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Lattice model for exchange-coupled ferromagnetic multilayer systems

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We present a variational method with the layer magnetization angle as the variational parameter, and Holstein-Primakoff transformation is applied to the variational Hamiltonian. The magnetization of a ferromagnetic superlattice system with interactions between magnetic layers with perpendicular and in-plane easy axes is estimated. Numerical results on the magnetization configurations under different applied fields, critical field, and critical anisotropic parameter are reported.

It is found that one can significantly improve the recording properties of a bulk magnetic memory material by placing a thin capping layer with in-plane easy anisotropy on the bulk layer which has a perpendicular easy axis. Some magnetic multilayer systems have already been shown to have a good potential to reach higher recording density and to reduce the recording time in a magneto-optical device. Theoretical studies have also been done for a continuous model of double-layer systems. In this Brief Report, we extend the continuous model to that on a discrete lattice. A multilayer lattice model with an interface between layers with perpendicular and in-plane easy axes is studied. We discuss the following anisotropic quantum Heisenberg ferromagnetic model:

$$H = \sum_{m,m'} \sum_{R,R'} H_{m,m'}(R,R')$$
$$+ \sum_{m,R} (D_m S_m^z(R))^2 - h S_m^z(R),$$

where

$$H_{m,m'}(R,R') = -\frac{1}{2} J_{m,m'}(R,R') S_m(R) \cdot S_{m'}(R'),$$

and the subscripts \(\{m, m'\}\) denote the layer numbers, the \(R\), or \(R'\), is the vector of a lattice in the layer, and \(h\) is proportional to the applied magnetic field. We only discuss the simple cubic case, in which the layers are arranged along the [001] direction. For a ferromagnetic system, the coupling constant \(J_{m,m'}\) in the Hamiltonian \(H\) is positive. Figure 1 shows the geometry of the layer structure where the \(z\) direction is perpendicular to the layer planes. The parameter \(D_m\) describes the anisotropy of magnetization. Local coordinates (LC) are introduced for each layer as shown in Fig. 1.

The direction of the \(y\) axis is fixed, and the \(x, z\) axes are rotated by an angle \(\theta\) for each layer which may be different from layer to layer. The spins \(\{S_m(R)\}\) are expressed in LC systems:

$$S_m(R) = [\cos(\theta_m) S_m^x(R) - \sin(\theta_m) S_m^z(R)] x$$
$$+ [\cos(\theta_m) S_m^x(R) + \sin(\theta_m) S_m^z(R)] y$$
$$+ S_m^z(R) z.$$

The Hamiltonian can be expressed by a function of the components of the spins in LC and the angles \(\{\theta_m\}\):

$$H = H[\{S_m^x(R), S_m^y(R), S_m^z(R)\}; \{\theta_m\}].$$

Then we apply the Holstein-Primakoff transitions to each spin operator in the transformed Hamiltonian and obtain

$$\hat{H} = U_0 + H_1 + H_2 + \cdots.$$

It is easy to obtain the expressions of \(U_0, H_1,\) and \(H_2;\) for example,

$$U_0 = S^2 N_{1} \sum_{m} D_m - \frac{N_{1} S^2}{2} \sum_{m \neq m'} I_{mm'} \cos(\theta_m - \theta_{m'})$$
$$- h S N_{1} \sum_{m} \cos(\theta_m) + \frac{SN_{1}}{2} (1 - 2S) \sum_{m} D_m \sin^2(\theta_m).$$

In first approximation, the ground-state energy \(E_0\) can be obtained from the minimum of \(U_0\) by means of an optimization with respect to the parameters \(\{\theta_m\}\). The necessary conditions are

$$\frac{\delta U_0}{\delta \theta_m} = 0, \quad m = 1, 2, \ldots.$$
They yield the following nonlinear equations:

\[ S \sum_{m} J_{m,m} \sin(\theta_m - \theta'_m) + \frac{1}{2} (1 - 2S) D_m \sin(2\theta_m) + h \sin(\theta_m) = 0, m = 1, 2, \ldots \]  

(8)

The above equations are the same as the conditions that \( H_i = 0 \).

In the classical case, the spin is a vector \( S \) with magnitude \( S \) and its direction can be changed continuously so that the energy of the system can be obtained easily from the Hamiltonian (1) where the spins \( \{ S_m(R) \} \) are vectors unlike the operators in quantum case. The classical energy of the system is

\[ U_0 = S^2 N_s \sum_m D_m - \frac{1}{2} N_s \sum_{m' \neq m} I_{m,m'} \cos(\theta_m - \theta'_m) - h S N_s \sum_m \cos(\theta_m) - S^2 N_s \sum_m D_m \sin^2(\theta_m). \]  

(9)

Comparing Eq. (9) with Eq. (6), we find that there is an additional term \( S N_s / 2 \sum_m D_m \sin^2(\theta_m) \) in Eq. (6). If \( S \) is very large, the additional term gives a lower order contribution so that Eq. (6) reduces to the classical result. The classical energy (9) in our discrete model can be converted easily to the equation (1) in the previous paper if we take the continuous limit. However, the difference is significant for small \( S \). In particular, for \( S = \frac{1}{2} \), the anisotropic terms of single ions in the Hamiltonian become constants. Therefore, the spin reconstruction induced by the anisotropic term of single ions should be neglected in this case.

Equation (8) always has trivial solutions \( \{ \theta_m = 0 \text{, or } \theta_m = 180^\circ \} \). However, we can find a nontrivial solution if the applied magnetic field is not too large. In this case, the system will undergo spin reconstruction and exhibit a nontrivial magnetization configuration. We have solved Eq. (8) numerically, and the results are shown in Figs. 2–5. The first example has ten layers of perpendicular easy axis ferromagnet \( (D_2 < 0) \) covered by two layers of ferromagnet \( (D_1 > 0) \) with in-plane easy axis. The coupling between the layers is denoted by \( I_1 = I_{m,m \pm 1} \) and that within the layers by \( I_2 = I_{m,m}(R,R') \). \( I_{12} \) denotes the coupling of the interface between easy axis and easy plane ferromagnets. Without losing generality, and showing some basic physical features of the system, we fix the parameters in Figs. 2 and 3 and Fig. 5 as the following:

\[ I_1/I_2 = 1.0, \quad I_{12}/I_2 = 1.0, \]

\[ \bar{D}_2 = \left[ 2 - \frac{1}{S} \right] D_2/I_2 = -2.5, \]

and

\[ \bar{D}_1 = \left[ 2 - \frac{1}{S} \right] D_1/I_2 = 0.5, \]

where \( S \) can be any value other than \( \frac{1}{2} \) that corresponds to the different values of \( D_2/I_2 \). Figure 2 gives the spin configurations for the cases of \( h' = h/\{I_2\} = 0, \quad 0.05, \) and

FIG. 2. Spin configurations: the angle distribution as a function of number of layers for three different applied magnetic fields \( h' = 0.0, \) 0.05, and 0.1.

FIG. 3. Resulting angle of the magnetization in the first layer relative to field \( h' \).

FIG. 4. Obtained relation of anisotropic parameter \( \bar{D}_1 \) and critical field \( h_c \).
Finally, I will discuss the coupling of the model with the classical field and report the numerical results. The model is based on the effective magnetic parameter $D_1$ which is dependent on the critical field $h_c$ shown in Fig. 4. We can find another critical value $D_1'$. The value of $h_c$ is zero when $D_1 \leq D_1'$. It means that the spin deviations can appear only when the effective anisotropic parameter $D_1$ is larger than a critical value. We also calculated a 21 layers model where the first ten layers are the in-plane easy axis ferromagnet with $D_1=0.5$ and the others with $D_2=-2.5$. The result is presented in Fig. 5. We can see a big jump of angle in crossing the interface. The magnetization in most of the regions far from interface remain the bulk value.

When we fix $D_1$ and decrease $D_2$, calculations show that the deviation angle $\theta_m$ near the interface and the critical applied field $h_c$ will increase. Finally, we must mention that all our calculations are for $S=\frac{1}{2}$ and further calculation to consider the quantum fluctuation will be carried out in the next step.

The present numerical calculation was performed at the Supercomputing Center of the Institute for Materials Research (IMR), Tohoku University. The authors are grateful to the crew for their continuous help. One of the authors (R.T.) would like to express his sincere thanks to the IMR for inviting him through the support of the Hitachi Company.

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0.1. The changes of spin directions are significant only for a few layers near the interface. Increasing the applied field $h$ results in a decreasing of angle $|\theta_m|$ of the layers. Figure 3 shows the relation of the angle of the magnetization in the first layer with applied field $h$ and a critical value $h_c'(=0.1846)$ can be found. The critical applied field $h_c$ is proportional to $h_c', h_c=SI_2h_c'$. Larger $S$ or larger ferromagnetic coupling $I_2$ will induce larger critical fields. If $h \geq h_c$, all of the spins in the system will point to the direction of the field and the deviations of the spin directions can appear only in the case $h < h_c$. Meanwhile, the value of $h_c$ will be changed if we change $D_1$ or $D_2$. The anisotropy $D_1$ dependence of the critical field $h_c$ is shown in Fig. 4. We can find another critical value $D_1'$. The value of $h_c$ is zero when $D_1 \leq D_1'$. It means that the spin deviations can appear only when the effective anisotropic parameter $D_1$ is larger than a critical value. We also calculated a 21 layers model where the first ten layers are the in-plane easy axis ferromagnet with $D_1=0.5$ and the others with $D_2=-2.5$. The result is presented in Fig. 5. We can see a big jump of angle in crossing the interface. The magnetization in most of the regions far from interface remain the bulk value.

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