GREEN FUNCTION METHOD FOR MAGNETIC SUPERLATTICES

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The spectrum of magnons, low temperature local magnetizations and magnetic susceptibility of magnetic superlattices are obtained using Green function and transfer-matrix methods. The elementary unit of thesuperlatticese under consideration consist of N different ferromagnetic layers.

INTRODUCTION

Growth and study of superlattices - artificial multi-layered systems -attracted considerable attention in recent years. Rapid development of modern technologies leads to their wide application, and this is causing increased interest to their experimental and theoretical investigation. A number of theoretical works are dedicated to magnetic superlattices [1-7]. Various models and methods of theoretical physics were used for their study. In most papers artificially created superlattices, consisting of layers of two magnetic materials, ferromagnetic and anti-ferromagnetic, are investigated. Examples of such superlattices are Fe/Cr, Co/Cr, Gd/Y, Dy/Y, etc. it has been shown that multi-layered systems have new, unique properties, not found in single-component systems. However, a large number of problems of the theory of magnetic superlattices remain unsolved.

The purpose of the present work is to consider more general model of a superlattice consisting of arbitrary number N (N=2,3,....) of magnetic layers, and to obtain its physical characteristics, such as spectrum of magnons, low-temperature magnetization, and magnetic susceptibility, b Green function method.

2.THE MODEL OF A SUPERLATTICE AND ITS HAMILTONIAN

Let us consider a model of a simple cubic ferromagnetic superlattice with arbitrary number N of layers [1]. Exchange interaction only between the nearest neighbors is taken into account. Interfaces are parallel to (001) plane. Each j-layer (j=1,2,....N) is characterized by the following common parameters: exchange integral J , lande factor g , and spin s . Ferromagnetic layers, in their turn, consits of nj atomic layers (j=1,2,...N). In addition, let us assume that external static magnetic field and anisotropic one-axis fields (restricted by two atomic layers at each interface) are directed perpendicularly to the interfaces.

The Hamiltonian of this system has the following form:

$$\hat{H} = -\frac{1}{2}\sum_{n,\nu,\delta_n} J_{n,n}\hat{\vec{S}}_{n,\nu}\hat{\vec{S}}_{n,\nu,\delta_n} - \sum_{n,\nu} J_{n,n+1}\hat{\vec{S}}_{n,\nu}\hat{\vec{S}}_{n+1,\nu} - \sum_{n,\nu} g_n\mu_B(H_0 + H_n^a)\hat{S}_n^z \quad (1)$$

where the first term describes exchange interaction inside atomic
layer, the second term describes interaction between neighboring atomic layers, and the last term include Zeeman"s energy and magnetic anisotropy energy. Here, is the number of the atomic layer, is the vector of lattice site in this layer (i.e. completely defines location of the atom in the superlattice), and δ_n is the vector of location of the nearest neighbors in the plane.

$J_{n,n}$ and $J_{n,n+1}$ exchange constants, g_n Lande factor, s_n spin and H_n anisotropic fields have the following form, depending on n:

$$J_{n,n} = \begin{cases} J^{(j)} & mL + \sum_{\sigma=1}^{j-1} n_\sigma + 2 \le n \le mL + \sum_{\sigma=1}^{j} n_\sigma - 1 \\ J^{(j)} + \Delta_2 & n = mL + \sum_{\sigma=1}^{j-1} n_\sigma + 1 \\ J^{(j)} + \Delta_1^{(j)} & n = mL + \sum_{\sigma=1}^{j} n_\sigma \end{cases} \quad (2)$$

$$J_{n,n+1} = \begin{cases} J^{(j)} & mL + \sum_{\sigma=1}^{j-1} n_\sigma + 1 \le n \le mL + \sum_{\sigma=1}^{j} n_\sigma - 1 \\ J^{(j,j+1)} + L & n = mL + \sum_{\sigma=1}^{j} n_\sigma \end{cases}$$

$$H_n^a = \begin{cases} 0 & mL + \sum_{\sigma=1}^{j-1} n_\sigma + 2 \le n \le mL + \sum_{\sigma=1}^{j} n_\sigma - 1 \\ H_1^{(j)} & n = mL + \sum_{\sigma=1}^{j-1} n_\sigma + 1 \\ H_2^{(j)} & n = mL + \sum_{\sigma=1}^{j} n_\sigma \end{cases}$$

$$\left.\begin{aligned} g_n &= g^{(j)} \\ S_n &= S^{(j)} \end{aligned}\right\} \quad mL + \sum_{\sigma=1}^{j-1} n_\sigma + 1 \le n \le mL + \sum_{\sigma=1}^{j} n_\sigma$$

where j=1,2,....N, L defined as $L=\Sigma n_\sigma$ (L_σ =1 - superlattice constant) m is the unit cell index (m=0±1, ±2,.... for infinite system and m=1,2,...for semi-infinite system). For j=N, j+1→1.

Here we used the Bloch's method of expansion by two-dimensional atomic planes, and now we can bind different planes by the method of transfer matrix.

3.GREEN FUNCTION OF SUPERLATTICE AND TRANSFER MATRIX METHOD

Let us define $G(k_n,)$-the low-temperature retarded Green function in k_n - space. In real space the retarded two-time Green function is defined as [8]:

$$G_{ij}(t-t') = -i\theta(t-t') \left\langle \left[S_i^-(t), S_j^-(t') \right] \right\rangle \qquad (3)$$

where i,j are lattice sites (i=nv).

$G(k_n,\omega)$ obeys Dyson's equation:

$$\omega G = 1 + HG \qquad (4)$$

or, in matrix form,

$$\omega \langle \vec{lk}_n | G | \vec{l'k}_n \rangle = \delta_{ll'} + \sum_j \langle \vec{lk}_n | H | \vec{jk}_n \rangle \langle \vec{jk}_n | G | \vec{l'k}_n \rangle \qquad (5)$$

Here Bloch wave functions $|k_n\rangle$ have the form:

$$\left| \vec{lk}_n \right\rangle = \frac{1}{\sqrt{N}} \sum_v \exp(i\vec{kv}) \left| \vec{lv} \right\rangle \qquad (6)$$

where N is the number of atoms in l-layer.

Matrix element of the Hamiltonian (1) in this basis will have the form:

$$\langle l|H|l'v\rangle = \left\{ E_0 + \sum_i J_{l,v} S_v + g_l \mu_B (H_0 + H_l^a) \right\} \delta_{ll'v} - J_{ll'v} (S_l S_{l'v})^{1/2} \qquad (7)$$

where $E_0=-J_0S_lS_j$ is the energy ground state of the superlattice. Let us transfor matrix element (7) using (6):

$$H_{n,n} = \langle n\vec{k}_n | H | n\vec{k}_n \rangle = E_0 + J_{n,n} S_n (Z_n = \gamma_n) + J_{n,n+1} S_{n+1} + J_{n,n-1} S_{n-1} + g_n \mu_B (H_0 + H_n^a) \qquad (8)$$

$$H_{n,n-1} = \langle n\vec{k}_n | H | (n-1)\vec{k}_n \rangle = -J_{n,n-1} (S_n S_{n-1})^{1/2} = H_{n-1,n} \qquad (9)$$

where Z_n is the number of the nearest neighbors in the plane, and

$$\gamma_n = \sum_{\delta_n} \exp(i\vec{k}\vec{\delta}_n) \qquad (10)$$

or, if one executes the sum (k_n =(k_x , k_y)),

$$\gamma_n = 2\left[\mathrm{Cos}(k_x a) + \mathrm{Cos}(k_y a) \right] \qquad (10a)$$

In order to find $G(k_n,\omega)$ Green function from Dyson's equation (5) we use transfer-matrix method, first proposed by Falikov [9]. For our case we introduce transfer-functions, which coorelate Green functions of the neighboring layers:

$$G_{n-1,l}(\vec{k}_n, \omega) = T_n G_{n,l}(\vec{k}_n, \omega)$$

$$T_n = T_n(\vec{k}_n, \omega) \qquad (11)$$

Let us write down Dyson's equation for $G_{n,l}(k_n,\omega)$:

$$\omega G_{n,l} = H_{n,n-1} G_{n-1,l} + H_{n,n} G_{n,l} + H_{n,n+1} G_{n+1,l} \qquad (12)$$

Taking into account (11), we obtain

$$\omega G_{n,l} = H_{n,n-1} T_{n-1}^{-1} G_{n,l} + H_{n,n} G_{n,l} + H_{n,n+1} T_n G_{n,l} \qquad (13)$$

or

$$\omega = H_{n,n-1} / T_{n-1} + H_{n,n} + H_{n,n+1} T_n \qquad (13a)$$

In order to find all T_n transfer-functions one has to solve a set of L equations of (12)-type for $G_{n,l}(k_n,\omega)$, n changing from 1 to L. As L could be a large number, the problem is difficult mathematically. However, it can be significantly simplified by one assumption. If n-th and n+j-th atomic layers are located in the bulk of the j-th layer, then $G_{n,l}$ and $G_{n+1,l}$ are describing similar physical states and should give identical results. Therefore, in this case one can assume T_n =1. Consequently, T_n =1 only at interface between j-th and j+1 layers, i.e. when n→n+1 transfer corresponds to j→ j+1. Thus, one can assume that

$$T_n = \begin{cases} 1 & mL+\sum_{\sigma=1}^{j-1} n_\sigma + 1 \le n \le mL+\sum_{\sigma=1}^{j} n_\sigma \\ T^{(j)} & n = mL+\sum_{\sigma=1}^{j} n_\sigma \end{cases} \quad (14)$$

Now let us calculate $T^{(j)}$. For this purpose we solve equation (12) for two atomic layers, n and n+1, at the interface between j-th and j+1-th layers. This means that $n=mL+\Sigma n_\sigma$.

Now we have two equations,

$$\omega = H_{n,n-1}/T_{n-1} + H_{n,n} + H_{n,n+1}T_n \quad (15)$$

$$\omega = H_{n,n+1}/T_n + H_{n+1,n+1} + H_{n+1,n+2}T_{n+1} \quad (16)$$

Taking into account (2), (8), (9) and (14) we obtain:

$$T_{n-1} = 1, \quad T_{n+1} = 1, \quad T_n = T^{(j)}$$

$$H_{n,n-1} = -J^{(j)}S^{(j)} \qquad H_{n,n+1} = -J^{(j,j+1)}(S^{(j)}S^{(j+1)})^{1/2}$$

$$H_{n+1,n+2} = -J^{(j+1)}S^{(j+1)} \qquad H_{n,n+1} = -J^{(j,j+1)}(S^{(j)}S^{(j+1)})^{1/2}$$

$$H_{n,n} = E_0 + (J^{(j)} + \Delta_2^{(j)})S^{(j)}(Z_n - \gamma_n) + J^{(j)}S^{(j)} +$$
$$+ J^{(j,j-1)}S^{(j-1)} + g^{(j)}\mu_B(H_0 + H_2^{(j)})$$

$$H_{n+1,n+1} = E_0 + (J^{(j+1)} + \Delta_2^{(j+1)})S^{(j+1)}(Z_n - \gamma_n) + J^{(j+1)}S^{(j+1)} +$$
$$+ J^{(j,j+1)}S^{(j)} + g^{(j+1)}\mu_B(H_0 + H_2^{(j+1)})$$

Substituting these expressions in (15) and (16), we get:

$$\omega = \Omega^{(j)} + KT^{(j)} \quad (17)$$

$$\omega = \Omega^{(j+1)} + K/T^{(j)}$$

where new denotions are introduced:

$$\Omega^{(j)} = E_0 + (J^{(j)} + \Delta_2^{(j)})S^{(j)}(Z_n - \gamma_n) + J^{(j,j-1)}S^{(j-1)} + \quad (18)$$
$$+ g^{(j)}\mu_B(H_0 + H_2^{(j)})$$

$$\Omega^{(j+1)} = E_0 + (J^{(j+1)} + \Delta_2^{(j+1)})S^{(j+1)}(Z_n - \gamma_n) + \quad (19)$$
$$+ J^{(j,j+1)}S^{(j)} + g^{(j+1)}\mu_B(H_0 + H_2^{(j+1)})$$

$$K = -J^{(j,j+1)}(S^{(j)}S^{(j+1)})^{1/2} \quad (20)$$

From (17) we find the final expression for $T^{(j)}$:

$$T^{(j)} = \left(\frac{\omega - \Omega^{(j)}}{\omega - \Omega^{(j+1)}}\right)^{1/2} \quad (21)$$

Now, knowing $T^{(j)}$, one can find G_{nn} Green function with the help of Dyson's equation for any layer:

$$\omega G_{n,n} = 1 + H_{n,n-1}G_{n-1,n} + H_{n,n}G_{n,n} + H_{n,n+1}G_{n+1,n} \quad (22)$$

Here $G_{n+1,n} = T_n G_{nn}$, and, in order to find $G_{n-1,n}$ one has to write out a sequence of n-1 equations of the following type:

$$\omega G_{n-1,n} = H_{n-1,n-2}G_{n-2,n} + H_{n-1,n-1}G_{n-1,n} + H_{n-1,n}G_{nn}$$
$$\omega G_{n-2,n} = H_{n-2,n-3}G_{n-1,n} + H_{n-2,n-2}G_{n-2,n} + H_{n-2,n-1}G_{n-1,n} \quad (23)$$

.....

$$\omega G_{1,1} = \ldots$$

By finding $G_{n-1,n}$ through $G_{n,n}$ from this system of recurrent equations, we find the final expression for $G_{n,n}(k_n,\omega)$. Obviously, for large n numbers the procedure is rather cumbersome, and therefore this method is better applicable for surface layers of a semi-infinite supelattice.

Let us for example find $G_{1,1}(k_{n1},\omega)$. Green function of the first surface layer. For simplicity we will assume that the parameters of the superlattice at the surface are the same as in the bulk.

$$G_{11}(\vec{k}_n,\omega) = (\omega - H_{11} - H_{12}T_1)^{-1}$$

If the first layer (n=1) is made of one magnetic material, and the second (n=2) is made of other material then

$$G_{11}(\vec{k}_n,\omega) = (\omega - \Omega^{(1)} - J^{(1)}S^{(1)} - KT^{(1)})^{-1} \quad (24)$$

General form of Green function of the second layer is the following:

$$G_{22}(\vec{k}_n,\omega) = (\omega - H_{22} - H_{12}H_{21}/(\omega - H_{11}) - H_{23}T^{(2)})^{-1}$$

etc.

4.DENSITY OF MAGNETIC STATES, MAGNETIZATION, AND MAGNETIC SUCCEPTIBILITY OF THE SUPERLATTICE.

Local density of states of magnons for 1-th layer of super-lattice can be found as follows:

$$D_1(\omega) = -\frac{1}{\sqrt{n}} n_j \sum_{\vec{k}_n} \langle \vec{k}_n | G(\vec{k}_n,\omega) | \vec{k}_n \rangle \quad (25)$$

where sum by kn goes over Brillouin zone [10].Knowledge of $D_1(\omega)$ enables to calculate local magnetization in the 1-th layer in the low-temperature limit [11]:

$$\mu_1 = \mu_0(1 - \langle n_1 \rangle) \quad (26)$$

where

$$\langle n_1 \rangle = \int_0^\infty \frac{D_1(\omega)d\omega}{\exp(\omega/\theta) - 1} \quad (27)$$

and μ_0 is spontaneous magnetization of the layer (at T=0).

The general expression of magnetic susceptibility tensor is the following:

$$\chi_{\alpha\beta}(\omega) = -\mu^2 \langle\langle S^\alpha | S^\beta \rangle\rangle_\omega \qquad (28)$$

where α, β=x,y,z, and $\mu=g\mu_B$ is the magnetic moment of the atom. Taking into account operators $S=S^x + iS^y$, the $\lambda(\omega)$ tensor can be written in the following form:

$$\chi(\omega) = \begin{pmatrix} \chi_\perp(\omega) & i\chi_x(\omega) & 0 \\ -i\chi_x(\omega) & \chi_\perp(\omega) & 0 \\ 0 & 0 & \chi_0 \end{pmatrix} \qquad (29)$$

where λ_0 is static succeptibility, and $\lambda_\perp$ and λ_x are the diagonal and non-diagonal components of dynamic succeptibility. According to Baryakhtar V.G. et al. [13], they can be expressed via Green functions, taking into account analytical properties of the latters, in the following general form:

$$\chi_\perp(\omega) = -\frac{(g\mu_B)^2}{2}\left\{G(\omega) + G^*(-\omega)\right\} \qquad (30a)$$

$$\chi_x(\omega) = -\frac{(g\mu_B)^2}{2}\left\{G(\omega) - G^*(-\omega)\right\} \qquad (30b)$$

For our superlattice and its Green function the components of magnetic succeptibility of the n-th layer take the form:

$$\chi_n^\perp(\omega) = \frac{(g_n\mu_B)^2}{2}\cdot\frac{1}{N}\sum_{\vec{k}_n}\left\{G_{n,n}(\vec{k}_n,\omega) + G_{n,n}^*(-\vec{k}_n,-\omega)\right\} \qquad (31a)$$

$$\chi_n^{(x)}(\omega) = \frac{(g_n\mu_B)^2}{2}\cdot\frac{1}{N}\sum_{\vec{k}_n}\left\{G_{n,n}(\vec{k}_n,\omega) - G_{n,n}^*(-\vec{k}_n,-\omega)\right\} \qquad (31b)$$

where sum by k_n goes over Brillouine zone.

Under the assumption on infinite size of the crystal, neglecting demagnetizing factors, we can find magnetic succeptibility in a simpler form, depending only on the external magnetic field and magnetization of the material. In this case, according to Tyablikov S.V. [12], magnetic succeptibility of a Heisenberg's ferromagnetic has the form:

$$\chi_\perp(\omega) = \frac{\chi_0}{1-(\omega/\omega_R)^2} \qquad (32a)$$

$$\chi_x(\omega) = \frac{\omega}{\omega_R}\chi_\perp(\omega) \qquad (32b)$$

where $\omega_r = \mu H$, and $\lambda_0 = \mu_0/H$, H is external magnetic field, and μ_0 is magnetization of the material at the temperature θ.

Then, for our superlattice magnetic succeptibility of the n-th layer has the form:

$$\chi_n^\perp(\omega) = \frac{\Omega_n^M\Omega_n^H}{(\Omega_n^H)^2 - \omega^2} \qquad (33a)$$

$$\chi_n^{(x)}(\omega) = \frac{\omega\Omega_n^M}{(\Omega_n^H)^2 - \omega^2} \qquad (33b)$$

where

$$\Omega_n^H = g_n M_B (H_0 + H_n^a) \qquad (34)$$

$$\Omega_n^H = g_n\mu_B\mu_n \qquad (35)$$

and n is the local low-temperature magnetization in the n-th layer defined by the formula (12).

Thus, in this form of magnetic succeptibility the influence of neighboring layers of superlattice is revealed by μ_n local magnetization, which is can be found via $G_{n,n}(k_n,\omega)$ Green function.

5. CONCLUSION

The results obtained above show that Green function method is applicable for superlattice as well. Calculation of physical parameters of a superlattice is reduced to Green function for separate layers. For a superlattice with two layers in a unit cell (different magnetic layers alter as ABABA...) density of states of magnons and local magnetization were calculated by this method in the paper by Zhou and Lin [2]. This method allows to investigate complex superlattices.

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MAGNIT IFRAT GƏFƏSLƏRI ÜCÜN GRIN FUNKSIYALARI METODU.

Elementar ozəyi ixtiyari sayda müxtəlif ferromagnit laylardan ibarət magnit ifrat gəfəsin modelinə baxilmisdir. Grin funksiyalari və transfer-matrisa metodlari vasitəsilə ifrat gəfəsin magnonlar spectri, alçagtemperaturlu magnitləşməsi və magnit gavrayiciliği hesablanmisdir.

Г.Р.ШАУЛОВ, У.С.ПАШАБЕКОВА

МЕТОД ФУНКЦИЙ ГРИНА ДЛЯ МАГНИТНЫХ СВЕРХРЕШЕТОК

Рассмотрена модель магнитной сверхрешетки, элементарная ячейка которой состоит из произвольного числа различных ферромагнитных слоев. Методами функций Грина и трансфер-матрицы получены спектр магнонов, низкотемпературная намагниченность и магнитная восприимчивость верхрешетки.

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