Curie temperature behavior in half-metallic ferromagnetic double perovskites within the electronic correlation picture

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The half-metallic ferromagnetic compound Sr_2FeMoO_6 is considered a fundamental material to understand the role of electronic parameters controlling the half-metallic ground state and high Curie temperature in double perovskite. We present an electronic approach using the Green's function technique and the renormalization perturbation expansion method to study the thermodynamical properties of double perovskites. The model is based on a correlated electron picture with localized Fe spins and conduction electrons interacting with the local spins via a double-exchange-type mechanism. Electron correlations within the conduction band are also included in order to study the Curie temperature T_C. Our results show an increases of T_C by increasing the carrier density in La-doped Sr_2FeMoO_6 compounds in contrast to the case of uncorrelated itinerant electrons.

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I. INTRODUCTION

Half-metallic materials, in which only one-spin direction is present at the Fermi level, have been investigated in view of their attractive properties for potential spintronic applications [1] and as potential candidates for memory devices by virtue of their large magnetoresistance (MR). The double perovskite Sr_2FeMoO_6 (SFMO) combines half-metallic ferromagnetic character with a high Curie temperature $T_C = 400$ K and substantial MR at low field [2]. The low-field MR in SFMO is strongly affected by the long-range ordering of Fe and Mo atoms [3,4]; disordered samples do not exhibit a low-field sharp magnetoresistive response, though the MR remains very similar to that of an ordered sample in the high-field regime. Disordering may modify the half-metallic character of the system: the experimental saturation magnetization ($\approx 3.2\mu_B$ per formula unit) is significantly lower than the saturation magnetization $4\mu_B$ expected from the polarized bands. Additionally, a spin polarization $P \approx 0.85$ has been measured [5] based on a tunnel junction device instead of the full polarization value $P = 1$ reached with saturation magnetization. These discrepancies have been attributed to some degree of disorder between Fe and Mo atoms. Decrease of the saturation magnetization with increasing disorder is expected as a result of the antiferromagnetic superexchange interaction between nearest-neighbor Fe atoms [6,7].

The ferromagnetism and half-metallicity in SFMO have been understood [8] in fully ordered systems on the basis of a strongly correlated picture, where the Fe^{3+} $(3d^5)$ are localized ions with a high-spin $S = 5/2$, together with Mo^{5+} $(4d^1)$ cores with one conduction electron (one per Mo atom) that can hop between Mo and Fe sites in the exchange split t_{2g} orbitals only with an orientation antiparallel to the localized spin, giving a $3d^6$ (Fe^{2+}) $S = 2$ configuration for the Fe sites. The kinetic energy of the conduction electrons stabilizes a ferromagnetic arrangement of the local spins, a mechanism similar to double exchange, and also leads to the opposite spin polarization of the conduction electrons.

The robustness of the ferromagnetic state, hence T_C, is governed by the kinetic energy gain which depends on the bandwidth $2w$ and the charge transfer energy, i.e., the energy to transfer an electron between Fe and M (M is a transition metal), $\Delta_0 = E$ (Fe d^5, $S = 5/2$; M d^1) $- E$ (Fe d^6, $S = 2$; M d^0), in the one-electron approximation $\Delta_0 = E_{\mathrm{M}} - E_{\mathrm{Fe}}$, accounting implicitly for the underlying Fe configuration, E_{M} and E_{Fe} being the site diagonal energies at the M and Fe sites respectively. One understands easily that for large Δ_0 the electrons become almost localized either on Fe or M depending on the sign of Δ_0, thus reducing strongly the kinetic energy and the stability of the ferromagnetic state. T_C depends essentially on Δ_0/w, and of course on the band filling. Various approaches [8,9] based essentially on this electronic model provide very similar behaviors for the dependence of T_C on Δ_0/w and n, as shown in Fig. 1. Although based on strong correlations on Fe sites, the above model is purely kinetic (tight-binding) and neglects the correlations among itinerant electrons. Throughout this paper this situation will be referred to as the "uncorrelated itinerant electrons case" or simply "uncorrelated case."

In these half-metallic ferromagnetic materials, the challenge is to obtain higher T_C. A substantial increase of T_C

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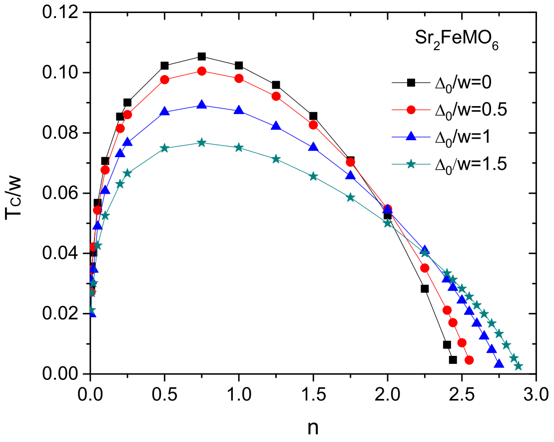

FIG. 1. Curie temperature T_C for the uncorrelated itinerant electrons case as function of the band filling n for different charge transfer energies Δ_0/w.

has been observed by increasing the number of conduction electrons resulting from the substitution of divalent Sr by trivalent La in $Sr_{2-y}La_yFeMoO_6$ [10]. It is clear from Fig. 1 that, in the framework of the above model, this increase of T_C cannot be accounted for by just increasing the carrier density. It has been suggested [8] that correlations within the conduction band could play a crucial role, giving rise by themselves to a ferromagnetic instability, the Stoner model of band ferromagnetism. Indeed, the idea is quite simple, and exchange splitting between ↑ and ↓ electrons stems from electron correlations in the Hubbard model $Un_{i\downarrow}n_{i\uparrow}$ by applying the mean-field approximation. This should reinforce the ferromagnetic (F) state generated by the kinetic energy mechanism leading to an increase of the Curie temperature T_C. On the other hand, it has been shown that Mo intra-atomic correlations, even moderate ones ≈1 eV, could play a key role in the understanding of the magnetic and electronic properties of disordered compounds [7,11]. Correlations on Fe are certainly stronger: values of the order of 2–4 eV have been reported [12–14]. In this paper, we will concentrate on the effect of the conduction electrons correlations on the Curie temperature behavior in ferromagnetic double perovskite. More details on the model are given in the following section.

II. MODEL

In the fully ordered double perovskite structure, Sr_2FeMoO_6, Fe and Mo occupy two interpenetrating sublattices α and β respectively, in a rocksalt structure. Oxygen atoms bridge the Fe and Mo ions to form alternating FeO_6 and MoO_6 octahedra. The electronic structure of the ferromagnetic compound Sr_2FeMoO_6, investigated by optical [15] and photoemission spectroscopies [12,16], is in good agreement with band structure calculations [2,16,17]. In the majority spin-up band, the occupied part of the bands near the Fermi level comes from filled t_{2g} and e_g bands with mainly Fe d character, although slightly hybridized with Mo d. These states will be modeled by frozen localized spins S_i corresponding to the Fe^{3+} d^5 configuration. Due to strong Hund coupling, parallel spins occupy the t_{2g} and e_g orbitals, giving the high spin configuration $S = 5/2$. We further simplify this picture by assuming that the localized spins can be either up (+) or down (−). The partly occupied minority spin-down band comes from three strongly mixed Fe and Mo degenerate t_{2g} states. The relevant states near the Fermi level are derived from Fe and Mo d orbitals. We will use a tight-binding Hamiltonian containing only Fe and Mo sites. This electronic scheme is consistent with *ab initio* calculations and with the current information on electronic states emerging from photoemission spectroscopy [12] and x-ray magnetic circular dichroism experiments [18].

Inclusion of on-site electronic correlations within the *ab initio* local density approximation + U (LDA+U) or the local spin density approximation (LSDA+U) does not modify qualitatively the electronic structure [12–14]; it merely enhance the exchange splitting of Fe, reinforcing the localized character of the Fe majority spin-up states. There are some attempts to include temperature in Sr_2FeMoO_6 double perovskite compounds using *ab initio* calculations [19], but most of the them are extremely difficult—owing to the computational time involved due to the averaging configuration to calculate the transition temperature by calculating the difference between the paramagnetic phase and the relevant magnetic phases—and have poor agreement with experimental results. Other attempts using first-principles calculations [20] to obtain the Curie temperature in the above systems also include the mean-field approximation within these type of calculations. The large computational time involved here, with results valid only for weak ferromagnetic systems and their T_C being far from experimental results, show us the importance of considering an alternative strongly correlated picture of the stable Fe d^5 configuration viewed as localized spins. This allows a rather simple but physical treatment of the temperature-induced spin disorder and calculation of T_C within the dynamical mean field scheme (DMF). Consistent with this approach, the alternating Bethe lattice (alternating Fa and Mo sites) produces an approximate density of states (DOS) mimicking the real DOS but preserving the essential features of the band structure calculations. In the ferromagnetic state, the minority spin-down DOS takes a semielliptic form around the Fermi energy; note that in addition one has also a Mo peak in the spin-up DOS above the Fermi energy corresponding to the unoccupied narrow Mo-derived band seen in the band structure calculations, thus preserving the half-metallic behavior.

As we mentioned in the Introduction, in studying T_C it is essential to take into account correlations both on Fe and Mo ions. Due to the degeneracy of the t_{2g} orbital, the Hubbard intra-atomic correlations among itinerant electrons, H_c^{Mo} and H_c^{Fe}, should contains both intraband and interband terms. Contrary to the assertion of Brey *et al.* [21], on Fe sites the interband term is the only interaction intervening, only one spin direction being possible on sites with + or − local spins, so

$$H_c^{\mathrm{Mo}} = (U^{\mathrm{Mo}} + 2J^{\mathrm{Mo}}) \sum_{i,\nu} n_{i\nu\uparrow} n_{i\nu\downarrow} + U^{\mathrm{Mo}} \sum_{i,\nu,\nu'\neq\nu} n_{i\nu\uparrow} n_{i\nu'\downarrow}$$

$$+ (U^{\mathrm{Mo}} - J^{\mathrm{Mo}}) \sum_{i,\nu,\nu'\neq\nu,\sigma} n_{i\nu\sigma} n_{i\nu'\sigma}, \tag{1}$$

$$H_c^{\mathrm{Fe}} = (U^{\mathrm{Fe}} - J^{\mathrm{Fe}}) \sum_{j,\nu,\nu'\neq\nu,\sigma} n_{j\nu\sigma} n_{j\nu'\sigma}, \tag{2}$$

where i,j correspond to sites occupied by Mo and Fe, and ν and ν' label the three t_{2g} orbitals.

Treating these terms in the mean-field approximation, we obtain the renormalized sites energies $\tilde{E}_{\mathrm{Fe},\sigma}(\pm)$ and $\tilde{E}_{\mathrm{Mo},\sigma}$. Here, $\tilde{E}_{\mathrm{Fe},\uparrow}(-)$ ($\tilde{E}_{\mathrm{Fe},\downarrow}(+)$) refers to Fe sites with itinerant electrons for spin ↑ (↓) and localized electrons with spins $-$ ($+$). For simplicity, we will denote these Fe site energies by $\tilde{E}_{\mathrm{Fe},\uparrow}$ ($\tilde{E}_{\mathrm{Fe},\downarrow}$):

$$\tilde{E}_{\mathrm{Fe},\sigma} = E_{\mathrm{Fe}} + \tfrac{2}{3} U_{\mathrm{eff}}^{\mathrm{Fe}} \langle n_{\alpha,\sigma}^{\mathrm{Fe}} \rangle, \tag{3}$$

$$\begin{aligned}\tilde{E}_{\mathrm{Mo},\sigma} = {} & E_{\mathrm{Mo}} + \left(U^{\mathrm{Mo}} + \tfrac{2}{3} J^{\mathrm{Mo}}\right) \langle n_{\beta,-\sigma}^{\mathrm{Mo}} \rangle \\ & + \tfrac{2}{3} U_{\mathrm{eff}}^{\mathrm{Mo}} \langle n_{\beta,\sigma}^{\mathrm{Mo}} \rangle,\end{aligned} \tag{4}$$

where $\langle n_{\alpha,\sigma}^{\mathrm{Fe}} \rangle$, $\langle n_{\beta,\sigma}^{\mathrm{Mo}} \rangle$ are the occupation numbers of electrons σ on Fe and Mo sites, $U_{\mathrm{eff}}^{\mathrm{Mo}} = U^{\mathrm{Mo}} - J^{\mathrm{Mo}}$, $U_{\mathrm{eff}}^{\mathrm{Fe}} = U^{\mathrm{Fe}} - J^{\mathrm{Fe}}$, and we used $\langle n_{i\nu\sigma} \rangle = \langle n_{i\sigma} \rangle / 3$ due to the degeneracy of the three t_{2g} orbitals. We shall take $U_{\mathrm{eff}}^{\mathrm{Fe}} = 3w$, $U_{\mathrm{eff}}^{\mathrm{Mo}} = w$, $J^{\mathrm{Mo}} = 0.1w$ since these values have been shown to provide good results in disordered compounds [11]. These sites energies have to be determined self-consistently from the density of states. $E_{\mathrm{Fe}} = 0$ will be taken as reference energy. In order to obtain the DOS per orbital for itinerant electrons on Fe and Mo sites, we calculate the local Green's functions within the renormalized perturbation expansion method [8,22], in an alternating Bethe lattice in the limit of infinite coordination number, $z \to \infty$, where zt^2 scales as $w^2/4$, w being half the bandwidth. In the figures of DOS we will take $w = 4$. The local average Green's functions take the dynamical mean-field (DMF) form $G_{ii,\sigma}^{-1} = \omega - \varepsilon_i - \sum_{l \neq i} t^2 G_{ll,\sigma}$, where ε_i is the corresponding on-site energy and the summation is over all nearest-neighbor sites. On a given Fe site, with all five d orbitals being occupied with the same spin direction, an itinerant electron is inevitably coupled antiferromagnetically to the Fe localized spins, giving a $3d^6$ ($S=2$) Fe^{2+} configuration. This imposes strong constraints on the hopping $t_{\mu_i,\sigma}$ of an electron with spin σ between a Mo site and an Fe site with local spin $\mu_i = \pm$, $t_{\mu_i,\sigma} = t$ only if μ_i and σ (↑ or ↓) are opposite, otherwise $t_{\mu_i,\sigma} = 0$ when μ_i and σ are parallel. These constraints are accounted for by the probabilities $\nu_{\pm} = (1 \pm m)/2$ that an Fe ion has its localized spin $+$ or $-$, with the magnetization due to the localized spins being $M = m\mu_B$.

The Green's functions for an itinerant electron with spin ↓ are given by

$$G_{\downarrow+}^{\alpha\mathrm{Fe}} = \frac{1}{\omega - \tilde{E}_{\mathrm{Fe},\downarrow} - \frac{w^2}{4} G_{\downarrow}^{\beta\mathrm{Mo}}}, \tag{5}$$

$$G_{\downarrow}^{\beta\mathrm{Mo}} = \frac{1}{\omega - \tilde{E}_{\mathrm{Mo},\downarrow} - \frac{w^2}{4} \nu_{+} G_{\downarrow+}^{\alpha\mathrm{Fe}}}, \tag{6}$$

while for spin ↑

$$G_{\uparrow-}^{\alpha\mathrm{Fe}} = \frac{1}{\omega - \tilde{E}_{\mathrm{Fe},\uparrow} - \frac{w^2}{4} G_{\uparrow}^{\beta\mathrm{Mo}}}, \tag{7}$$

$$G_{\uparrow}^{\beta\mathrm{Mo}} = \frac{1}{\omega - \tilde{E}_{\mathrm{Mo},\uparrow} - \frac{w^2}{4} \nu_{-} G_{\uparrow-}^{\alpha\mathrm{Fe}}}, \tag{8}$$

where $\tilde{E}_{\mathrm{Fe},\sigma}$ and $\tilde{E}_{\mathrm{Mo},\sigma}$ are effective Fe and Mo site energies respectively, which include electronic correlation.

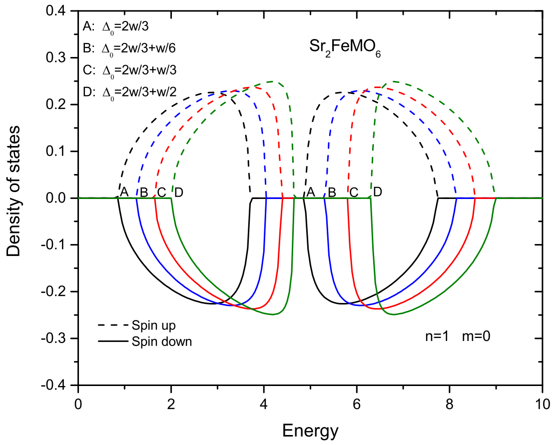

FIG. 2. Total density of states for the $\mathrm{Sr_2FeMO_6}$ system as a function of the energy in the paramagnetic state ($m = 0$) for different values of the transfer energy Δ_0. Here, the electronic correlation parameters are given by $U_{\mathrm{eff}}^{Fe} = 3w$, $U_{\mathrm{eff}}^{\mathrm{Mo}} = w$, and $J^{\mathrm{Mo}} = 0.1w$.

In the ferromagnetic state, it is convenient to define the charge transfer energy (Δ) for ↓ spin electrons,

$$\begin{aligned}\Delta &= \tilde{E}_{\mathrm{Mo},\downarrow} - \tilde{E}_{\mathrm{Fe},\downarrow} \\ &= E_{\mathrm{Mo}} - E_{\mathrm{Fe}} + \tfrac{2}{3} U_{\mathrm{eff}}^{\mathrm{Mo}} \langle n_{\beta,\downarrow}^{\mathrm{Mo}} \rangle - \tfrac{2}{3} U_{\mathrm{eff}}^{\mathrm{Fe}} \langle n_{\alpha,\downarrow}^{\mathrm{Fe}} \rangle,\end{aligned} \tag{9}$$

where $E_{\mathrm{Mo}} - E_{\mathrm{Fe}} = \Delta_0$, Δ_0 being the bare charge transfer energy defined in the uncorrelated case.

It has been shown that the charge transfer energy is quite small in SFMO [8], therefore, $\Delta = 0$ is considered here in order to reproduce the mixed-valence character in $\mathrm{Fe}^{2.5+}$ and $\mathrm{Mo}^{5.5+}$ observed experimentally [23,24]. For this $\Delta = 0$ value, Δ_0 is obtained directly from Eq. (9) since then $\langle n_{\beta,\downarrow}^{\mathrm{Mo}} \rangle = \langle n_{\alpha,\downarrow}^{Fe} \rangle = \frac{n}{2}$ for a general electronic concentration (n), giving $\Delta_0 = 2nw/3$ for the above-mentioned values of the correlation parameters. In particular, for SFMO ($n = 1$) we have $\Delta_0 = 2w/3$.

The total density of states, $\rho(m,\omega,\Delta_0) = \sum_\sigma [\rho_\sigma^{Fe}(m,\omega,\Delta_0) + \rho_\sigma^{\mathrm{Mo}}(m,\omega,\Delta_0)]$, allows us write $n = 3\int_{-\infty}^{E_F} \rho(m,\omega,\Delta_0) d\omega$ to determine the Fermi energy E_F. We calculate the kinetic energy of the conduction electrons $E_{kin}(m,\Delta_0) = 3\int_{-\infty}^{E_F} \rho(m,\omega,\Delta_0)\omega\, d\omega$. In order to obtain the thermodynamical values of $m(T)$ we need to calculate the minimum of the free energy $F = E_{kin}(m,\Delta_0) - TS(m)$, where $S(m) = \ln(2) - \nu_+ \ln(2\nu_+) - \nu_- \ln(2\nu_-)$ is the entropy term of the local spins, consistent with our approximation that these are either up or down. The Curie temperature T_C is determined from $m(T_C) = 0$ [8].

III. RESULTS AND DISCUSSION

In Fig. 2, we show the total density of states for different values of the charge transfer energy Δ_0 in the paramagnetic state ($m = 0$). This figure shows the shift of the density of states and how the gap increases with increasing Δ_0 ($\Delta_0 = 2w/3$ for SFMO). The shift toward higher energies of all bands results from the correlations and increasing Δ_0 according to Eqs. (3) and (4). When Δ_0 increases, the Fe occupation increases while the Mo occupation decreases, so the Fe level is shifted to higher energy due to the correlations according to Eq. (3) (we take

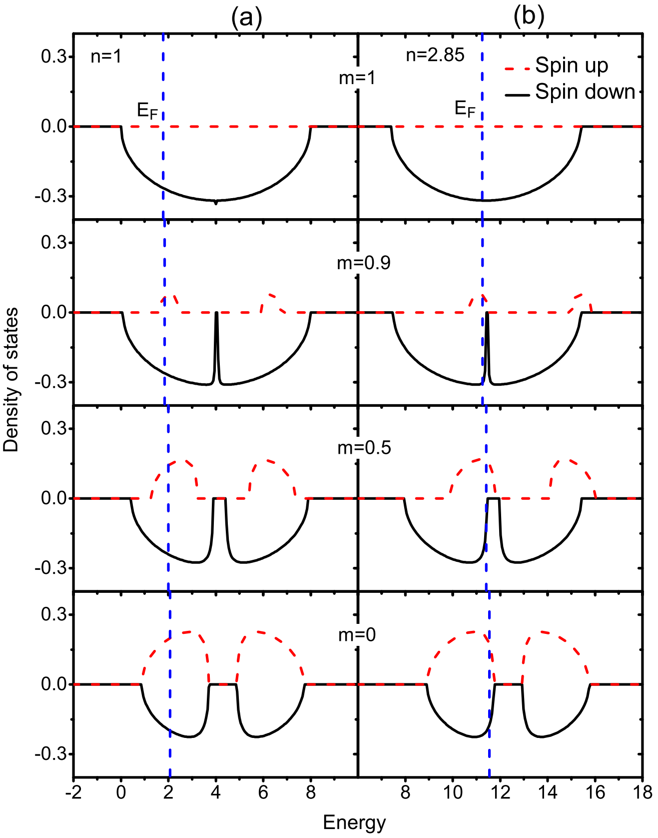

FIG. 3. Evolution of the density of states vs energy ($\Delta_0 = 2nw/3$) for (a) $n = 1.0$ and (b) $n = 2.85$. The electronic correlation parameters are the same as those given in Fig. 2. Vertical dashed lines indicates the Fermi energy E_F.

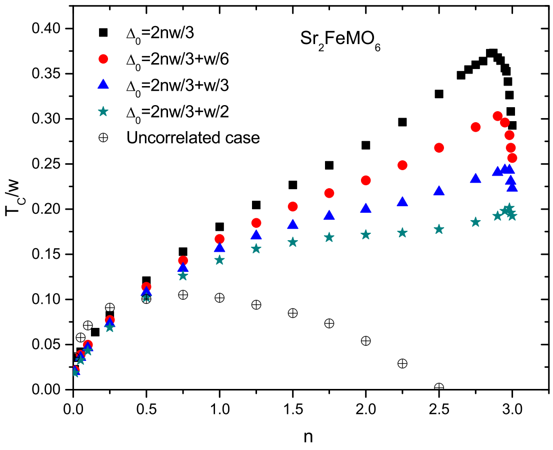

FIG. 4. Variation of the Curie temperature as a function of the band filling in Sr_2FeMO_6 (here, M is a transition metal) for different values of Δ_0; the electronic correlation parameters are the same as in Fig. 2. The T_C without itinerant electron correlations is also included as reference.

$E_{Fe} = 0$) and the Mo level is also shifted upward because of Δ_0, but this increase is less than the change of Δ_0 because the Mo occupation diminishes [according to Eq. (4)]. Fe and Mo levels are both shifted to higher energy, leading to the upward shift of the two bands. In all cases, the effective charge transfer is smaller than Δ_0 but increases with Δ_0, although less than Δ_0. Therefore, the splitting between the two bands increases with Δ_0, but this is smaller than what would occur from Δ_0. The behavior of the DOS is further observed in Fig. 3, where we show the results for the density of states and Fermi energy (E_F) for different values of the magnetization (m). In Fig. 3(a) results for stoichiometric Sr_2FeMoO_6 ($n = 1.0$) are given, and Fig. 3(b) shows results for band filling $n = 2.85$, where the T_C has a maximum as seen in the upper curve of Fig. 4. Here, $\Delta_0 = 2nw/3$ so that in both cases in the F state ($m = 1$) $\Delta = 0$, thus giving a semielliptic down-spin DOS of width $2w$ centered at the energy $4n$. For $m = 1$ we observe that the system retains its half-metallic character with the partially filled Fe-Mo down-spin minority band and unoccupied Mo up-spin states above the Fermi level. Over the whole range $0 < m < 1$ the system loses its half-metallic character and we observe the appearance of up-spin states at E_F because the orientation of localized spin (Fe) changes from (+) to (−). For the paramagnetic state, $m = 0$, we observed a behavior similar to that obtained by E. Carvajal *et al.* [8], which indicates two identical bands separated by a gap. The main difference is the shift to the right observed on the DOS due to the renormalization of the levels by the correlations.

In Fig. 4, we represent T_C/w for different values of Δ_0, as a function of band filling n. Δ_0 and n are considered as parameters in order to generalize the results to a wide variety of ordered double perovskites Sr_2FeMO_6 (M is a transition metal) or even with Fe replaced by another transition metal with different Δ_0 and n. However, we should keep in mind that the correlation parameters could be different from those we used to represent Sr_2FeMoO_6. The upper curve (black squares) corresponds to $\Delta_0 = 2nw/3$, i.e., $\Delta = 0$ (remember that Δ is defined in the F state) for which T_C reaches a fairly high maximum around $n = 2.85$. The uncorrelated case corresponding to $\Delta_0 = 0$ is also included as a reference. For $n = 1$ (Sr_2FeMoO_6) there is a substantial increase of T_C/w due to the correlations between the lower ($\Delta_0 = 0$) and higher points ($\Delta_0 = 2w/3$), which are relevant to reproduce the correct experimental behavior ($\Delta = 0$).

In Fig. 5, we show how T_C/w depends on Δ_0/w for $n = 1$; the value $\Delta_0/w = 2/3$ is shown by a vertical line separating the regions $\Delta > 0$ and $\Delta < 0$. For Δ_0/w large, $\Delta/w > 0$, itinerant electrons are mostly localized on Fe and $T_C/w \to 0$ as in the uncorrelated case without an important effect on T_C. On the other side, $\Delta/w < 0$, more electrons are on Mo sites and T_C/w continues to increase as a result of a Stoner-like mechanism arising essentially from the first two terms in H_c^{Mo} (an exchange splitting stemming from the interaction between ↑ and ↓ electrons). However, this should be taken as a tendency because for large occupation numbers the mean-field treatment of the correlations could be questionable. For this reason we have limited Fig. 5 to $\Delta_0/w > 0.2$. The inset of Fig. 5 shows the linear behavior of Δ as a function of Δ_0.

Now, let us focus on the doped $Sr_{2-y}La_yFeMoO_6$ system. The number of carriers increases by substitution of Sr (divalent) by La (trivalent) as $n = 1 + y$ [10]. To describe this family we keep $\Delta_0 = 2w/3$ as in pure Sr_2FeMoO_6 and vary only $n(y)$. In Fig. 6, we show some results for the DOS for $y = 0.5$ and $y = 1$. In the F state, in comparison with Sr_2FeMoO_6 [Fig. 3(a)]

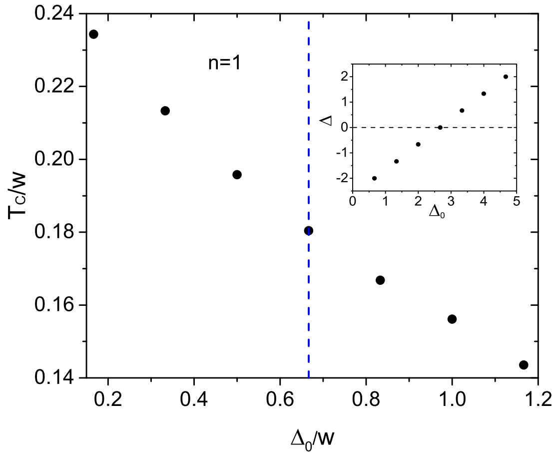

FIG. 5. Variation of the Curie temperature as function of Δ_0/w for the Sr_2FeMoO_6 system. The vertical dashed line separate the regions $\Delta > 0$ and $\Delta < 0$. The inset shows Δ as function of Δ_0.

the DOS now presents a gap in the middle of the band which reflects the fact that $\Delta \neq 0$ due to the correlations and the band filling, while $\Delta = 0$ (no gap) for $y = 0$ ($n = 1$). The doped system retains its half-metallic character because added electrons occupy the spin-down band. We also observe the shift of the bands to higher energy as a result of the renormalization of energy levels by the correlations increasing with increasing carrier concentration.

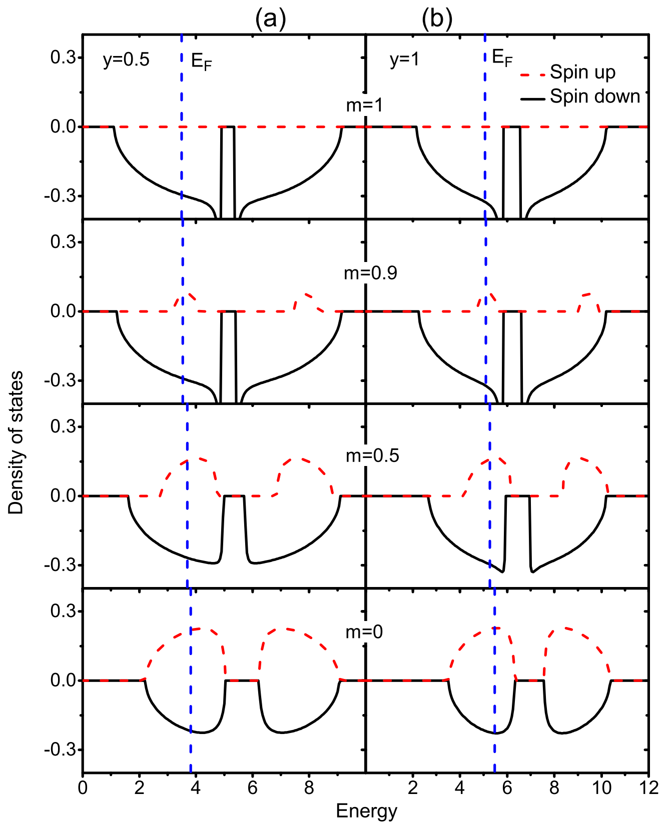

FIG. 6. Density of states as function of energy for different values of La doping (a) $y = 0.5$ and (b) $y = 1$. Vertical dashed lines indicates the Fermi energy E_F.

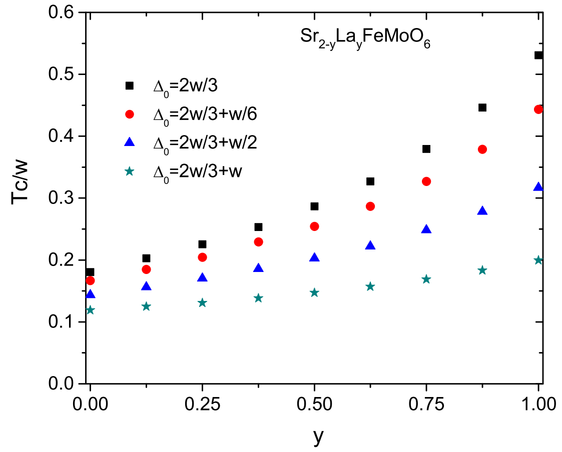

FIG. 7. Curie temperature as function of La doping in the $Sr_{2-y}La_yFeMoO_6$ system for different values of Δ_0; the electronic correlation parameters are the same as in Fig. 2.

In Fig. 7 we present T_C/w as a function of y for $0 \leqslant y \leqslant 1$ as in the experimental results [10]. T_C/w shows an important increase for all values of Δ_0. At first sight, the increase of T_C is in qualitative agreement with experiment [10], but clearly for $\Delta_0 = 2w/3$ relevant for Sr_2FeMoO_6 the rate of increase of T_C/w vs y is by far too large as compared with the experimental results. Much larger values of Δ_0/w would be required, values no longer compatible with the mixed valence character 2.5 for Fe. However, we have to remember that La doping induces disorder between Fe and Mo sites [10], which is detrimental to the Curie temperature T_C. This disorder could be due to Fe ions migrating to Mo sites in order to balance the charge induced by La doping into the cell. Therefore, with disorder the variation of T_C/w vs y will certainly be slower than that obtained here. Including disorder in our approach is possible [7], but we do not know how disorder varies with La doping in these compounds.

In conclusion, we have presented an electronic correlation study within the dynamical mean-field approximation of the double perovskite systems Sr_2FeMO_6 (where M is a transition metal, like Mo or Re) and $Sr_{2-y}La_yFeMoO_6$, where the on-site Hubbard interaction in Fe and Mo sites was taken as $U_{\mathrm{eff}}^{Fe} = 3w$ and $U_{\mathrm{eff}}^{\mathrm{Mo}} = w$ respectively. The electronic correlation (interband and intraband) for Fe and Mo and the charge transfer energy together with the band filling effects play a fundamental role on the behavior of the Curie temperature in both systems. In the Sr_2FeMO_6 compound the Curie temperature has a maximum for $n = 2.85$ and $\Delta_0 = 2nw/3$ and for the $Sr_{2-y}La_yFeMoO_6$ system we obtain that T_C increases with La doping, in qualitative agreement with experimental results.

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