Magnon-phonon effects in ferromagnetic manganites

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A model is presented for the magnon-phonon interaction in three-dimensional cubic ferromagnetic systems. The Heisenberg Hamiltonian for localized spins is used. The calculated magnon and phonon dampings are compared with the experiments and good agreement is found. It is estimated that there is a significant broadening in the magnon linewidth at the end of the zone and that the phonon linewidth is not affected by this mechanism. The modified magnon spectrum is also evaluated and compared to experimental measurements. It is found that the model predicts softening of the magnon mode at the end of the zone consistent with the experiments. The contribution from both Mn and O atoms is included. The developed model can be applied to systems with reduced dimensions and systems with different than cubic symmetry.

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I. INTRODUCTION

Spin waves have been studied extensively in magnetic systems. The theory is designed to investigate the ground state and the low-lying excitation states of a system with localized coupled spins.[1] In insulating ferromagnets the spin waves (or magnons) are usually well defined through the entire Brillouin zone and studying the magnon dispersion relations can provide useful information about the material. A suitable description is the Heisenberg Hamiltonian with nearest-neighbor exchange coupling constant.

Ferromagnets of the type $A_{1-x}B_x\mathrm{MnO}_3$ (manganite perovskites), where A is a rare earth and B is an alkaline earth, can reach different states by varying A and B.[2] The theoretical basis for understanding the manganites is the so-called double-exchange (DE) model. This is a Kondo lattice model with an exchange constant J in the limit of infinite J.[3] Some inelastic neutron scattering measurements suggest that the spin waves can be mapped with a nearest-neighbor Heisenberg Hamiltonian.[4] An approximate spin-wave theory found that the DE model in the infinite-J limit and the nearest-neighbor Heisenberg model are equivalent, and that the latter model is independent of the concentration and the spin of the carriers.[5] The dispersions can be reproduced very well for those manganites that have relatively high T_C and relatively low residual resistivity ρ.

Recent inelastic neutron scattering measurements show that new effects are seen in manganites with lower T_C and higher resistivity ρ.[6,7] The result is that a large magnon broadening and softening are observed at the end of the zone at low temperatures. The large magnon linewidth cannot be reproduced by the single DE model, which means that additional contributions have to be considered. The experiments suggest that the onset of the linewidth broadening and softening of the mode appear when the magnon dispersion crosses the longitudinal optical branch of the phonons. Thus, the most probable cause of the anomalous broadening has lattice character and the interaction between the magnetic excitations and the lattice excitations needs to be considered explicitly.

In this paper we will describe a model that governs the interaction between magnons and phonons. A generic model was proposed in Ref. 8, but no explicit form of the Hamiltonian was given and no specific calculations were presented. In principle, the coupling between magnetic moments and lattice can modify the spin waves in two different ways. One way is that the anisotropy of the spin waves can be affected through mixing with the phonons. The other way is when there is a significant magnetoelastic interaction or magnon-phonon coupling. The latter way is the subject of this work. We try to answer the question if the coupling between spin and lattice degrees of freedom are responsible for the observed effects[7] by presenting a simple model and evaluating the damping and the energy dispersion of the magnons.

The paper is organized as follows. In Sec. II the Hamiltonian and the explicit matrix elements are written. We also discuss different limits. In Sec. III the magnon and phonon broadenings are estimated and a comparison with the experimental results for the ferromagnetic manganites is given. In Sec. IV the renormalized magnon dispersion is estimated and compared with experimental findings. Section V is left for conclusions, where we discuss the model and its possible generalizations.

II. FORMALISM FOR THE MAGNON-PHONON COUPLING

Studying the spin dynamics of materials is very important because it gives insight into the underlying physics of the compounds. It has been measured that for several manganites at dopings $x=[0.15,0.5]$ the spin dynamics throughout the Brillouin zone is equivalent to a nearest-neighbor Heisenberg ferromagnet.[4] In this doping regime the compounds are ferromagnetic metals and are described by the double-exchange model, which accounts for the strong ferromagnetic coupling between the itinerant e_g and localized t_{2g} carriers. Furukawa[5] argued that the result is consistent with the double-exchange model. He showed that starting from the DE model the material behaves like a nearest-neighbor Heisenberg ferromagnet and the stiffness constant reflects the itinerant nature of the carriers. According to Ref. 5 in the limit of infinite double-exchange constant J_H, the stiffness

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constant is found to be $D=t(\mathbf{R}_i-\mathbf{R}_j)a^2/(2S)\Sigma_{\mathbf{k}}f_{\mathbf{k}}\cos k_x a$, where $f_{\mathbf{k}}$ is the Fermi occupation number and $t(\mathbf{R}_i-\mathbf{R}_j)$ is the hopping integral in a single e_g band. This suggests that in order to study the problem of coupling between magnetic and lattice excitations for this doping regime, it is correct to assume that there are ''effective'' magnetic moments located on sites i,j coupled by a ferromagnetic Heisenberg interaction. Also the interaction constant $J(\mathbf{R}_i-\mathbf{R}_j)$ can be taken to be proportional to the hopping integral t.[9] Therefore, the Hamiltonian is

$$H=-\sum_{i,j} J(\mathbf{R}_i-\mathbf{R}_j)\mathbf{S}_i\cdot\mathbf{S}_j. \tag{1}$$

Here $\mathbf{R}_{i,j}$ stands for the positions of the Mn magnetic ions, $\mathbf{S}_{i,j}$ is the ''effective'' localized spin, and $J(\mathbf{R}_i-\mathbf{R}_j)\sim t(\mathbf{R}_i-\mathbf{R}_j)$ is the exchange interaction constant. The direct overlap integral t between nearest-neighbor Mn sites in the manganites is zero since due to the perovskite lattice the Mn atoms are bridged by an O atom. Therefore, $t(\mathbf{R}_i-\mathbf{R}_j)$ is estimated by a second-order perturbation with respect to the electron transfer between Mn $3d$ and O $2p$ orbitals: V_{pd}.[10] Thus, $t=V_{pd}^2/\Delta$ where V_{pd} is the overlap integral in Slater-Koster terms[11] and $\Delta=|\epsilon_p-\epsilon_d|$ is the energy difference between the occupied O $2p$ and unoccupied $3d$ levels. It is estimated by photoemission experiments that for the manganites $t\sim 0.72$ eV.[12] Furthermore, the charge transfer energy Δ is measured to be about 4 eV.[13] Thus, one finds for the pd transfer integral $V_{pd}\sim 1.7$ eV.

There are two types of magnon-phonon interactions. One type is to consider a form of Hamiltonian that is bilinear in the magnon and phonon operators.[14,15] This kind is responsible for the mixing (or hybridization) of the magnon and phonon modes and it does not cause the broadening. If hybridization were significant, this would affect both magnon and phonon dispersions through mixing of the excitations. The experiments[7] show that the phonon linewidth hardly changes and the magnon and phonon excitations exist separately through the whole zone. The effect of hybridization was calculated in the 1970s and 1980s for many rare-earth materials.[14,15]

Another way of looking at the problem is when the scattering of a magnon is done with an emission or absorption of a phonon. In this case the coupling manifests itself through the distortion of the lattice. Indeed, studies show the importance of the fact that conduction electrons strongly couple to lattice distortions in the manganites.[16] To introduce the phonons in the picture the magnetic ions are allowed to vibrate around their equilibrium position:

$$\mathbf{R}_i=\mathbf{R}_i^0+\mathbf{u}_i, \tag{2}$$

$$\mathbf{u}_i=\sum_{\mathbf{Q}} X_{\mathbf{Q}}\hat{\eta}_{i,\mathbf{Q}}e^{i\mathbf{Q}\cdot\mathbf{R}_i^0}A_{\mathbf{Q}}, \tag{3}$$

$$X_{\mathbf{Q}}=\sqrt{\frac{\hbar}{2NM\omega_{\mathbf{Q}}}}, \tag{4}$$

$$A_{\mathbf{Q}}=b_{-\mathbf{Q}}^{\dagger}+b_{\mathbf{Q}}, \tag{5}$$

where $\mathbf{R}_i^0$ is the equilibrium positions of the ions on lattice sites i, $\mathbf{u}_i$ is a small displacement, $\hat{\eta}_{\mathbf{Q}}$ is the polarization vector, N is the number of ions, M is the mass of one ion, and $b_{-\mathbf{Q}}^{\dagger}$ and $b_{\mathbf{Q}}$ are the phonon creation and anihilation operators, respectively. The phonon operator is denoted by $A_{\mathbf{Q}}$. The next step is to expand the exchange coupling constant $J(\mathbf{R}_i-\mathbf{R}_j)=\beta V_{pd}^2/\Delta$ around the equilibrium positions. β denotes the numerical factor $\Sigma_{\mathbf{k}}f_{\mathbf{k}}\cos k_x a/4S^2$. In this way one obtains up to first order in the displacements and for a unit volume

$$H=H_0+H', \tag{6}$$

$$H_0=-\sum_{ij} J(\mathbf{R}_i^0-\mathbf{R}_j^0)\mathbf{S}_i\cdot\mathbf{S}_j, \tag{7}$$

$$\begin{aligned}H'=2\beta\frac{V_{pd}}{\Delta}\sum_{ij,\mathbf{Q}}\{&X_{\mathbf{Q}}^{Mn}\hat{\eta}_{i,\mathbf{Q}}\cdot\nabla V_{pd}(\mathbf{R}_i-\mathbf{R}_l)e^{i\mathbf{Q}\cdot\mathbf{R}_i^0}\\&-X_{\mathbf{Q}}^{Mn}\hat{\eta}_{j,\mathbf{Q}}\cdot\nabla V_{pd}(\mathbf{R}_l-\mathbf{R}_j)-X_{\mathbf{Q}}^{O}\hat{\eta}_{l,\mathbf{Q}}\cdot[\nabla V_{pd}(\mathbf{R}_i-\mathbf{R}_l)\\&+\nabla V_{pd}(\mathbf{R}_l-\mathbf{R}_j)]e^{i\mathbf{Q}\cdot\mathbf{R}_l^0}\}A_{\mathbf{Q}}\mathbf{S}_i\cdot\mathbf{S}_j,\end{aligned} \tag{8}$$

where the two nearest-neighbor Mn atoms at site i and site j are taken to be inequivalent and the O atom is in the middle between them at $\mathbf{R}_l$. The gradient of V is evaluated at equilibrium. The O ion appears because the overlap integral V_{pd} depends on the relative distance between the Mn and O positions.

The unperturbed Hamiltonian can be diagonalized by different approaches.[1] The Dyson-Maleev transformation is chosen here: $S_{i,j}^{\dagger}=\sqrt{2S}a_{i,j}$, $S_{i,j}^{-}=\sqrt{2S}a_{i,j}^{\dagger}$, $S_{i,j}^{z}=S-a_{i,j}^{\dagger}a_{i,j}$. Considering only nearest neighbors, $\delta=\mathbf{R}_i^0-\mathbf{R}_j^0$, the Hamiltonian H_0 and the energy of the magnetic excitations after a Fourier transformation are obtained to be

$$H_0=\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}, \tag{9}$$

$$\epsilon_{\mathbf{k}}=2S\sum_{\delta} J(\delta)[1-\gamma_{\mathbf{k}}(\delta)], \tag{10}$$

where $a_{\mathbf{k}}$ denotes the magnon operator and $\gamma_{\mathbf{k}}(\delta)=e^{i\mathbf{k}\cdot\delta}$. For a cubic crystal in the nearest-neighbor approximation $J(\delta)$ is replaced by an overall constant J_0.[1] In the limit of small wave vectors the energy dispersion is quadratic with a stiffness constant $D=2SJ_0a^2$. Thus, the excitations are isotropic and gapless. In further estimates we take the experimental values cited in Ref. 7: $D=0.165$ eV Å^2, stiffness constant, and $a=3.86$ Å lattice parameter.

Next, we consider H' which describes the interaction between the localized spins and the phonons. Both type of ions Mn and O contribute to the magnon-phonon coupling. Special attention should be given to the gradient of the pd overlap integral. Using the expression for V_{pd} in Ref. 11 the symmetry of the p and d functions is such that the derivative of the exchange constant points along the lattice axis:

$$\nabla V_{pd}(\mathbf{R}_i-\mathbf{R}_l)=q_0\tilde{V}(\delta)\hat{\delta} \tag{11}$$

Here q_0 is the Slater coefficient describing the exponential decrease of the functions and $\hat{\delta}=(\mathbf{R}_i^0-\mathbf{R}_j^0)/|\mathbf{R}_i^0-\mathbf{R}_j^0|$. q_0 is of the order of 1 Å^{-1}. $\tilde{V}(\delta)$ is of the order of the original integral $V(\delta)$ and for the purposes of these calcuations they will be taken to be equal.

The interaction Hamiltonian conserves the spin quantum number. The form in Eq. (8) was obtained for a cubic symmetry and can be written explicitly

$$H'=\sum_{\mathbf{k},\mathbf{Q}}[M^{Mn}_{\mathbf{k},\mathbf{Q}}a^\dagger_{\mathbf{k}+\mathbf{Q}}a_{\mathbf{k}}+M^{O}_{\mathbf{k},\mathbf{Q}}a^\dagger_{\mathbf{k}+\mathbf{Q}/2}a_{\mathbf{k}}]A_{\mathbf{Q}}, \tag{12}$$

$$M^{Mn}_{\mathbf{k},\mathbf{Q}}=2i\beta\frac{V_{pd}^2}{\Delta}\sum_{\mathbf{k},\mathbf{Q}}X^{Mn}_{\mathbf{Q}}(\hat{\eta}_Q^{Mn_1}+\hat{\eta}_Q^{Mn_2})\hat{\delta}[\sin(\mathbf{k}+\mathbf{Q})\cdot\mathbf{a}-\sin\mathbf{k}\cdot\mathbf{a}-\sin\mathbf{Q}\cdot\mathbf{a}], \tag{13}$$

$$M^{O}_{\mathbf{k},\mathbf{Q}}=-4i\beta\frac{V_{pd}^2}{\Delta}\sum_{\mathbf{k},\mathbf{Q}}X^{O}_{\mathbf{Q}}\hat{\eta}^O_{\mathbf{Q}}\cdot\hat{\delta}[\sin(\mathbf{k}+\mathbf{Q}/2)\cdot\mathbf{a}-\sin\mathbf{k}\cdot\mathbf{a}-\sin\mathbf{Q}/2\cdot\mathbf{a}]. \tag{14}$$

The lattice constant $\mathbf{a}$ and the unit vector $\hat{\delta}$ change only in the positive direction of the x, y, and z axes.

III. DAMPING OF THE MAGNONS AND PHONONS

Since the form of the interaction Hamiltonian has been determined, one can analyze it by using Green's functions technique. It is evident that there is an analogy between this type of coupling and the usual electron-phonon coupling—the electron operators which are fermions are substituted with boson operators for the magnons. The difference is that here one takes into account the magnetic ordering of the system. Thus, the bosonic operators $a_{\mathbf{k}}$ for the elementary magnetic excitation are introduced, and the coupling is between two bosonic fields. While in the case of electron-phonon interaction, the coupling is between fermionic and bosonic fields.

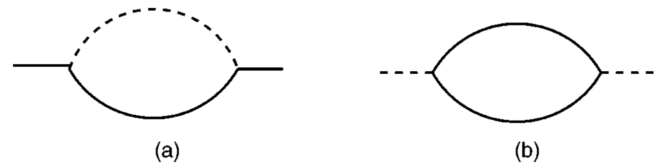

FIG. 1. Self-energy diagrams of the first-order magnon-phonon coupling for (a) magnons, and (b) phonons.

The following Green's functions for the magnons can be defined:

$$G(\mathbf{k},\tau)=-\langle T_\tau a_{\mathbf{k}}(\tau)a^\dagger_{\mathbf{k}}(0)\rangle, \tag{15}$$

$$\tilde{G}(\mathbf{k},\tau)=-\langle T_\tau a^\dagger_{\mathbf{k}}(\tau)a_{\mathbf{k}}(0)\rangle, \tag{16}$$

$$D(\mathbf{Q},\tau)=-\langle T_\tau A_{\mathbf{Q}}(\tau)A_{-\mathbf{Q}}(0)\rangle. \tag{17}$$

The lowest-order perturbation theory is applied to determine the damping of the magnetic excitations. The unperturbed Green's functions are

$$G^0(\mathbf{k},\tau)=\frac{1}{ik-\epsilon_{\mathbf{k}}}, \tag{18}$$

$$\tilde{G}^0(\mathbf{k},\tau)=-\frac{1}{ik+\epsilon_{\mathbf{k}}}, \tag{19}$$

$$D^0(\mathbf{Q},\tau)=-\frac{2\omega_{\mathbf{Q}}}{\omega^2+\omega^2_{\mathbf{Q}}}, \tag{20}$$

where $D^0(\mathbf{Q},\tau)$ is the one for the phonons. The self-energy diagrams for the magnons and phonons are given in Fig. 1. The imaginary part of the self-energy of the magnons is a measure of the damping: $-\mathrm{Im}\,\Sigma(\mathbf{k})=\hbar/2\tau$. The lowest-order perturbation expansion reads

$$\begin{aligned}-\mathrm{Im}\,\Sigma(\mathbf{k})=\pi\sum_{\mathbf{Q}}&|M^{Mn}_{\mathbf{k},\mathbf{Q}}|^2\{(N_{\omega_{\mathbf{Q}}}-N_{\epsilon_{\mathbf{k}+\mathbf{Q}}})[\delta(\epsilon_{\mathbf{k}}+\hbar\omega_{\mathbf{Q}}-\epsilon_{\mathbf{k}+\mathbf{Q}})-\delta(\epsilon_{\mathbf{k}}-\hbar\omega_{\mathbf{Q}}+\epsilon_{\mathbf{k}+\mathbf{Q}})]+(1+N_{\omega_{\mathbf{Q}}}-N_{\epsilon_{\mathbf{k}+\mathbf{Q}}})[\delta(\epsilon_{\mathbf{k}}-\hbar\omega_{\mathbf{Q}}\\&-\epsilon_{\mathbf{k}+\mathbf{Q}})-\delta(\epsilon_{\mathbf{k}}+\hbar\omega_{\mathbf{Q}}+\epsilon_{\mathbf{k}+\mathbf{Q}})]\}+|M^O_{\mathbf{k},\mathbf{Q}}|^2[(N_{\omega_{\mathbf{Q}}}-N_{\epsilon_{\mathbf{k}+\mathbf{Q}/2}})][\delta(\epsilon_{\mathbf{k}}+\hbar\omega_{\mathbf{Q}}-\epsilon_{\mathbf{k}+\mathbf{Q}/2})-\delta(\epsilon_{\mathbf{k}}-\hbar\omega_{\mathbf{Q}}+\epsilon_{\mathbf{k}+\mathbf{Q}/2})]\\&+(1+N_{\omega_{\mathbf{Q}}}-N_{\epsilon_{\mathbf{k}+\mathbf{Q}/2}})[\delta(\epsilon_{\mathbf{k}}-\hbar\omega_{\mathbf{Q}}-\epsilon_{\mathbf{k}+\mathbf{Q}/2})-\delta(\epsilon_{\mathbf{k}}+\hbar\omega_{\mathbf{Q}}+\epsilon_{\mathbf{k}+\mathbf{Q}/2})],\end{aligned} \tag{21}$$

$$N_{\omega_{\mathbf{Q}}}=\frac{1}{e^{\beta\hbar\omega_{\mathbf{Q}}}-1}, \tag{22}$$

$$N_{\epsilon_{\mathbf{k}}}=\frac{1}{e^{\beta\epsilon_{\mathbf{k}}}-1}, \tag{23}$$

where $M_{\mathbf{k},\mathbf{Q}}$ stands for the matrix elements in Eqs. (13) and (14).

Now let's look at the different limits. It is instructive to consider the small-wave-vector limit first, because one is able to obtain simple expressions. In this case $\epsilon_{\mathbf{k}}=Dk^2$ and the longitudinal acoustic phonons with $\omega_{\mathbf{Q}}=sQ$ are taken. The δ functions give the limits of the integration. The matrix elements are expanded with respect to small wave vectors:

$$M^{Mn}_{\mathbf{k},\mathbf{Q}}=-8Si\beta\frac{V^2_{pd}}{\Delta}X^{Mn}_{\mathbf{Q}}\hat{\eta}^{Mn}_{\mathbf{Q}}\cdot\hat{\delta}[(\mathbf{k}\cdot\mathbf{a})^2(\mathbf{Q}\cdot\mathbf{a})+(\mathbf{k}\cdot\mathbf{a})\times(\mathbf{Q}\cdot\mathbf{a})^2], \tag{24}$$

$$M^{O}_{\mathbf{k},\mathbf{Q}}=8Si\beta\frac{V^2_{pd}}{\Delta}X^{O}_{\mathbf{Q}}\hat{\eta}^{O}_{\mathbf{Q}}\cdot\hat{\delta}[(\mathbf{k}\cdot\mathbf{a})^2(\mathbf{Q}\cdot\mathbf{a}/2)+(\mathbf{k}\cdot\mathbf{a})\times(\mathbf{Q}\cdot\mathbf{a}/2)^2]. \tag{25}$$

Now the imaginary part of the magnon self-energy is evaluated. Since we are interested in the low-temperature regime, the only significant term is the one that has no occupation numbers, since they do not contribute at $T\rightarrow 0$. Thus,

$$-\mathrm{Im}\,\Sigma(\mathbf{k})=\pi\sum_{\mathbf{Q}}\left[|M^{Mn}_{\mathbf{k},\mathbf{Q}}|^2\delta(\epsilon_{\mathbf{k}}-\hbar\omega_{\mathbf{Q}}-\epsilon_{\mathbf{k}+\mathbf{Q}})+|M^{O}_{\mathbf{k},\mathbf{Q}}|^2\delta(\epsilon_{\mathbf{k}}-\hbar\omega_{\mathbf{Q}}-\epsilon_{\mathbf{k}+\mathbf{Q}/2})\right]. \tag{26}$$

To the lowest limit of k one calculates

$$-\mathrm{Im}\,\Sigma(\mathbf{k})=fJ_0[ka]^6, \tag{27}$$

where $f\sim(\hbar J_0 a^6/s)(1/M_{Mn}+1/M_O)$ for the case $\mathbf{k}=k\hat{z}$ and a similar expression for $\mathbf{k}=(k\hat{x},k\hat{y},0)$. The following should be noticed here. First, the effect of the magnon-phonon coupling on the damping of the magnons is proportional to k^6. This means that the damping is very small since the limit of small wave vectors is considered. If one takes $k=0.1k_D$, where k_D is at the end of the zone, then the imaginary part of the self-energy is proportional to 10^{-6}. Second, since the Mn ion is heavier than the O ion, the contribution from the O to the magnon-phonon coupling is actually more significant than the contribution to from the Mn. The ratio of the masses, M_{Mn}/M_O, shows that the contribution from the O ion is about 1.6 more. Third, the k^6 behavior suggests that the magnon-phonon damping increases significantly with increasing the value of the wave vector.

Indeed, experiments indicate that at the end of the zone for the magnons there is an anomalous increase in the damping.[7] This happens when the longitudinal optical phonon dispersion crosses the magnon dispersion. The developed Hamiltonian allows us to calculate the effect—the general expressions from Eqs. (12)–(14) should be used and the energy for the longitudinal optical phonons, $\hbar\omega=\mathrm{const}$, should be taken.

Again, we calculate the most significant term from Eq. (21), the one that has no occupation numbers. The energy of the longitudinal optical phonons is $\hbar\omega_{\mathbf{Q}}=\mathrm{const}=25$ meV.

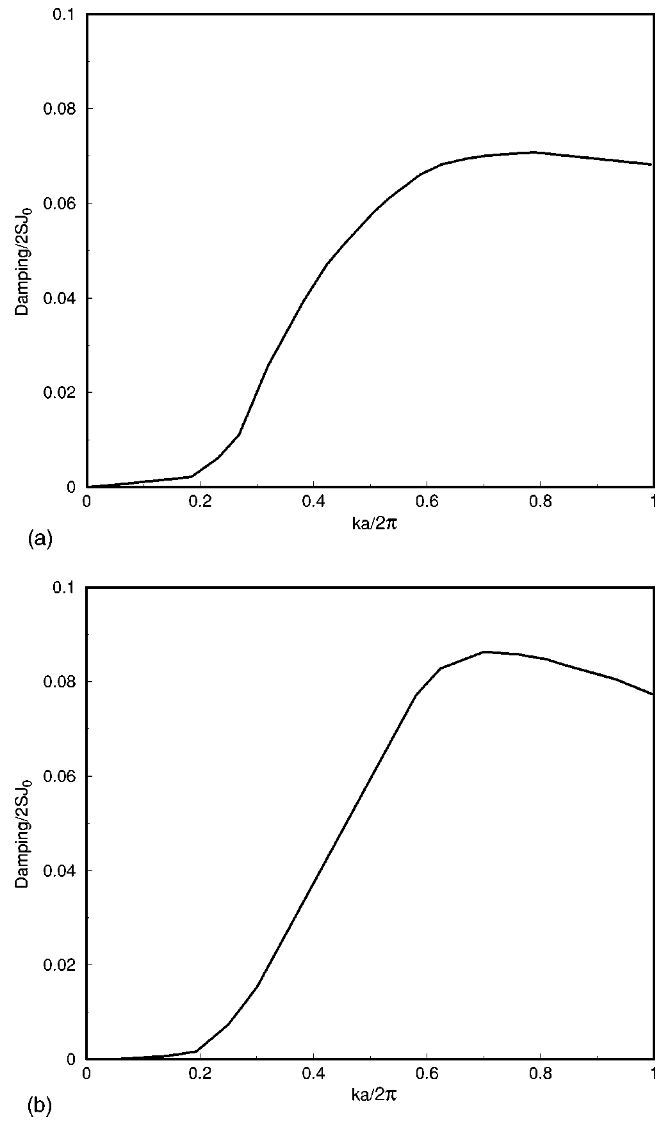

FIG. 2. Magnon damping as a function of the parameter $ka/2\pi$ (a) along the z axis and (b) in the xy plane.

In Fig. 2 the damping is plotted as a function of the parameter $ka/2\pi$ for both cases: k is along the z axis and k is in the xy plane. The linewidth of the magnons rises relatively steeply after a certain value of the wave vector, which suggests that the effect becomes more important. When compared with the data from Ref. 7 it is evident that the characteristic behavior of the damping is relatively well reproduced. For energies of the magnons smaller than the optical phonon frequency ω_0 the damping of the magnons is small. When the crossing in the dispersions occurs, the broadening becomes large, which means that the process of a magnetic excitation scattered into a new one according to the conservation energy expressed in the δ function becomes significant.

The phonon linewidth can also be calculated by evaluating the self-energy diagram from Fig. 1(b). Since the coupling conserves the spin quantum number, the only relevant term here is

$$-\mathrm{Im}\,\Pi(\mathbf{Q})=\pi\sum_{\mathbf{k}}\,[|M^{Mn}_{\mathbf{k},\mathbf{Q}}|^2(N_{\epsilon_{\mathbf{k}}}-N_{\epsilon_{\mathbf{k+Q}}})\,\delta(\epsilon_{\mathbf{k}}+\hbar\omega_{\mathbf{Q}}-\epsilon_{\mathbf{k+Q}})+|M^{O}_{\mathbf{k},\mathbf{Q}}|^2(N_{\epsilon_{\mathbf{k}}}-N_{\epsilon_{\mathbf{k+Q/2}}})\times\delta(\epsilon_{\mathbf{k}}+\hbar\omega_{\mathbf{Q}}-\epsilon_{\mathbf{k+Q/2}})]. \tag{28}$$

For the case of $T\to 0$, the occupation numbers are negligible. Thus, the phonon damping is zero. Therefore, even though the magnon-phonon interaction can be significant, no broadening in the phonons is shown. This is consistent with the experiments where no significant change in the phonon linewidth was measured.[6,7]

IV. RENORMALIZATION OF THE MAGNON SPECTRUM

In the previous section we evaluated the damping of the magnons to the first approximation in the perturbation series. We now study the propagation of the magnetic excitations. At low temperatures the dynamics of the spin waves is described by the single-magnon dispersion. The important question which arises is to which extent the magnon spectrum is affected by the magnon-phonon coupling. To answer qualitatively one needs to express the full spectrum in terms of the magnon self-energy

$$\epsilon_{\mathbf{k}}=\epsilon_{0,\mathbf{k}}+\mathrm{Re}\,\Sigma(\mathbf{k}), \tag{29}$$

where the unperturbed magnon dispersion $\epsilon_{0,\mathbf{k}}$ was defined in Eq. (10). Again we look at the lowest-order interaction and one obtains for the real part of the magnon self-energy

$$\begin{aligned}\mathrm{Re}\,\Sigma(\mathbf{k})=\sum_{\mathbf{Q}}\,&|M^{Mn}_{\mathbf{k},\mathbf{Q}}|^2\Bigg[(N_{\omega_{\mathbf{Q}}}-N_{\epsilon_{\mathbf{k+Q}}})\Bigg(\frac{1}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k+Q}}+\hbar\omega_{\mathbf{Q}}}\\&-\frac{1}{\epsilon_{\mathbf{k}}+\epsilon_{\mathbf{k+Q}}-\hbar\omega_{\mathbf{Q}}}\Bigg)+(1+N_{\omega_{\mathbf{Q}}}-N_{\epsilon_{\mathbf{k+Q}}})\\&\times\Bigg(\frac{1}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k+Q}}-\hbar\omega_{\mathbf{Q}}}-\frac{1}{\epsilon_{\mathbf{k}}+\epsilon_{\mathbf{k+Q}}+\hbar\omega_{\mathbf{Q}}}\Bigg)\Bigg]\\&+|M^{O}_{\mathbf{k},\mathbf{Q}}|^2\Bigg[(N_{\omega_{\mathbf{Q}}}-N_{\epsilon_{\mathbf{k+Q}/2}})\Bigg(\frac{1}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k+Q}/2}+\hbar\omega_{\mathbf{Q}}}\\&-\frac{1}{\epsilon_{\mathbf{k}}+\epsilon_{\mathbf{k+Q}/2}-\hbar\omega_{\mathbf{Q}}}\Bigg)+(1+N_{\omega_{\mathbf{Q}}}-N_{\epsilon_{\mathbf{k+Q}/2}})\\&\times\Bigg(\frac{1}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k+Q}/2}-\hbar\omega_{\mathbf{Q}}}-\frac{1}{\epsilon_{\mathbf{k}}+\epsilon_{\mathbf{k+Q}/2}+\hbar\omega_{\mathbf{Q}}}\Bigg)\Bigg].\end{aligned} \tag{30}$$

At low temperatures the terms multiplied by the occupation factor $N_{\omega_{\mathbf{Q}}}$ or $N_{\epsilon_{\mathbf{k}}}$ are neglected. Consider the case of small magnon wave vectors and longitudinal acoustic phonons. The matrix elements are given in Eqs. (24) and (25). To lowest order of the magnon wave vector when k is along the z axis it is easy to obtain

$$\mathrm{Re}\,\Sigma(\mathbf{k})=-Dgk^2, \tag{31}$$

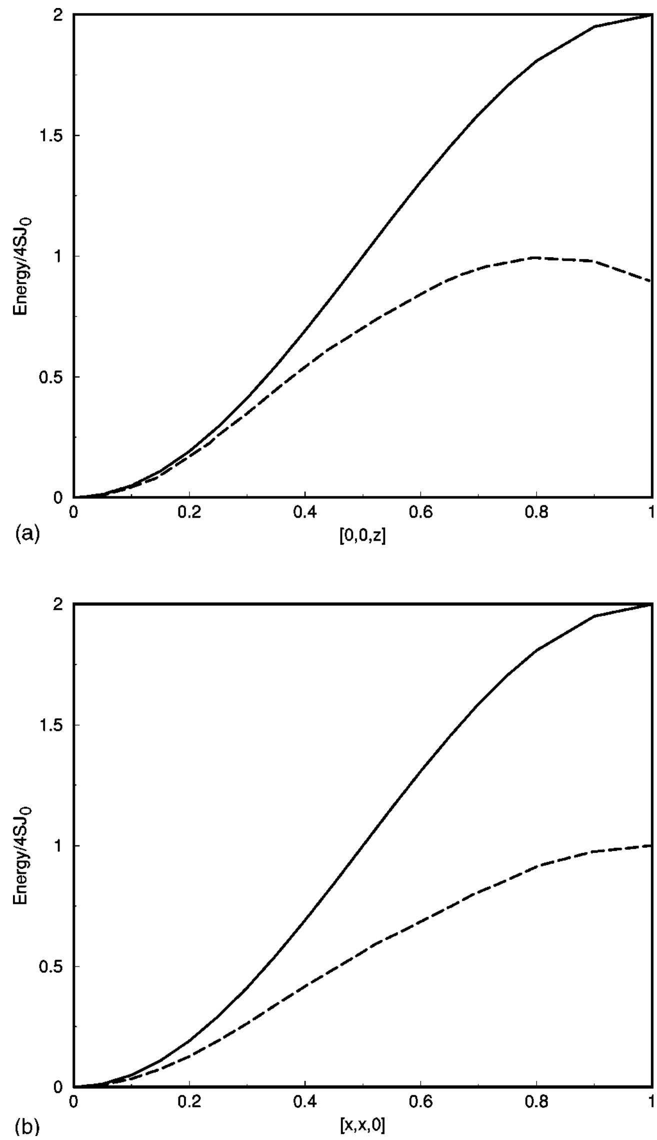

FIG. 3. Magnon dispersion as a function of $ka/2\pi$ (a) along the z axis and (b) in the xy plane. The solid line represents the nearest-neighbor Heisenberg Hamiltonian and the dashed line represents the renormalized dispersion due to the magnon-phonon interaction.

$$g=\frac{\hbar(Q_Da)^4}{7\pi^4 sa}\left[\frac{1}{M_{Mn}}+\frac{1}{M_O}\right]. \tag{32}$$

Note that a Debye cutoff Q_D is introduced in the integration over the Q variable. For three-dimensional (3D) systems $Q_D=(6\pi^2)^{1/3}/a$. If typical constants for the manganites are used, g is estimated in the range of 0.01. When k is in the xy plane, a similar expression for the $\mathrm{Re}\,\Sigma(\mathbf{k})$ is found, although the formula for g is more cumbersome, but the numerical value is still in the order of 0.01. Thus, in this limit the magnon-phonon coupling introduces only a small negative correction to the stiffness constant and it is not important.

Now we examine the limit of large magnon wave vectors with longitudinally polarized phonons. In this case the integrals are evaluated numerically. In Fig. 3 we plot the magnon dispersion with and without the coupling. It is evident that for small k the correction to the magnon energy is not significant. But at larger k the effect of the interaction is much more pronounced. According to the reported data in Ref. 7 the magnon mode experiences softening and its dispersion is very close to the LO phonons after the crossing point of about $ka/2\pi = 0.3$. Indeed, the estimated values for the correction to the magnon spectra is always negative and it becomes large when k is large. Figure 3 shows that the behavior of the calculated magnon energy is very similar to the measured one. Thus, the presented model favors the argument that such behavior should be attribured to a channel related to the coupling between magnons and phonons.

V. DISCUSSION

One of the most interesting features of the manganese perovskites is the existence of colossal magnetoresistance (CMR). Investigating the mechanisms for the magnon damping and softening is very important in order to understand their magnetic and electronic properties. It is claimed that to describe the magnon dispersion properly one needs to include orbital fluctuations and phonons via Jahn-Teller distortion.[17] The Jahn-Teller-based electron-lattice coupling is known to be important at temperatures near and above T_C. The experiments, discussed in this paper, were performed at very low temperatures where the Jahn-Teller effect is very small. They show that the magnons are heavily damped at the end of the zone.[7] One possibility considered was that a strong spin-orbit exchange interaction is the reason.[18] Another possibility is that this is due to strong magnetoelastic effects or the interaction between magnons and phonons is important. In this paper we focused on the role of the latter kind of coupling.

The interaction between the lattice and the ferromagnetically ordered carriers is obtained by allowing a modulation of the exchange coupling constant with respect to the lattice displacements and that the spin quantum number is conserved. The performed calculations are for phonons with longitudinal polarization in the acoustic and optical regimes. It was shown that the long-wavelength magnons would not be affected, but the damping in the short-wavelength limit becomes large. We also find that the phonon linewidth is not changed. This is consistent with the experiments.

Another feature is the effect on the phonons could be more significant with elevating the temperature. The reason is that the damping is proportional to the boson occupation number, which becomes more important at higher temperatures. This would require more experiments. Finally, we also calculated how the magnon dispersion changes if one takes into account the magnon-phonon coupling. It was found that the effect is really small at small wave vectors and it is significant near the zone boundary. Thus, the conclusion is that with this simple model one is able to describe the observed effects of broadening and softening in those manganites in which the nearest-neighbor Heisenberg model is valid. Indeed, the role of the interplay between spin and lattice degrees of freedom needs to be included in the analysis for a more complete understanding of the physics in these compounds.

The present model also allows for the Mn and O ions to be treated explicitly. Because the direct overlap between Mn ions is zero, the exchange coupling constant is the second perturbation order of the hopping from Mn to O site. Therefore, the interaction Hamiltonian contains the positions and masses of both types of sites: Eqs. (12)–(14). Since the O ion is lighter, one concludes that its contribution to the effect is a few times more significant than the contribution from the Mn. This is consistent with experiments reported in Ref. 16 which show that at temperatures as low as 50 K the displacements of the O ions is about 2 times larger than the displacements of the Mn ions. The model also allows for different types of phonon polarization to be evaluated.

Dimensionality has been shown to be an important consideration in the behavior of many materials. The proposed model can be generalized to ferromagnets that have reduced dimensions. In fact, we calculated the magnon damping in the 2D case using the expression for the magnon damping from Eq. (20) with the same values of the exchange constant and lattice parameters as used earlier in the paper and we obtained that the broadening becomes even larger at the end of the zone. This means that the effect of the magnon-phonon coupling could be more pronounced in materials that consist of quasi-2D planes. More experiments for ferromagnetic layered compounds in this direction are necessary.

In summary, two things are accomplished in this paper. First, a model for treating the interaction between magnons and phonons in systems with localized spins is established, which can be applied to materials with symmetry different than cubic and different types of phonon polarization. The explicit form of the matrix elements is obtained, and thus one can look into different limits. Second, the calculations for the magnon and phonon dampings and magnon softening are in agreement with the experimental findings: namely, that there is an anomalous broadening of the magnon linewidth and softening of the energy dispersion near the zone end and that the phonon linewidth is hardly changed.

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[1] J. Callaway, *Quantum Theory of the Solid State* (Academic Press, San Diego, 1991).
[2] H.Y. Hwang, S.-W. Cheong, P.G. Radaeli, M. Marezio, and B. Batlogg, Phys. Rev. Lett. **75**, 914 (1995).
[3] C. Zenner, Phys. Rev. **82**, 403 (1951).
[4] T.G. Perring, G. Aeppli, S.M. Hayedn, S.A. Carter, J.P. Remeika,

and S.-W. Cheong, Phys. Rev. Lett. **77**, 711 (1996); Y. Endoh and K. Hirota, J. Phys. Soc. Jpn. **66**, 2264 (1997).

[5] N. Furukawa, J. Phys. Soc. Jpn. **65**, 1174 (1996).

[6] H.Y. Hwang, P. Dai, S.-W. Cheong, G. Aeppli, D.A. Tennant, and H.A. Mook, Phys. Rev. Lett. **80**, 1316 (1998).

[7] P. Dai, H.Y. Hwang, J. Zhang, J.A. Fernandez-Baca, S.-W. Cheong, C. Kloc, Y. Tomioka, and Y. Tokura, Phys. Rev. B **61**, 9553 (2000).

[8] N. Furukawa, J. Phys. Soc. Jpn. **68**, 2522 (1999).

[9] I.V. Solovyev and K. Terakura, Phys. Rev. Lett. **82**, 2959 (1999); P. Mahadevan, I.V. Solovyev, and K. Terakura, Phys. Rev. B **60**, 11 439 (1999).

[10] P.W. Anderson and H. Hasegawa, Phys. Rev. **100**, 675 (1955).

[11] J.C. Slater and G.F. Koster, Phys. Rev. **94**, 1498 (1954); W. A. Harrison, *Electronic Structure and the Properties of Solids, The Physics of the Chemical Bond* (Freeman, San Francisco, 1980).

[12] S. Saitoh, A.E. Bocquet, T. Mizokawa, H. Namatame, A. Fujimori, M. Abbate, Y. Takeda, and M. Takano, Phys. Rev. B **51**, 13 942 (1995).

[13] J.H. Jung, K.H. Kim, T.W. Noh, E.J. Choi, and J.J. Jui, Phys. Rev. B **57**, R11 043 (1998).

[14] S. Lovesey, *Theory of Neutron Scattering from Condensed Matter* (Clarendon Press, Oxford, 1984).

[15] J. Jensen and A. R. Mackintosh, *Rare Earth Magnetism* (Clarendon Press, Oxford, 1991).

[16] P. Dai, J. Zhang, H.A. Mook, S.-H. Liou, P.A. Dowben, and E.W. Plummer, Phys. Rev. B **54**, 3694 (1996).

[17] G. Khaliullin and R. Kilian, Phys. Rev. B **61**, 3494 (2000).

[18] S. Ishihara, M. Yamanaka, and N. Nagaosa, Phys. Rev. B **56**, 686 (1997).