraction occupied by each phase is shown in Fig. 7 from which we can see that phase separation takes place around the critical conditions for the first-order transitions.

As mentioned previously, the origin of the resistivity maximum that appears near the critical temperature is still not well understood. As already mentioned, this peak is obtained in the DE-H model,[7–9] when the electron coupling γ takes values in a relatively narrow range. The calculations of the resistivity in these previous works show that ρ decreases monotonically with T if $\gamma<1.2$. On the other hand, if $\gamma>1.6$, the resistivity rapidly increases with $1/T$. This last behavior is probably due to the formation of polarons, whose resistivity exhibit such a dependence with T. Although the spin scattering could contribute to develop a maximum at T_c, the resistivity of the polarons increases so rapidly that the peak is not observed. In order to estimate the variation in the resistivity due to polaron formation, we shall use the expression for ρ_{pol} in the strong-coupling adiabatic limit $(\omega/t\rightarrow 0)$,

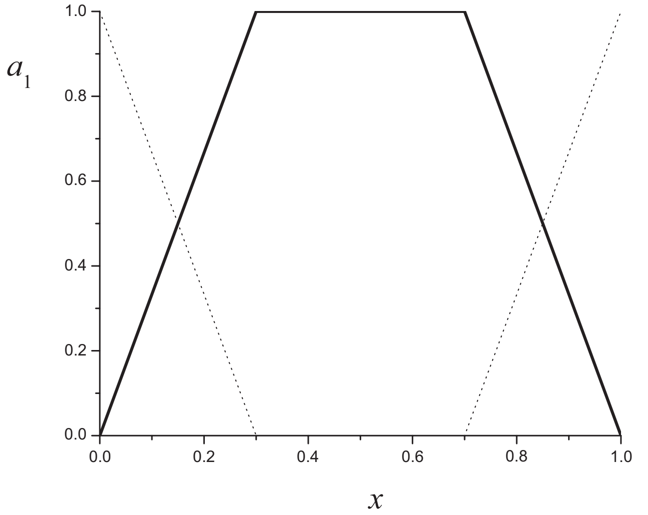

FIG. 7. Volume fraction occupied by F (solid line) and P (dashed line) regions, for $g=2$, $\alpha=0.2$, and $k_BT=0.05$.

$$\rho_{\mathrm{pol}}(T)=AT\exp\left(\frac{\epsilon_a}{k_BT}\right), \tag{17}$$

where $\epsilon_a\approx\epsilon_p/2$ is the activation energy[1] and $\epsilon_p=g^2\omega$ is the polaron binding energy. From the Kubo's formula for resistivity, it follows[20] that $\rho\propto 1/t^2$. Then, we can write $A\propto 1/W^2$, where A is the parameter appearing in Eq. (17). In various works it was found that this expression agrees very well with the resistivity in manganites in the region $T>T_c$,[21–23] revealing the presence of small polarons in the paramagnetic phase.[24] It is worth mentioning that in principle it is difficult to differentiate the polaronic resistivity from the resistivity of an ordinary semiconductor, which has a similar dependence to Eq. (17) (without the prefactor T). However, in Ref. 25 it has been shown that a band insulator theory cannot explain the differences between the gap value obtained from thermopower and the one obtained from resistivity measurements. On the other hand, these differences may be explained assuming polaronic interactions.

We studied the variation of $\rho_{\mathrm{pol}}(T)$ using Eq. (17) with the values of g and W obtained in the mean-field solutions. In order to consider a realistic value of ω, we included the third term in Eq. (8) and minimized the free energy given by

$$\mathcal{F}=\Omega_e(\lambda)-NT[\ln z(\lambda)-\lambda m(\lambda)]-\omega g^2(\lambda)\sum_i n_i. \tag{18}$$

In order to take realistic values of the parameters, we used the estimations of the activation energy and phonon frequency given in Ref. 23, $\epsilon_a=0.08$ eV and $\omega=0.036$ eV, which gives $g_0=2$. On the other hand, the bare bandwidth has been estimated in Ref. 5 to be of order 2.5 ever. Since in our model $D=12t$, this gives $\omega\approx 0.2t$. In Fig. 8 the values of $\log(\rho_{\mathrm{pol}})$ for $g_0=2$, $\alpha=0.4$, and $\omega=0.2$ $(t=1)$ are shown.

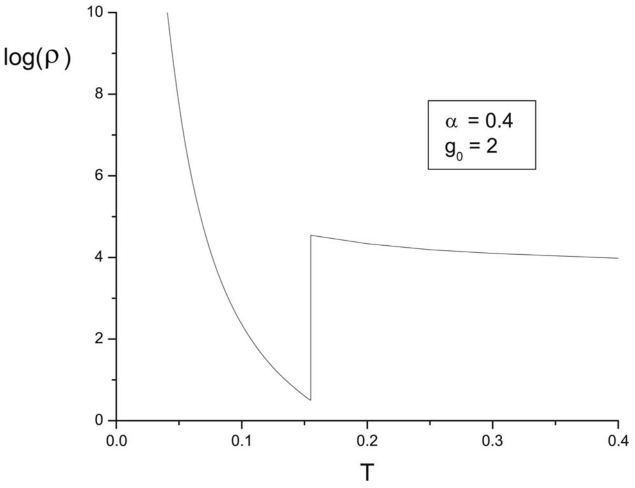

FIG. 8. Logarithm of the polaronic part of the resistivity obtained from the expression $\rho_{\mathrm{pol}}(T)=\frac{BT}{W^2}\exp(\frac{g^2\omega}{k_BT})$, using the values of g and W obtained in the mean-field solutions for $g_0=2$, $\omega=0.2$, and $\alpha=0.4$ (B is a constant).

From this figure we can see that a peak accompanied by a pronounced depletion of ρ is observed at $T=T_c$. This is caused by a rapid reduction of g (in this case from $g=2$ in the P state to $g=1.2$ in the F state). As it can be seen from Fig. 8, relatively small changes in g produce drastic changes in ρ_{pol}. Moderate variations of γ or other system parameters will not suppress the presence of these peaks. These appear in region III of Fig. 4. Of course, we have not considered the scattering of the electrons by the spins. We expect that this effect will superpose to the polaronic ones and contribute to increase the resistivity peak.

We note that the reduction of g allows a transition from small polarons (large coupling) in the P state to large polarons (small coupling) in the F state. This transition has been reported by a number of groups.[26–28] The variation in the resistivity for $T<T_c$ also supports reduction in the electron-phonon coupling in the ferromagnetic region. It has been shown that resistivity in the ferromagnetic phase of the manganites can be well described with a dependence of the form $\rho=\rho_0+AT^2+BT^{4.5}$, where the first term is a constant, and the two last terms correspond to electron-electron (e-e) interaction and electron-magnon scattering, respectively.[21,29] A kind of transition between two polaronic regimes, as the one found here, could explain the small influence of polaronic effects in the resistivity below T_c. We comment that we do not attempt to describe accurately the resistivity of the *F* phase with Eq. (17) because it is valid for the strong-coupling regime. Thus, the resistivity of Fig. 8 describes the transition between two phases with different e-ph coupling, both in the strong-coupling case. It is worth mentioning that the form of this curve is similar to the one obtained in $La_{0.85}Sr_{0.15}MnO_3$. At $T_c=240$ K, this compound experiments a transition from a P insulator to an F insulator[30] (see inset in Fig. 40 of Ref. 1).

A recent study of the quasiparticle excitation spectrum of $La_{0.77}Ca_{0.23}MnO_3$ using scanning tunneling microscopy by Seiro *et al.*[24] revealed that the spectra present a polaronic gap in the F and P phases. However, the gap is reduced when the system enters in the F phase. Since the polaronic gap measured in the experiment is of magnitude ϵ_p, the dependence of the gap with the temperature is compatible with the reduction in the e-ph interaction in the F state that is obtained in the present model.

V. CONCLUSIONS

In this work, we study a DE-H model with an electron-phonon interaction that depends on the magnetic ordering. By a simple argument, in examining the calculation of the electron-phonon coupling, we show that g is affected by the magnetic interactions. This occurs principally when the Hund's coupling is strong, which is precisely the regime that is considered to be relevant for the manganites. Introducing a field parameter to control the magnetization and making some assumptions about the spatial form of the electron-ion interaction, we calculated a dependence of g with the magnetization m. When α ($\sim dg/dm$) is above a critical value that depends on g_0, the F-P transitions become discontinuous. This is not only because the DE mechanism and the polaron formation are affected mutually in an indirect form but also because there is an interplay between these two mechanisms. In the spin-disordered state, the electron-phonon interaction is enhanced, favoring the appearance of small polarons. In turn, the polaronic effect reduces the electrons mobility decreasing the efficiency of the DE mechanism. This highly nonlinear effect induces a sharp magnetic transition. These first-order transitions may occur directly between the F and P states or between two F states. The last case appears only in a narrow region of the parameter space and probably will not be present in a more refined treatment of the model than the mean-field approach considered here. On the other hand, we can expect that a crossover from smooth to sharp transitions will persist in region II if fluctuations are included. The abrupt transitions of region III (Fig. 4) have a shape that resembles the magnetic transitions experimentally observed in the manganites. We estimated the changes in the polaronic resistivity using the expression of ρ_{pol} in the adiabatic limit. A strong peak in the resistivity of polaronic origin appears at the critical temperature when the transitions are abrupt. This is very robust and appears in region III of the phase diagram of Fig. 4. This allows to explain the presence of the resistivity maximum in a series of compounds, for which γ and other properties may be different. For some values of the parameters, the discontinuous transitions are accompanied by a crossover from large polarons in the FM phase to small polarons in the PI phase, in agreement with several experimental observations.[26–28] In summary, the obtained results show that the DE-H model with an electron-phonon coupling that varies with the magnetization reproduces some properties of the manganites that are still not well understood. It is not our intention to neglect the importance of other factors, such as structural disorder or phase separation in order to explain the manganites behavior, but instead of proposing another mechanism that could be important to complete the description of these systems.

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APPENDIX

The spin-dependent part of the electron-ion interaction is an exchange interaction given by

$$J(R) = \int \int \phi_1(r)\phi_2(r')V(r'-r)\phi_2(r')\phi_1(r)drdr' . \tag{A1}$$

The orbital functions $\phi_i(r)$ are centered on different points separated by a distance R. In order to study the dependence of this interaction with R, we follow Campbell *et al.*[31] and assume that the e-e interaction is a screened potential of the form $V(r'-r)=A\exp(-a|r-r'|)$, $r-r'$ being the distance between the electrons. We also assume that the functions ϕ_i are of the form $\phi(r)=C\exp(-\kappa r)$. Here $1/a$ is the screening length and $1/\kappa$ is the localization length. We evaluated J for different values of a, κ, and R. We obtained that when a and κ are nearly equal, the variation of $J(R)$ follows the variation of $V(R)$. When $a>\kappa$, $J(R)$ falls more rapidly than $V(R)$. In the case $a<\kappa$, the opposite occurs. Then, the assumption that $J(R)$ has the same spatial dependence than $V(R)$ is valid for some particular physical conditions. On the other hand, it is worth mentioning that the overall results do not depend strongly on the functional dependence of g with m. Thus, this assumption was performed to allow an analytical calculation but does not introduce results which disappear if other dependence is adopted.

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