Magnon energy gap in a periodic anisotropic magnetic superlattice

D. S. Deng, X. F. Jin, and Ruibao Tao*
State Key Laboratory of Applied Surface Physics, and Department of Physics, Fudan University, Shanghai 200433, China
(Received 1 July 2002; published 30 September 2002)

A periodic anisotropic magnetic superlattice is proposed, and the magnon energy band of this system is investigated by local coordinates and a spin-Bose transformation quantum approach. A modulated energy gap exists in the energy band of [001] spin wave excitation, and the energy-gap–applied-field diagram has three phases derived from quantum fluctuation. Furthermore, a complete band gap extending through the Brillouin zone denoted as ‘‘spin crystal’’ can also occur in this system.

DOI: 10.1103/PhysRevB.66.104435 PACS number(s): 75.70.Cn

The study of the periodic medium is an interesting topic. It has been well known that electrons as a ‘‘de Broglie wave’’ in the periodic crystal potential form an energy band. Analogous to this original idea, Yablonovitch[1] pioneered the concept of the photonic crystal, denoted as electromagnetic waves in periodic dielectric material.[2] Subsequently extended to other cases, a special energy gap was also investigated in periodic elastic composites[3] or periodic ferroelectric media.[4]

Meanwhile, the magnon as a kind of spin excitation is an interesting and important magnetic research subject. Recently, Berger[5] and Slonczewski[6] proposed emission magnons at a magnetic multilayer interface as a spin wave induced by the driven current. Furthermore, based on up or down spin freedom rather than only charge in traditional electronics, spintronics becomes an intriguing and emerging field.[7,8] In view of all these inspiring findings, a natural question is: What is the nature of the magnon gap in the periodic magnetic multilayer?

In this paper, a periodic anisotropic magnetic superlattice (PAMSL) is proposed, and the magnon energy band is investigated by our previous *local coordinates + spin-Bose transformations* lattice quantum approach. We find that a modulated energy gap appears in the energy band of the [001] spin wave excitation, and the diagram of the energy gap versus applied field has three phases derived from quantum fluctuation. Furthermore, a complete band gap extending through the Brillouin zone can also occur in this system.

There have been a few papers about spin wave in ultrathin magnetic films.[9] Camley *et al.*[10] in 1983 reported on an analysis of the long-wavelength spin waves originating from dipolar stray fields in magnetic/nonmagnetic multilayered structures. Hillebrands[11] then took into account magnetic interface anisotropy and exchange contributions by adding them to the boundary condition. Barnas[12] showed exchange-dominated spin waves with a transfer-matrix formalism method. These previous works were devoted to the important study of magnon spectra, but unfortunately did not focus on the magnon energy gap.

In fact, Vasseur *et al.*[13] calculated the magnon band structure of two-dimensional periodic composites with evidence of an energy gap. Krawczyk *et al.*[14] computed a spin wave with a gap in the layered composite materials. Up until now, in the framework of the Landau-Lifshitz torque equation and magnetostatic Maxwell equations,[15] these theoretical methods of energy gap in the above two papers are classical and in the long-wavelength approximation. However, to discuss the existence of a gap, one needs to research the short-wavelength cases in the Brillouin zone. On the other hand, the previous classical approaches ignore quantum fluctuations that might significantly affect magnon excitation. Therefore, with consideration of both discrete effect (related to short wavelength) and quantum effect, it is further interesting to study the spin wave spectrum and explore the magnon gap from a discrete quantum spin Heisenberg model.

In the paper, the schematic structure of this PAMSL is composed of two kinds of ferromagnetic (FM) films F_1 and F_2 with different anisotropy periodically arranged as indicated in Fig. 1. The system is denoted as $\{D_1^{t1}D_2^{t2}\}_N$, where N is the number of periodic superlattice cells, D_1 and D_2 are perpendicular anisotropy of films F_1 and F_2, and $t1$ and $t2$ are the F_1 and F_2 monolayer numbers. For such system, the Hamiltonian we will discuss is[16]

$$H=-\frac{1}{2}\sum_m \sum_{n,n'} \sum_{R,R'} J_{n,n'}S_n(R)S_{n'}(R') -\sum_m \sum_{n,R} D_n[S_n^z(R)]^2-B\sum_m \sum_{n,R} S_n^x(R). \qquad (1)$$

Here m denotes the number of superlattice unit cells, and $\{n,n'\}$ and $\{\mathbf{R},\mathbf{R}'\}$ denote the layer number and the vector of lattices in the unit cell. $J>0$ is the ferromagnetic interaction, D_n is the perpendicular anisotropy, and the magnetic field B is applied along the x direction at the layer plane. Note that only zero temperature calculations are presented and the dipolar interaction is neglected for simplicity here.

After spin-Bose transformation through the approach of the ‘‘local coordinates (LC) (Ref. 16)+spin-Bose transformation,’’ such as Holstein-Primakoff[17] (HP) or the complete Bose transformation (CBT),[18] the Hamiltonian in the harmonic approximation is[19]

$$H=U_0+H_1+H_2, \qquad (2)$$

where

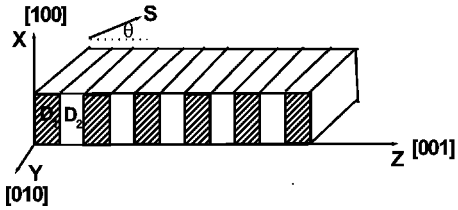

FIG. 1. The schematic structure of periodic anisotropic magnetic superlattice (PAMSL) $\{D_1^{t1}D_2^{t2}\}_N$, θ the angle between the spin and the z axis.

$$U_0=\text{const}-\frac{S^2}{2}\sum_m\sum_{n,n'}\sum_{R,R'}J_{n,n'}\cos(\theta_n-\theta_{n'})+\frac{S}{2}(2S-1)\sum_m\sum_{n,R}D_n\sin^2\theta_n-BS\sum_m\sum_{n,R}\sin\theta_n. \quad (3)$$

In first approximation, the ground-state energy E_0 can be obtained from the minimum of U_0 by means of a variation method with the layer magnetization angle $\{\theta_n\}$ as the variational parameter. It yields the following nonlinear equations:

$$S\sum_{n'}J_{n,n'}\sin(\theta_n-\theta_{n'})+\tfrac{1}{2}D_n(2S-1)\sin(2\theta_n)-B\cos\theta_n=0,\quad n=1,2,\cdots. \quad (4)$$

The conditions of Eq. (4) are just the same as for $H_1=0$. After the Fourier transformation to $\mathbf{k}(k_x,k_y,k_z)$ space, the harmonic term H_2 becomes

$$H_2=\sum_{n,n'}\sum_{\mathbf{k}}F_{n,n'}(\mathbf{k},\theta)a_n^+(\mathbf{k})a_{n'}^-(\mathbf{k})+\sum_{n,n'}\sum_{\mathbf{k}}G_{n,n'}(\mathbf{k},\theta)\times[a_n^+(\mathbf{k})a_{n'}^+(-\mathbf{k})+a_n^-(\mathbf{k})a_{n'}^-(-\mathbf{k})], \quad (5)$$

where

$$F_{n,n}(\mathbf{k},\theta)=J_{n,n}SZ_1(1-\gamma_{k1})+Dn\left(S-\frac{1}{2}\right)(2\cos^2\theta_n-\sin^2\theta_n)+Z_2J_{n,n'}S\times\cos(\theta_n-\theta_{n'})+B\sin\theta_n, \quad (6)$$

$$F_{n,n'}(\mathbf{k},\theta)=-\frac{S}{2}J_{n,n'}[1+\cos(\theta_n-\theta_{n'})]Z_2\gamma_{k2},\quad (n\neq n'), \quad (7)$$

and

$$G_{n,n}(\mathbf{k},\theta)=-\frac{1}{4}\sqrt{2S(2S-1)}D_n\sin^2\theta_n, \quad (8)$$

$$G_{n,n'}(\mathbf{k},\theta)=\frac{S}{4}J_{n,n'}[1-\cos(\theta_n-\theta_{n'})]Z_2\gamma_{k2},\quad (n\neq n'), \quad (9)$$

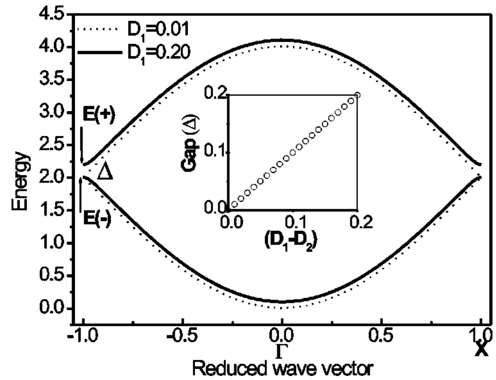

FIG. 2. Magnon excitation spectrum in the [001] direction. For the periodic anisotropy the case, magnon energy band bifurcates two branches with an energy gap (Δ). Energy gap (Δ) as the function of (D_1-D_2) shown by inset. Other parameters are $I_1=1.00$, $D_2=0.01$, $B=0$. (The [001] excitation is independent of coupling within layer I_2.)

$$\gamma_{k1}=\frac{1}{Z_1}\sum_{\delta_1}\exp(i\mathbf{k}\cdot\boldsymbol{\delta}_1),\qquad \gamma_{k2}=\frac{1}{Z_2}\sum_{\delta_2}\exp(i\mathbf{k}\cdot\boldsymbol{\delta}_2), \quad (10)$$

where $\boldsymbol{\delta}_1$ and Z_1 are the vector and number of the nearest-neighbor sites in the (x,y) plane, $\boldsymbol{\delta}_2$ and Z_2 are those of the nearest-neighbor sites along the z axis, is $I_1=J_{n,n'}$ the coupling between the different anisotropy layers, and $I_2=J_{n,n}$ is that within the same anisotropy layers. Here we will discuss the $\{D_1^1D_2^1\}_{100}$ PAMSL system in the simple-cubic structure and set quantum spin $S=1$. The periodic boundary condition is used. The Hamiltonian of Eq. (5) can be diagonalized by a (U,V) transformation;[19] then the magnon excitation energy ϵ_k can be obtained.

Figure 2 illustrates the magnon excitation energy in the [001] direction (perpendicular to the layers) without applied field for two cases: uniform and periodic anisotropy (corresponding to $D_1=D_2$ and $D_1\neq D_2$, respectively). It is normal that the energy band is continuous for the former case. By contrast, in the later case, one distinct feature is that *an energy gap* (Δ) *exists in the periodic anisotropic superlattice energy band*. And it clearly demonstrates that the energy band of the magnon propagating in the [001] direction will bifurcate two branches with a gap. Physically, this situation is analogous to the phonon excitation gap of lattice vibration ("acoustic mode" and "optical mode") in the periodic atomic chain with two different kinds of atoms in a unit cell.[20] For uniform anisotropy, the magnon gap will disappear naturally. The magnon gap as the function of anisotropy (D_1-D_2) is shown by inset of Fig. 2.

Note the novelty that the energy band of PAMSL can be modulated with the applied magnetic field. For the photonic crystal or acoustic crystal, the energy band gap is determined by the material proprieties and microstructure. In contrast, as for PAMSL, the magnon energy band depends on not only the material anisotropy and microstructure, but also on the spin configuration. So with applied transverse magnetic field, the reconstructing spin configuration will result in the modulation of energy band gap.

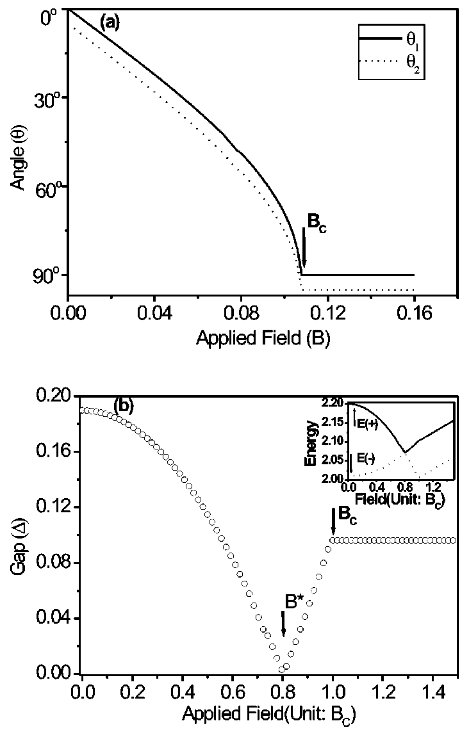

FIG. 3. (a) Spin configuration dependent on the $[100]$ field. The curve for θ_2 is displaced vertically for clarity. Magnetization saturation field is denoted by critical field B_C. (b) Energy-gap–applied-field phase diagram. Tip field B^* and critical field B_C divides the energy gap into three phases. Inset: $E(+)$ and $E(-)$ relationship with field; here $E(+)$ and $E(-)$ are the same as in Fig. 2. Parameters: $I_1=1.0, D_1=0.20, D_2=0.01$ (independent of coupling within layer I_2).

The spin configuration $\{\theta_1,\theta_2\}$ relationship with the $[100]$ transverse field is presented in Fig. 3(a). Here the spin configuration is obtained from numerical calculations for the nonlinear Eq. (4), and B_C is the $[100]$ saturated magnetization field. Figure 3(b) indicates the phase diagram of the energy gap via applied field for the $[001]$ spin wave excitation. The field (B^*) is associated with the tip energy gap. One obvious characterstic is that the fields B^* and B_C divide the energy gap into three phases, i.e., energy gap (i) decreasing with field; (ii) increasing with field; (iii) unchanging with field. From the classical view, the periodic effective fields, i.e., $\{JS\cos(\theta_1-\theta_2)-D_1S\cos^2\theta_1-B\sin\theta_1,\quad JS\cos(\theta_1-\theta_2)-D_2S\cos^2\theta_2-B\sin\theta_2\}$, will become a uniform effective field $\{JS-B\}$ above saturation magnetization field with $\{\theta_1=\theta_2=\pi/2\}$. And the energy gap will monotonically reduce to zero with field. Thus the tip gap and platform gap in phases (ii) and (iii) are not expected. In fact, these effects should be the result of quantum fluctuations, since the additional anisotropy term S_x^2 has no classical counterpart after the LC $+$spin-Bose transformation.[16,19,21]

It is also worth exploring whether a complete gap can exist in a three-dimensional (3D) direction. Figure 4 demonstrates the full band structure in this simple-cubic structure superlattice without applied field. The ΓM excitation is a $[110]$ $\mathbf{k}_\parallel$ (in the layers) spin wave; the ΓX excitation is a $[001]$ $\mathbf{k}_\perp$ (normal to the layers) spin wave; and MR, XR excitations are combined by both $\mathbf{k}_\parallel$ and $\mathbf{k}_\perp$ spin waves. In this case, the energy band has a complete magnon band gap (indicated by the shaded area in the figure), which extends through the Brillouin zone. This magnon gap may be potentially useful for the application such as microwave absorption.

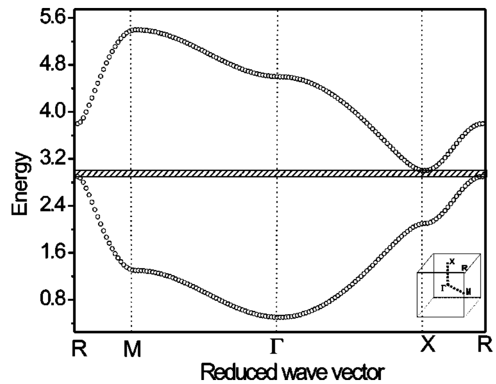

FIG. 4. Magnon band structure for PAMSL with simple-cubic structure. A complete gap extending the Brillouin zone with zero applied field is indicated by the shaded area. The parameters are $I_1=1.0$, $I_2=0.1$, $D_1=0.1$, and $D_2=1.0$.

The unit cell in PAMSL can also be extended to other thickness cases. For the $\{D_1^2D_2^2\}_{100}$ superlattice with two atomic layers in each constituent, the $[001]$ magnon excitation spectrum shown in Fig. 5 has four energy branches with multiple gaps. For the real experimental sample, fluctuations due to surface roughness or layer thickness, in fact, possibly influence the magnon spectrum through the occurrence of local states or a gap decrease in the energy band. But the spectrum could be stable with such weak fluctuations, since fluctuations might be suppressed by the gap for the lowest ground-state excitation. In this case, the magnon gap with an applied field is complicated because several energy branches should be investigated.

Several points also should be discussed. The preceeding discussion for simple-cubic structure can be generalized to face-centered cubic (fcc) or body-centered cubic (bcc) structure. Also note that for the case of quantum spin $S=\frac{1}{2}$

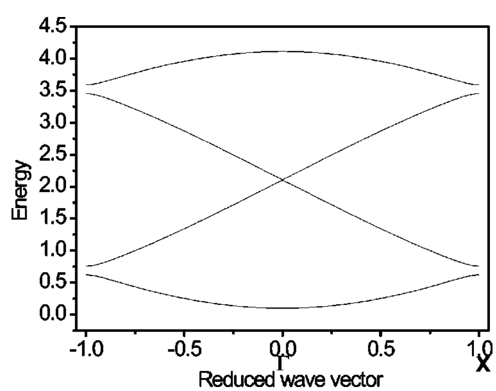

FIG. 5. Magnon excitation spectrum in the $[001]$ direction with multiple gaps in the $\{D_1^2D_2^2\}_{100}$ superlattice (two atomic layers for each constituent). The parameters are $I_1=I_2=1.00$, $D_1=0.20$, $D_2=0.01$, $B=0$.

PAMSL, the anisotropy term in the Hamiltonian will be only a constant of ground-state energy and the energy gap in the magnon band should disappear. With applied field, the 3D energy band calculation method mentioned above will fail because spin configuration loses the crystal symmetry in response to the applied field. Also the first principle approach to verify the existence of the 3D magnon gap system denoted as ''spin crystal'' is still open, since our calculation is based on the harmonic approximation of spin excitation.

In summary, a periodic anisotropic magnetic superlattice is proposed, and the main results of PAMSL are (i) a modulated energy gap exists in the energy band of [001] spin wave excitation; (ii) the energy-gap–applied-field diagram has three phases derived from quantum fluctuation; (iii) a complete band gap extending through the Brillouin zone can also occur. At present, how to create the PAMSL is still an open issue experimentically. These theoretical predictions are not only interesting for fundamental physics research, but also can be tested experimentally by Brillouin light scattering spectra. We hope PAMSL magnetic media with a modulated gap could link with a photonic crystal for electromagnetic wave propagation, and might shed light on the future of spintronics.

One of the authors, D.S.D., is grateful to Dr. L. Zhou for the helpful discussions on analytic calculation. This work is supported by National Natural Science Foundation of China, Shanghai Research Center of Applied Physics and a research grant for nanomaterials science, Chinese Science Academy.

*Email address: rbtao@fudan.ac.cn

[1] E. Yablonovitch, Phys. Rev. Lett. **58**, 2059 (1987).

[2] See, e.g., J. Joannoupoulous, R. Meade, J. Winn, *Photonic Crystals* (Princeton Univ. Press, New York, 1995), and references therein.

[3] M.S. Kushwaha, P. Halevi, L. Dobrzynski, and B. Djafari-Rouhani, Phys. Rev. Lett. **71**, 2022 (1993), and references therein.

[4] Yan-qing Lu, Yong-yuan Zhu, Yan-feng Chen, Shi-ning Zhu, Naiben Ming, and Yi-Jun Feng, Science **284**, 1822 (1999).

[5] L. Berger, Phys. Rev. B **54**, 9353 (1996).

[6] J.C. Slonczewski, J. Magn. Magn. Mater. **159**, L1 (1996).

[7] G.A. Prinz, Phys. Today **48**(4), 58 (1995).

[8] G.A. Prinz, Science **282**, 1660 (1998); (unpublished).

[9] R.E. Camley and R.L. Stamps, J. Phys.: Condens. Matter **5**, 3727 (1993).

[10] R.E. Camley, T.S. Rahman, and D.L. Mills, Phys. Rev. B **27**, 261 (1983).

[11] B. Hillebrands, Phys. Rev. B **37**, 9885 (1988).

[12] J. Barnas, Phys. Rev. B **45**, 10 427 (1992).

[13] J.O. Vasseur, L. Dobrzynski, B. Djafari-Rouhani, and H. Puszkarski, Phys. Rev. B **54**, 1043 (1996).

[14] M. Krawczyk, J.-C. Lévy, D. Mercier, and H. Puszkarski, Phys. Lett. A **282**, 186 (2001).

[15] L. Landau and E. Lifshitz, Phys. Z. Sowjetunion **8**, 153 (1935).

[16] Ruibao Tao, Xiao Hu, and Yoshiyuki Kawazoe, Phys. Rev. B **52**, 6178 (1995).

[17] T. Holstein and H. Primakoff, Phys. Rev. **59**, 1098 (1940).

[18] Ruibao Tao, J. Phys. A **27**, 3621 (1994).

[19] Lei Zhou, Ruibao Tao, and Yoshiyuki Kawazoe, Phys. Rev. B **54**, 9924 (1996).

[20] M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford Univ. Press, Oxford, 1954).

[21] The S_x^2 term with harmonic approximation is $S_x^2=\frac{1}{4}(S^++S^-)^2 =(S/2)+(\sqrt{2S(2S-1)}/4)\quad(a^+a^++a^-a^-)+(S-\frac{1}{2})a^+a^- +O(a^3)$.