

# Magnon–phonon coupling in two-dimensional Heisenberg ferromagnetic system

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## Abstract

A magnon–phonon interaction model is set up for a two-dimensional insulating ferromagnetic system. By using Matsubara function theory, we have studied the magnon spectrum and calculated the magnon dispersion curve on the main symmetric point and line in the Brillouin zone for various parameters of the system. The results show that at the boundary of Brillouin zone, there is a strong magnon softening. The contributions of longitudinal and transverse phonons on the magnon softening are compared and the influences of various parameters are also discussed.

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## 1. Introduction

The research on magnon–phonon coupling may date back to 1970s when A.I. Akhiezer first proposed that lattice deformation leads to the change of the spin coupling coefficient (exchange integral) [1]. The magnon–phonon coupling which relates to exchange interaction in local spin Heisenberg system is a kind of important interaction [1].

In the middle of 1970s, Jensen and Houmann [2] investigated the spin wave of Tb with the hexagonal close-packed structure ( $D_{6h}^4$ ) considering the magnon–phonon coupling. They analyzed the group symmetry of the Hamiltonian in the form of magnon–phonon coupling and explored the coupling interaction by applying the matrix representation  $D_{lm,\alpha}^{l'm'}(ij)$  of the rotation operator in quantum angular momentum theory [2]. The Hamiltonian related to the magnon–phonon coupling was written as

$$H_{\text{spin-lattice}} = \sum_{i \neq j} \sum_{\alpha} \sum_{lm} \sum_{l'm'} \delta R_{\alpha}(ij) D_{lm,\alpha}^{l'm'}(ij) \tilde{O}_{l,m}(J_i) \tilde{O}_{l',m'}(J_j) + \text{H.c.},$$

where  $i$  and  $j$  denote different Tb atoms,  $\delta R_{\alpha}(ij) = (\mathbf{R}_i - \mathbf{R}_j)_{\alpha}$  is projecting component along coordinate axis,  $\tilde{O}_{l,m}(J_i)$  is Racah operator related with the irreducible tensor in angular momentum multi-coupling [2]. Then by solving the chain of closed equation of motion of each Hamiltonian of the system the analytical solution of the spin wave energy of Tb can be acquired from the corresponding secular equation. Though the results concord well with experiment, the shortcoming of this method is that the solution of secular equation whose dimension exceeded four is very difficult to find unless that the matrix elements may be diagonalized separately.

Up to around 1990, the magnon–phonon coupling mechanism aroused the interest of researchers again due to the finding of layered antiferromagnetic superconductor such as the single-layer system  $(\text{La}_2, \text{Sm}, \text{Nd}, \text{Pr})\text{CuO}_4$  [3–6] and the double-layer system  $\text{YBa}_2\text{Cu}_3\text{O}_6$  [6–8] of spin  $S = \frac{1}{2}$  named as cuprates which were investigated by Singh et al. [3], Sulewski et al. [4] and Sugai et al. [5,6]. The single-layer system such as  $(\text{Pr}, \text{La})_2\text{NiO}_4$  of spin  $S = 1$  named as nickelates were investigated by Sugai et al. [6] and Andres et al. [9] and the broadening of the Raman energy spectrum was found.

The research work by Knoll et al. may be considered to be the turning point in solving this problem. Knoll et al.

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accurately measured the dependence of the energy spectrum of  $\text{YBa}_2\text{CuO}_6$  on temperature and found that the two-magnon spectral feature width depends sensitively on temperature and there exists significant magnon softening at high temperature [7]. Sanger [10,11] developed Knell's work in consideration of magnon–phonon coupling and obtained comparatively good result. At the same time Tucker, Wang and co-workers [12,13] also applied the magnon–phonon coupling in investigating the phonon softening problem in antiferromagnetic material and diluted ferromagnetic material and obtained good result either.

In the middle of 1990s, Hwang et al. [14], Roder et al. [15] and Millis et al. [16] reasonably explained high  $T_c$  material by employing the double-exchange model proposed by Zener [17] and Anderson and Hasegawa [18]. However, with the decreases of  $T_c$  and the electric energy band width the magnetic transportation properties become significant and the explanation of the enhanced first-order phase transition requires further considering strong Jahn–Teller effect that is based on phonon correlation. Dai et al. [19] and Radaelli et al. [20] confirmed these points and showed that the static and dynamic lattice deformation becomes more important for insulator state at zero temperature in their research. Hwang et al. [21], Dai et al. [22] and Solov'ev et al. [23] investigated some Mn perovskites by inelastic neutron scattering experiment and found that for  $T < T_c$  the magnon spectrum becomes softening near the Brillouin zone boundary, for  $T \rightarrow T_c$  the spectrum line near the Brillouin zone boundary broadens significantly, for  $T > T_c$  no evidence shows the existence of excitation such as spin wave. More exactly, the spectrum line broadening exists at low temperature either. The new phenomena discovered in mixing-valenced Mn perovskite  $\text{Pr}_{0.63}\text{Sr}_{0.37}\text{MnO}_3$  and  $\text{A}_{0.7}\text{B}_{0.3}\text{MnO}_3$  (A and B are rare earth and alkaline-earth elements, respectively) cannot be explained by the classical double-exchange model. Through analyzing the softening of the magnon and the optical-mode phonon Hwang and Dai inferred that the abnormal spin dynamic behavior at low temperature most probably originates to the strong magnon–phonon coupling [21,22]. Furthermore, considering the interaction of the magnon with the long optical-mode phonon Woods [24] investigated the three-dimensional ferromagnetic perovskite  $\text{A}_{1-x}\text{B}_x\text{MnO}_3$  by theoretical calculation and obtained that the magnon becomes significantly softening and the long optical-mode phonon is unaffected by the magnon–phonon coupling. Although the results concord with the experiment, the phenomenon of spectrum line broadening cannot be explained well by their work. It is thought that neglecting the phonon characteristic and taking the long-wave approximation were the joint inadequacy of their work.

For the collective excitations (magnon, phonon, etc.), there exist general characters between the two- and three-dimensional models of the same form Hamiltonian. However, there is much difference for the magnetization

intensity of the two- and three-dimensional models because for the two-dimensional model, the relationship between the reduced magnetization and the temperature cannot be explored. Furthermore, it is quite inconvenient to qualitatively study the three-dimensional system's elementary excitation since the phonon dispersion solution of analytical form for the three-dimensional multiple lattices cannot be obtained unless applying the first principle to find the numerical solution of the elementary excitation (phonon energy) of the lattice vibration. Regarding the general character between two- and three-dimensional models we may infer the properties of three-dimensional model from two-dimensional model. The research on two-dimensional case will be of theoretical significance in investigating real material properties.

Therefore, in this paper, we employ the lattice dynamics instead of using the long-wave approximation to obtain the phonon energy and to explore in detail the influence of magnon–phonon interaction on magnon's dispersion. The relation of  $\omega_\sigma(\mathbf{q})$  to  $\mathbf{q}$  becomes nonlinear and the contribution from the transverse phonon can be distinguished from that of the longitudinal phonon.

## 2. Magnon–phonon interaction model and the Hamiltonian of the system

For insulating ferromagnet, Heisenberg exchange model can be established on the basis of the local spin model. The Hamiltonian is

$$H^{S+SP} = \sum_{\langle l, l' \rangle} -J(|\mathbf{R}_l - \mathbf{R}_{l'}|) \hat{\mathbf{S}}_l \cdot \hat{\mathbf{S}}_{l'}, \quad (1)$$

$\langle l, l' \rangle$  denotes that only the nearest neighbor is considered,  $\mathbf{R}_l = \mathbf{R}_l^0 + \mathbf{u}_l$ ,  $\mathbf{R}_{l'} = \mathbf{R}_{l'}^0 + \mathbf{u}_{l'}$ , here  $\mathbf{R}_l^0, \mathbf{R}_{l'}^0$  are the balance positions in the iron lattice.  $\mathbf{u}_l, \mathbf{u}_{l'}$  are small displacements deviating from the balance positions. Expand the exchange integral  $J(|\mathbf{R}_l - \mathbf{R}_{l'}|)$  to  $(\mathbf{R}_l^0 - \mathbf{R}_{l'}^0)$  in Taylor series only retaining the first-order approximation of  $(\mathbf{u}_l - \mathbf{u}_{l'})$ , we have

$$H^{S+SP} = H^S + H^{SP}, \quad (2)$$

where

$$H^S = - \sum_{\langle l, l' \rangle} J(|\mathbf{R}_l^0 - \mathbf{R}_{l'}^0|) \hat{\mathbf{S}}_l \cdot \hat{\mathbf{S}}_{l'}, \quad (3)$$

$$H^{SP} = \sum_{\langle l, l' \rangle} |\nabla J(|\delta|)| \left[ (\mathbf{u}_l - \mathbf{u}_{l'}) \cdot \frac{\delta}{|\delta|} \right] \hat{\mathbf{S}}_l \cdot \hat{\mathbf{S}}_{l'}. \quad (4)$$

Eq. (3) is the Hamiltonian related with spin, Eq. (4) is the Hamiltonian related with spin–phonon interaction,  $H^{S+SP}$  is the combination of  $H^S$  and  $H^{SP}$ ,  $\delta = \mathbf{R}_l^0 - \mathbf{R}_{l'}^0$ .

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