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Model of the interplay of band Jahn-Teller effect with magnetic order mediated by exchange interactions

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A model calculation is presented with the aim to study the interplay between magnetic and structural transitions. The model consists of an orbitally doubly degenerate conduction band and a periodic array of local moments. The band electrons interact with the local spins via the *s-f* interaction. The interaction of the band electrons with phonons is introduced by including band Jahn-Teller (J-T) interaction. The model Hamiltonian, including the above terms, is solved for the single particle Greens function. In doing this an ansatz for self-energy of electrons, which was developed earlier, has been utilized. The quasiparticle density of states (QDOS) and hence the orbital populations are calculated treating the ferromagnetism of local moments in the mean field approximation. The critical value of electron-phonon interaction (G) for the appearance of the band J-T distortion is higher in the ferromagnetic state. The strain appears at a critical temperature (T_s) when G is greater than the critical value. The onset of ferromagnetism at T_C ($<T_s$) arrests the growth of the strain. It is concluded that the magnetization hinders the structural transition. The quasiparticle density of states are presented to interpret these results.

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I. INTRODUCTION

Interplay of order parameters originating from different degrees of freedom of electrons is very relevant in condensed matter. One of the recent interests in this area is related to the mutual influence of band Jahn-Teller (J-T) effect and ferromagnetic order. The former results from the removal of orbital degeneracy and the latter from the lifting of spin degeneracy. The magnetic order can originate either from the same electrons that are involved in the band J-T effect or from the electrons in some other states. The first case corresponds to narrow band solids which are usually described by the twofold degenerate Hubbard model and is applicable to intermetallic compounds. The interplay between the above two order parameters had been considered earlier and it was shown that the magnetic order tends to suppress the spontaneous distortion resulting from charge-lattice interaction. In the present work, we are considering a situation where the electrons involved in J-T splitting and the magnetic order are different. The doped manganites[1,2] and Heusler alloys[3–5] are some of the real systems that represent this case. Doped manganites shows a rich variety of phenomena such as several forms of magnetic, orbital and charge ordering.[6,7] The interesting physics of manganites is due to the dynamics of the d electrons of the Mn ion. In the host material $LaMnO_3$, which is a Mott insulator, there are four electrons per Mn ion. The d orbitals are split by the crystal field in to two, namely the triply degenerate (ignoring the spin) t_{2g} states which are well localized and the doubly degenerate e_g states which are extended and form a doubly degenerate band. Out of the four d electrons, three occupy the t_{2g} states and the remaining electron is in the e_g band. The Mn ion is in Mn^{3+} state. Due to the large Hund's rule coupling in this system, the three t_{2g} electrons have their spins oriented parallel to each other making a localized spin of $S=3/2$. This is again strongly Hund's rule coupled to the e_g electron. Since the e_g is an extended state, the electron in this state can hop from lattice site to lattice site. The hopping combined with Hund's rule coupling is responsible for the long range magnetic order that exists in this system. This is known in literature as the double exchange mechanism. Another way of looking at the system is that there is a localized spin at each lattice site and the band electrons interact with these spins via an intraatomic exchange interaction. This is known in literature as the Kondo-lattice model (KLM). Similar scenario also prevails in Heusler alloy like Ni_2MnGa, where Mn possesses localized moment and the magnetic properties of the host system can be understood from the KLM with the carrier concentration (e_g electrons) of one per Mn atom. When the trivalent rare-earth ion is partly replaced by divalent ions like Ca, Sr, or Ba, the material exhibits CMR properties undergoing transition from the paramagnetic-insulator state to the ferromagnetic-metal one. The localized spin of $S=3/2$ is retained but there is a decrease in the electron concentration in the e_g band. The carrier concentration is less than one per atom. While studying the CMR and the associated magnetic and insulator-metal transitions, it was realized that KLM alone is not sufficient to understand the physics of manganites. It is now accepted that electron-phonon interaction plays an important role.[8–11] These materials crystallize in perovskite structure and the Mn ion has O_6 octahedron as its immediate environment and therefore interacts strongly with the distortions in the octahedron. Obviously, this introduces J-T effect which lifts the degeneracy of the e_g band. The spontaneous distortion associated with the J-T effect exists when the lowering of the band energy is more than the increase in elastic energy due to the strain. The simplest way to describe the band J-T effect is to incorporate the interaction of the e_g electrons with the lattice distortions (phonons) in the KLM model. When this is done, it is pertinent to examine the interplay between the band J-T effect and magnetism in the model system. There are experimental results supporting such an interplay in manganites and in Heusler alloys. It was observed that the J-T distortion in (La-Y)CaMnO$_3$ (Ref. 12) and (La, Pr, Ca) MnO$_3$ (Ref. 13) is reduced in ferromagnetic state. The suppression of the J-T distortion in (Nd,Sm)$_{1/2}$Sr$_{1/2}$MnO$_3$ in ferromagnetic state under high magnetic field has also been reported.[14] The coexistence of the J-T distorted phase and the ferromagnetic phase have been reported in Rh$_2$CoSn.[3] J-T splitting exists in these systems below the transition temperature T_C.

Therefore, in order to study the interplay of structural and magnetic transitions, we consider a model where the band electrons, which are approximated to be *s* electrons in doubly degenerate extended states, interact intra-atomically with a periodic array of localized spins (a Kondo lattice). We provide for the spontaneous lifting of the degeneracy of the band states by including a band J-T interaction. The lifting of the degeneracy is signalled by the appearance of strain. The presence of the long range magnetic order is characterized by the nonzero value of the magnetization. We study, self-consistently, the strain as a function of the J-T coupling constant for different carrier (e_g electron) concentrations and the dependence of the strain on temperature. In the latter case, the magnetization of the local moments which is caused by the exchange interaction between the e_g and t_{2g} electrons (Kondo interaction) determines, decisively, the temperature dependence of the strain.

II. MODEL HAMILTONIAN AND ITS APPROXIMATE SOLUTION

The e_g electrons moving in the doubly degenerate band are described by

$$H_s = \sum_{\alpha=1}^{2}\sum_{ij\sigma}(T_{ij}-\mu\delta_{ij})c^\dagger_{\alpha i\sigma}c_{\alpha j\sigma} = \sum_{\alpha\mathbf{k}\sigma}(\epsilon(\mathbf{k})-\mu)c^\dagger_{\alpha\mathbf{k}\sigma}c_{\alpha\mathbf{k}\sigma}. \tag{1}$$

T_{ij} is the hopping integral for hopping of the electrons from lattice site i to j. $c^\dagger_{\alpha i\sigma}(c_{\alpha i\sigma})$ is the creation(annihilation) operator for an electron in the α-state on the lattice site i with spin σ. $\alpha=1,2$ is the band index. μ is the chemical potential. $\epsilon(\mathbf{k})$ is the band energy related to T_{ij} by

$$T_{ij} = \frac{1}{N}\sum_{\mathbf{k}}\epsilon(\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}. \tag{2}$$

The band electrons interact with the localized spins via the intraatomic exchange interaction of the coupling strength J and this is described by

$$H_{sf} = -J\sum_{j,\alpha}\sigma_{\alpha,j}\cdot\mathbf{S}_j = -\frac{1}{2}J\sum_{\alpha,j\sigma}(z_\sigma S^z_j n_{\alpha j\sigma} + S^{-\sigma}_j c^\dagger_{\alpha j-\sigma}c_{\alpha j\sigma}). \tag{3}$$

σ is the spin of the band electron and $\mathbf{S}$ is the localized spin (total spin of the three t_{2g} electrons). $n_{\alpha j\sigma}$ is the number operator for the electron in the state α at the lattice site j with spin σ. At the outset itself we assume a ferromagnetic interaction ($J>0$). z_σ is a sign factor, $z_\sigma=\delta_{\sigma\uparrow}-\delta_{\sigma\downarrow}$ and $S^\sigma_j=S^x_j+iz_\sigma S^y_j$.

The electron density in the degenerate band couples to the static elastic strain through the J-T interaction. In the case of a tetragonal distortion, this interaction is described by[15–17]

$$H_{JT} = Ge\sum_{\mathbf{k},\sigma}(n_{1\mathbf{k}\sigma}-n_{2\mathbf{k}\sigma}) = Ge\sum_{i\sigma}(n_{1i\sigma}-n_{2i\sigma}). \tag{4}$$

G is the strength of the J-T coupling and e is the lattice strain given by

$$e = \frac{G}{NC_0}\sum_{i\sigma}(\langle n_{1i\sigma}\rangle - \langle n_{2i\sigma}\rangle), \tag{5}$$

where C_0 is the elastic constant. It is clear that H_{JT} tries to create a difference in the occupation of the two degenerate bands. The difference in occupation leads to the building up of the strain. Thus, under suitable conditions, there is a spontaneous splitting of the bands and building up of strain which indicates a structural transition. The building up of the strain however leads to an increase in the lattice elastic energy which is given by

$$H_L = \frac{1}{2}NC_0e^2, \tag{6}$$

where N is the total number of atoms. Since this term is a c number and we are not looking for the ground state whose energy has to be minimum, we leave this term out of our consideration. Then the Hamiltonian of the model system we are considering is

$$H = H_s + H_{sf} + H_{JT}. \tag{7}$$

The model Hamiltonian Eq. (7) obviously cannot be solved exactly. However, in an earlier work,[18] we have proposed, for the Hamiltonian without the J-T term, an approximation scheme, which is reliable in the limit of low carrier concentration. We will exploit that scheme in solving the present model. First, without resorting to any approximation, we can absorb the J-T term into H_s by modifying the band energies for the two bands as

$$\epsilon_\alpha(\mathbf{k}) = \epsilon(\mathbf{k}) + (-1)^\alpha Ge. \tag{8}$$

Then we have

$$\mathcal{H}_s = \sum_{\alpha\mathbf{k}\sigma}(\epsilon_\alpha(\mathbf{k})-\mu)c^\dagger_{\alpha\mathbf{k}\sigma}c_{\alpha\mathbf{k}\sigma} \tag{9}$$

and the total Hamiltonian is given by

$$H = \mathcal{H}_s + H_{sf}. \tag{10}$$

In order to calculate the strain (caused by the structural transition), one has to calculate the one-electron Greens function

$$G_{\alpha\mathbf{k}\sigma}(E) = \langle\langle c_{\alpha\mathbf{k}\sigma};c^\dagger_{\alpha\mathbf{k}\sigma}\rangle\rangle_E = \frac{1}{E-\epsilon_\alpha(\mathbf{k})-\Sigma_{\alpha\sigma}(E)}. \tag{11}$$

That means, one has to calculate the self-energy $\Sigma_{\alpha\sigma}(E)$ of the electron in the presence of H_{sf}. There are some exact results available for the self-energy in certain limiting cases, namely, the zero bandwidth limit for all temperatures[19] and the finite bandwidth but ferromagnetic saturation ($T=0$) limit.[20,21] In addition, using Mori formalism, the result for the second order perturbation theory is also available.[22] We propose an ansatz for the self-energy that reproduces the known limiting results and in addition, satisfies the strong coupling limit. This can be taken care of by making a high energy expansion and evaluating the first four spectral moments.[22] We thus have a self-energy which fulfills (a) the zero bandwidth limit for all temperatures and coupling strengths, (b) $T=0$ limit for all bandwidths and coupling constants, (c) the weak coupling limit ($\mathcal{O}J^2$), and (d) has the correct high energy behavior. The ansatz for $\Sigma_{\alpha\sigma}(E)$ is given by

$$\Sigma_{\alpha\sigma}(E) = -\frac{1}{2}Jm_\sigma + \frac{1}{4}J^2 \frac{a_\sigma G_{\alpha 0}\left(E - \frac{1}{2}Jm_\sigma\right)}{1 - b_\sigma G_{\alpha 0}\left(E - \frac{1}{2}Jm_\sigma\right)}. \qquad (12)$$

Here

$$G_{\alpha 0}(E) = \frac{1}{N}\sum_{\mathbf{k}} G_{\alpha\mathbf{k}}(E) = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{E - \epsilon_\alpha(\mathbf{k})} \qquad (13)$$

$m_\sigma = z_\sigma \langle S^z\rangle$. The ansatz assumes a **k**-independent self-energy. As H_{sf} is a local interaction, the energy dependence of the self-energy is the deciding factor in relation to the electron density of states. The parameters a_σ and b_σ and are fixed by rigorous high energy expansions to fulfill the first four spectral moments:

$$a_\sigma = S(S+1) - m_\sigma(m_\sigma + 1), \quad b_\sigma = b_{-\sigma} = \frac{1}{2}J. \qquad (14)$$

It should be mentioned that this ansatz is valid only in the limit of low carrier density. Since we are interested in simulating systems with low carrier density, it is justified to use the above ansatz. From $G_{\alpha\mathbf{k}\sigma}(E)$ one can obtain the spectral density $S_{\alpha\mathbf{k}\sigma}(E)$ and the density of states $\rho_{\alpha\sigma}(E)$ from the well known relations

$$S_{\alpha\mathbf{k}\sigma}(E) = -\frac{1}{\pi} Im\, G_{\alpha\mathbf{k}\sigma}(E) \qquad (15)$$

$$\rho_{\alpha\sigma}(E) = \frac{1}{N}\sum_{\mathbf{k}} S_{\alpha\mathbf{k}\sigma}(E). \qquad (16)$$

From the knowledge of the density of states, the expectation values can be evaluated:

$$\langle n_{\alpha\sigma}\rangle = \int dE f_-(E)\rho_{\alpha\sigma}(E), \qquad (17)$$

where $f_-(E) = 1/(1+e^{\beta E})$ is the Fermi function with $\beta = 1/kT$. The chemical potential μ is fixed by the constraint

$$n = \sum_{\alpha\sigma} \langle n_{\alpha\sigma}\rangle = \text{const}. \qquad (18)$$

For a given set of the model parameters n, J, S, and G and for a fixed T, the occupancies of both lower and upper subbands for each spin direction is computed self-consistently. After having the self-consistent solution, the lattice strain

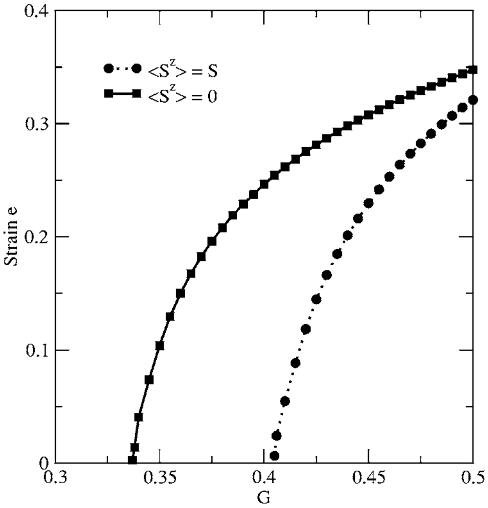

FIG. 1. Lattice strain as a function of electron-phonon coupling constant G at $T=0$ with and without localized magnetization. $n=0.7$, $J=1$, $S=3/2$, and $C_0=1$.

$$e = \frac{G}{C_0}\sum_\sigma (\langle n_{1\sigma}\rangle - \langle n_{2\sigma}\rangle) \qquad (19)$$

is calculated. The average occupation of e_g orbitals $\langle n_{\alpha\sigma}\rangle$ can be numerically obtained using a model density of states for the "free" e_g band:

$$\rho_0(E) = A\sqrt{1 - \left|\frac{E}{D}\right|}\ \ln\left|\frac{D^2}{E^2}\right|, \qquad (20)$$

where A is a normalization constant and D is half the width of free Bloch band. In order to calculate $\langle n_{\alpha\sigma}\rangle$, we require $\langle S^z\rangle$, since this enters into the self-energy. The local moment system is described within the mean field approximation and is represented by Brillouin function. The effective field seen by the local moment is determined by mutual exchange interaction which fixes T_C. Numerical results are given where all the energy parameters are normalized in terms of the free bandwidth ($2D$). Ideally, one should get the magnetization $\langle S^z\rangle$ self-consistently out of the calculation. However, it is a very involved problem. Therefore, we treat it as a parameter and obtain its value at any temperature from the Brillouin function assuming a value for T_C.

Using the above theory, the results for the density of states and the strain are presented in the next section.

III. RESULTS AND DISCUSSION

First we consider the $T=0$ case for two extreme situations of the local magnetization, namely, the paramagnetic ($\langle S^z\rangle = 0$) and the saturated ferromagnetic ($\langle S^z\rangle = S$) state. In Fig. 1 we have plotted the strain as function of the J-T coupling constant G. We find that unless the value of G exceeds a critical value, there is no spontaneous splitting of the orbitally degenerate bands. The splitting of the bands takes place

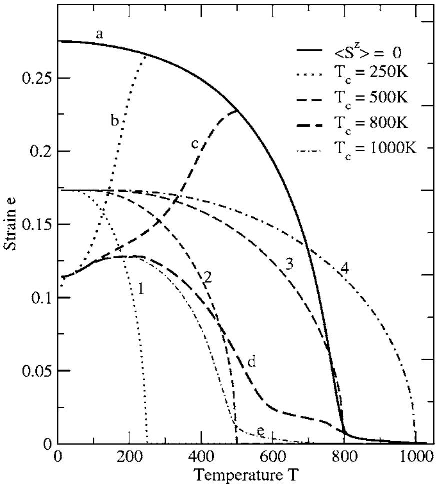

FIG. 2. Lattice strain as a function of temperature for various values of T_c (curves a, b, c, d, and e). $n=0.7$, $J=1$, $S=3/2$, $C_0=1$, and $G=0.42$. Brillouin function is also plotted (curves 1, 2, 3, and 4) in the same figure as a guide for the eye.

and the lower of the split bands is occupied more by the electrons than the upper one in order to lower energy. This is energetically favored only for a sufficiently large G. When G is further increased, the lower of the split bands is more populated and therefore the strain increases as shown in the figure. Though not shown in the figure, the critical value of G also depends on the carrier concentration. Larger is n, smaller is the critical value of G. Another feature which is displayed in Fig. 1, is the role of the magnetization $\langle S^z \rangle$. Critical value of G to induce J-T effect is much higher for the saturated local magnetization situation as compared to that of the paramagnetic situation. With increase of G, it is observed that the gap between the two curves decreases. The difference in the critical value of G appears to be a result of the competition between the mechanisms leading to the lifting of orbital and spin degeneracies of the e_g state. In the ferromagnetic situation, the effective field lifts the spin degeneracy so that stronger electron lattice interaction is necessary for the strain to appear. As the strain becomes larger, the energy gain by the J-T distortion dominates over the energy gain by lifting of the spin degeneracy. So the influence of magnetization becomes less important. The interplay becomes more interesting when the energy gain due to the two mechanisms is comparable.

In order to examine this interplay in more detail, we study the temperature dependence of the strain in Fig. 2. The structural transition temperature T_s is the temperature at which the strain goes to zero. We choose the parameters such that $T_s=800$ K. Then we study the effect of magnetization on strain by varying T_C such that (i) $T_C < T_s$, (ii) $T_C \approx T_s$, and (iii) $T_C > T_s$. Figure 2 displays the T dependence of the strain (curves a, b, c, d, and e) and the magnetization (which is a Brillouin function for a given T_C) for different T_C's (curves 1, 2, 3, and 4). Whatever is T_C, at $T=0$, $\langle S^z \rangle = S$. Therefore, the effect of the magnetization on the strain is independent of T_C and leads to a maximum decrease of strain. As T_C increases, the strain goes up with increasing T and the rate of increase is higher for lower T_C so long as $T_C < T_s$. Therefore, there always appears a peak in the curves. When $T_C \approx T_s$, the peak is very faint and the strain becomes very small well before T_s is reached. For $T_C > T_s$, the strain is nonzero only when T is much lower than T_C (curve e of Fig. 2).

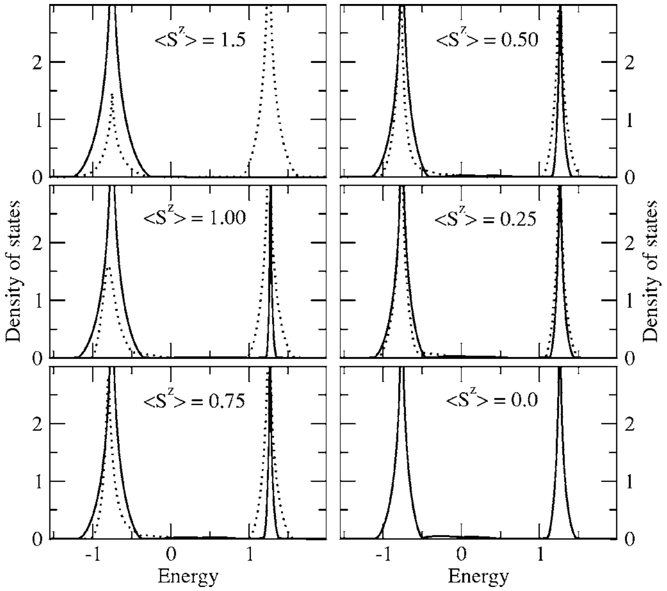

FIG. 3. Quasiparticle density of states as a function of energy for various values of localized magnetization $\langle S^z \rangle$ in the absence of Jahn-Teller distortion, i.e., for $G=0$. Full line for spin up and dotted line for spin down. $J=1$ and $S=3/2$.

It is clear that at $T=0$, the presence of magnetization causes a redistribution of electrons between the orbital levels by creating a population difference between the spin levels. Such redistribution is the cause of suppression of strain. As T increases, the spin level occupancies tend to equalize and that polarizes the orbital levels further resulting in the increase in the strain compared to its $T=0$ value. Since for smaller T_C the magnetization decreases faster with increasing T, the increase in strain is also faster. For $T_C > T_s$, due to the choice of parameters, as expected, there is no strain between $T_s < T < T_C$. When T is much lower than T_C, the occupancy of the spin levels is stabilized and the system can lower energy by further redistribution of electrons between the orbital states. That is why the strain is finite for T much less than T_C (curve e of Fig. 2). The results obtained are interpreted with the help of the quasiparticle density of states (QDOS). Before discussing the results of the full problem, to fix up a reference for further discussion, we want to present in Fig. 3, the QDOS for the case of a pure KLM, that is, for the case of $G=0$. The QDOS consists of two subbands for each spin direction separated by an energy of the order of $\frac{1}{2}J(2S+1)$. The separation of the bands is independent of T but the spectral weights of these subbands, however, depend on T through the value of $\langle S^z \rangle$. For example, at $T=0$ ($\langle S^z \rangle = S$), the spectral weight of the upper subband for $\uparrow$-states is zero. The reason for this is easy to understand. At $T=0$, the local moment system is saturated. Therefore, for an $\uparrow$-electron there is no chance to spin-flip by involving a corresponding spin-flip of the local moment system. That means, at $T=0$, as far as the $\uparrow$-electron is concerned, only

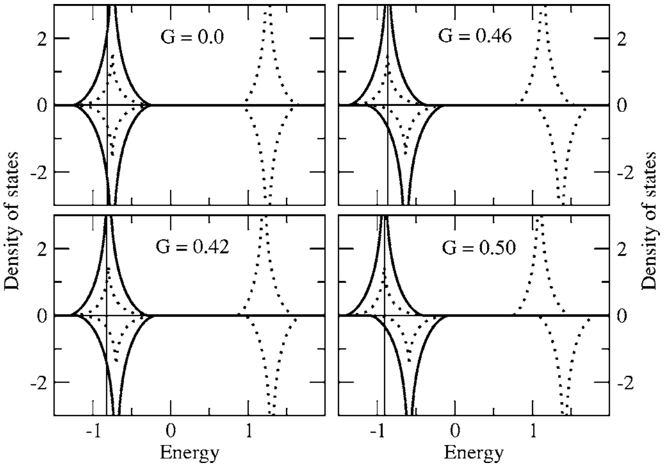

FIG. 4. Quasiparticle density of states (for lower subband (α=1) in the positive half of the frame and for upper subband (α=2) in the negative half of the frame) as a function of energy for various values of electron-phonon coupling constant G. Full line for spin up and dotted line for spin down. Thin vertical line shows the position of the chemical potential. n=0.7, J=1, S=3/2, C_0=1, $\langle S^z \rangle = S$, and T=0.

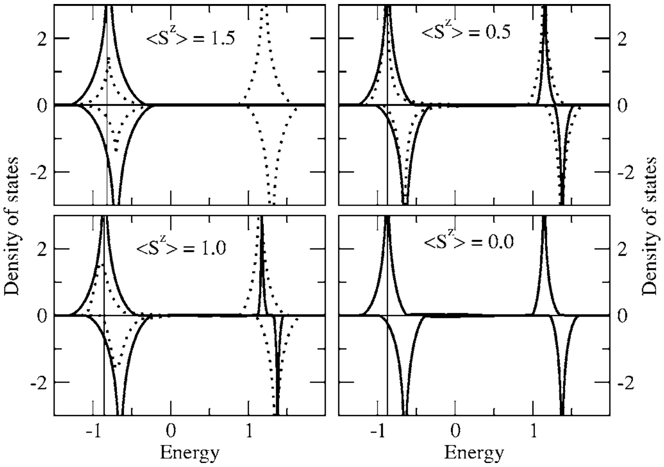

FIG. 5. Quasiparticle density of states (for lower subband in the positive half of the frame and for upper subband in the negative half of the frame) as a function of energy for various values of localized magnetization $\langle S^z \rangle$. Full line for spin up and dotted line for spin down. Thin vertical line shows the position of the chemical potential. n=0.7, J=1, S=3/2, C_0=1, T=0, and G=0.42.

the Ising part of H_{sf} operates resulting simply in a rigid shift of QDOS. As we see from Fig. 3, the spectral weight of the ↓-states in the lower subband is finite. This is because, for a ↓-electron, even at T=0, spin-flip is possible. Furthermore, when a ↓-electron flips its spin, it lands as an ↑-electron. Therefore the nonzero QDOS of the ↓-electron should be in the same energy region as that of ↑-electron. For a ↓-electron there is another possibility. It can have repeated magnon emission and absorption. That is, in a sense, it propagates in the lattice dressed by a cloud of magnons. This is a stable quasiparticle, which we call the magnetic polaron. Obviously, at T=0, there is no possibility of magnetic polaron for ↑-electron. As T increases ($\langle S^z \rangle$ decreases), the spin-flip processes are allowed for both the spin directions and therefore the spectral weights in both the subbands are nonzero for both the spin directions. At $T = T_C$ ($\langle S^z \rangle = 0$), the spectral weights of ↑- and ↓-states in the two subbands become equal as it should be. We note the asymmetry with respect to the center of the free band. This originates from the renormalization of the atomic levels by the s-f interaction.[19]

Now we consider the further splitting of these bands due to the J-T effect. That is, when the degeneracy of the e_g band is lifted due to the J-T effect, each of the subbands of Fig. 3 for each spin direction discussed above is again split into two as shown in Fig. 4. Noting the position of the chemical potential, we see that the upper subbands for both values of α can be ignored since they are never populated. Only we have to keep in mind the change in their spectral weights. From now on, when we speak of subbands they are the two e_g bands, corresponding to α=1,2 as displayed in the positive and negative halves of the frame.

We want to understand the dependence of the strain on the coupling constant G and the influence of $\langle S^z \rangle$. In Fig. 4, we take the case of saturation ($\langle S^z \rangle = S$). When G is less than the critical value, the two e_g bands are degenerate. As G approaches the critical value of 0.42, there is a slight splitting of the two subbands and the difference in their population becomes nonzero. At the same time, it should be noticed that the position of both the subbands shifts to lower energy, so that, on the whole, the energy of the system is lowered by the splitting. For a small increase in G, the splitting increases and the increase in strain is very large. Further, the shifting of the subbands to lower energy is also large so that the energy of the system is much lower. Any further increase in G does not have much effect on the quasiparticle spectrum anymore which means the strain saturates. It should be emphasized that the strain is not introduced by hand but comes self-consistently out of the model.

In Fig. 5 we now fix the value of G at 0.42, so that the model prefers the J-T split situation and look at the influence of $\langle S^z \rangle$. At saturation ($\langle S^z \rangle = S$), the spectral weight of ↑-subband is such that the α=1 subband is slightly more populated compared to the α=2 subband. As a result, a small strain appears. As $\langle S^z \rangle$ decreases, this spectral weight is modified in such a way that the occupation of the α=1 subband is more than that of the α=2. This results in an increase of the strain with T as depicted in Fig. 2. This trend continues until $\langle S^z \rangle = 0$ and at that point, the strain is as if there is no exchange interaction in the model. In short, the effect of magnetization is to hinder J-T splitting.

In order to examine the interplay of magnetization and the strain as a function of T, it is necessary to include the temperature variation of both the strain and the magnetization. Therefore, we consider a specific case of T_C=250 K and T_s=800 K and the corresponding QDOS at different temperature are displayed in Fig. 6. Starting from T=0, the α =1 subband occupation increases as T increases up to T_C. Above T_C, the situation is reversed and both the α subbands are equally occupied at T_s. Therefore, the maximum of strain occurs at T_C as shown in curve b of Fig. 2.

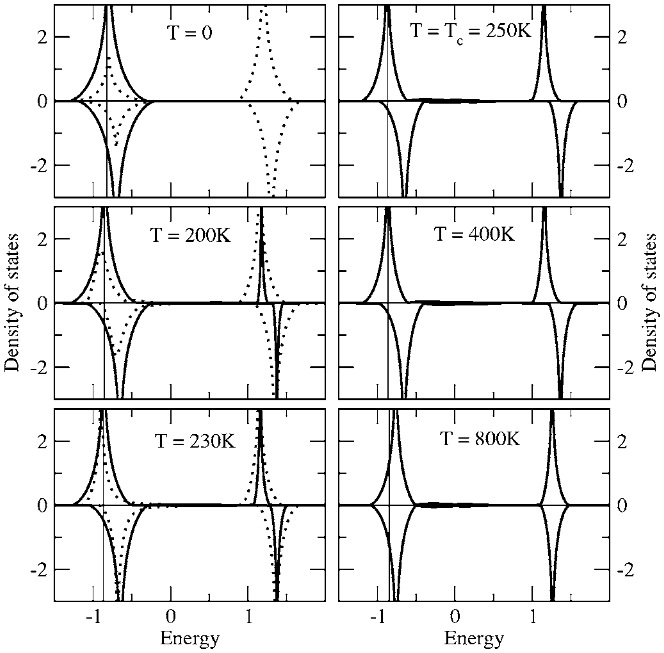

FIG. 6. Quasiparticle density of states (for lower subband in the positive half of the frame and for upper subband in the negative half of the frame) as a function of energy for various values of temperature T. Full line for spin up and dotted line for spin down. Thin vertical line shows the position of the chemical potential. $n=0.7$, $J=1$, $S=3/2$, $C_0=1$, and $G=0.42$.

IV. CONCLUSIONS

The model Hamiltonian is solved by first absorbing the J-T term into the band electron term and then utilizing an interpolation ansatz for the self-energy. The band splitting and through it the strain in the lattice due to J-T interaction has been determined self-consistently. The strain as a function of the coupling constant at $T=0$ is studied with and without the presence of local moment ordering. It is found that a minimum value of G is required for the strain to appear. This critical G is larger if the local moments are ordered or alternately if there is an external magnetic field. The temperature dependence of the strain is studied by assuming different values for the magnetic transition temperature. The study indicates that there is a strong interplay between the magnetic and structural transitions. It is observed that the growth of the strain appearing at T_s ($>T_C$) is arrested with the onset of ferromagnetism and tends to a lower value determined by the magnetization at $T=0$. This means the removal of spin degeneracy is not conducive to the removal of orbital degeneracy. The results are explained on the basis of the QDOS. The basic ingredients of the model are the band J-T effect, long range magnetic order and their mutual interaction. The possibility of different hopping between the degenerate bands is not considered for simplicity and therefore the results correspond to large J-T effect. The interorbital hopping, which is sometimes considered, would remove partially the degeneracy of the state. Also the magnetism which should evolve within the model is treated as a parameter. The detailed comparison with experiment is therefore not attempted. However, the general trends of the results related to suppression of J-T strain and coexistence of two phases are in tune with the experimental[12–14] observations in a Ca-doped manganite and Heusler alloy. The calculation is based on the ansatz used for self-energy which is valid only in the limit of low charge carrier concentration. If this needs to be relaxed, the interaction among the band electrons has to be taken into account and naturally the ansatz for the self-energy has to be modified.

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