Green Function Method for Ferromagnetic Superlattice Nanotubes

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Spin-waves excitations propagating along the superlattice nanotubes are investigated by use of the many-body Green function method of quantum statistical theory. The elementary unit cell of superlattice nanotubes constructed of l atomic layers of ferromagnetic material a and r atomic layers of different ferromagnetic material b. The exchange coupling between two neighboring magnetic atoms of material a (or b) in intralayer and interlayer are $J_a(J_b)$ and $Y_a(Y_b)$, respectively. Exchange interactions between neighboring spins of two adjacent a and b materials is Y. An external magnetic field h is applied along the z-direction. Continuous and discrete components of the total wave vector are used to take into account the periodicity of the nanotubes along the z-axis and circumferential direction. Within the framework of random-phase approximation the expressions of Green functions for different spins of nanotubes, which are modeled as having a hexagonal cross section, are derived by recurrence relation technique. The results are illustrated numerically for a particular choice of parameters. The spin-wave spectra for reduced frequency ω/J_a versus the wave-vector component, which characterizes periodicity in the z direction for the system under consideration, are demonstrated. Moreover, in order to clarify the effect of exchange interaction and the number of atomic layers l and r in the elementary unit cell on dispersion law, the results are presented for the various values of discrete components of wave-vector. It is found that four energy ranges exist for the spin waves propagating along the z direction. When both k_a and k_b are real superlattices, dispersion curve exhibits brood pass band and narrow stop bands.

Keywords: Nanotubes, Superlattice, Spin waves, Green function, Interlayer exchange coupling.

1. INTRODUCTION

Currently, there is an increasing emphasis on the magnetic properties of nanosized materials. The reason for this is that they have extraordinary properties compared to bulk materials and have the potential to be used in magnetoelectronic devices [1-4]. Multidimensional structures play an important role in multifunctional bioanalysis, biosensors, magnetic cell division and gene delivery. Therefore, the magnetic properties of these systems are of particular interest to many scientists, both experimental and theoretical [5-8]. Experimentally, many requests have been made to fabricate such nanomaterials using electron beam lithography, vapor-liquid solid and wet chemical methods [9-11]. Theoretically, different superlattices, nanotubes and nanowires can be modeled with finite spins of the selected size, and the magnetic properties of these structures are actively studied using various techniques, such as Green function technique (GF), mean field approximation (MFA), effective field theory (EFT) and Monte Carlo (MC) simulation techniques [12-16].

Compared to bulk systems, both superlattice and nanotubes systems show new magnetic and electronic features. The magnetic behavior of nanoscale magnetic objects is strongly dependent on size, shape and composition. The study of spin waves is very useful in defining the fundamental parameters that characterize these structures.

The organization of this work is as follows: in section 2 we give the model and formalism of the GF. Section 3 is devoted to results and discussions.

2. MODEL AND FORMULATION

The schematic representation of the system can be seen in Fig. 1 in two different perspectives. Elementary cell of hexagonal ferromagnetic superlattice nanotubes (SLNTs) consists of l atomic layers of material a and r atomic layers of material b, having exchange constants J_a and J_b in intralayer and Y_a and Y_b in interlayer, respectively. On the other hand, the exchange interaction between neighboring spins on two adjacent a and b materials is Y. Each atomic layer is assumed to be the xy plane and lattice constant of the SLNTs is $D = (l + r)d$.
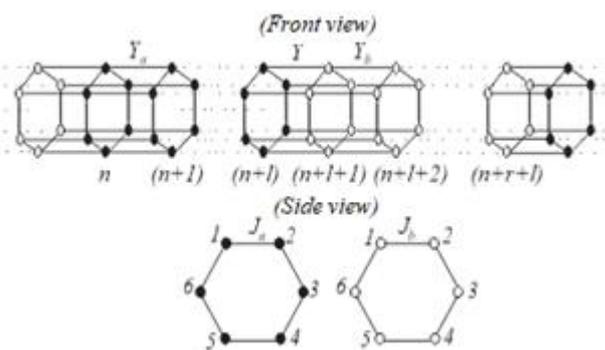

Fig. 1 – Model of hexagonal ferromagnetic nanotubes in which l atomic layers of material a alternate with r atomic layers of material b. The nanotubes are infinite in the direction perpendicular to the axes z

In studying magnetic properties of such systems, two periodic conditions have been taking into account. Therefore, the total wave vector has two components $k_{tot} = f(k, q)$. The wave-vector component denoted as k is

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within the first Brillion zone and characterizes periodicity in the z direction. The other component denoted as q characterizes periodicity in the xy plane and takes the following discrete values [17]:

$$q = \pi v/3d, v = 0,1,2,...,5 . \qquad (1)$$

The Hamiltonian of the system can be written in the form

$$H = H_a + H_b + H'_a + H'_b,$$
$$H_{a(b)} = -J_{a(b)} \sum_{j,\tau,\delta} S_j^\tau S_j^{\tau+\delta} - Y_{a(b)} \sum_{j,\tau} \left(S_j^\tau S_{j-1}^\tau + S_j^\tau S_{j+1}^\tau \right) - h \sum_{j,\tau} S_j^\tau, (2)$$
$$H'_{a(b)} = - \sum_{j,\tau,\delta} \left(Y_{a(b)} S_j^\tau S_{j-1}^\tau + Y S_j^\tau S_{j+1}^\tau \right).$$

Here, $\lambda_a = h + 2J_a\langle S^z\rangle + 2Y_a\langle S^z\rangle - 2J_a\langle S^z\rangle \cos qd$, also the random-phase approximation (RPA) decoupling and discrete Fourier transformation in circumferential direction (in the xy plane) [17, 18] have been made.

Here, j is the number of layers, while τ represents the position in this layer and the sum on δ is over nearest neighbors only. H_a and H_b describe exchange interactions between the neighboring spins and Zeeman's energy when j belongs to materials a and b, respectively. Also, h is the externally applied field along the SLNTs under consideration and it is assumed to be parallel to the z axis. Exchange interactions between neighboring spins on two adjacent a and b materials are described by the terms H'_a and H_b.

We evaluate a retarded GF of the form $\langle\langle S_{n,\tau'}^+ S_{m,\tau}^- \rangle\rangle$ denoted as $G_{n,m}^{\tau',\tau}$. Assuming that n-th and m-th layers belong to material a, by using the model Hamiltonian (2) the explicit equation for the GF can be written as:

$$\left(\omega - \lambda_a\right)G_{n+1,m}^{1,\tau} + Y_a\langle S^z\rangle\left(G_{n+2,m}^{1,\tau} + G_{n,m}^{1,\tau}\right) = 2\langle S^z\rangle\delta_{n+1,m}\delta_{1,\tau} . \qquad (3)$$

On the other hand, one can also write the equations of GFs for the spins whose one of the neighboring spins belongs to different material.

$$\begin{cases} \left(\omega - \lambda'_a\right)G_{n+1,m}^{1,\tau} + Y_a\langle S^z\rangle G_{n+l-1,m}^{1,\tau} + Y\langle S^z\rangle G_{n+l+1,m}^{1,\tau} = 2\langle S^z\rangle\delta_{n+l,m}\delta_{1,\tau}, \\ \left(\omega - \lambda'_b\right)G_{n+l+1,m}^{1,\tau} + Y_b\langle S^z\rangle G_{n+l+2,m}^{1,\tau} + Y\langle S^z\rangle G_{n+l,m}^{1,\tau} = 2\langle S^z\rangle\delta_{n+l+1,m}\delta_{1,\tau}, \end{cases} \qquad (4)$$

where,

$$\lambda'_{a(b)} = h + 2J_{a(b)}\langle S^z\rangle + Y_{a(b)}\langle S^z\rangle + Y\langle S^z\rangle - 2J_{a(b)}\langle S^z\rangle \cos qd .$$

Equations (3) and (4) can be solved by recurrence relation technique to relate the Green functions for different spins at the first and second atomic layers of elementary unit cell [19, 20]

$$\begin{pmatrix} G_{n+l+2,m}^{1,\tau} \\ G_{n+l+1,m}^{1,\tau} \end{pmatrix} = T''_a T_a^{l-1} \begin{pmatrix} G_{n+1,m}^{1,\tau} \\ G_{n,m}^{1,\tau} \end{pmatrix} + T'_a \sum_{k=2}^{l} T_a^{l-k} \begin{pmatrix} 2\delta_{n+k-1,m}\delta_{1,\tau}/Y_a \\ 0 \end{pmatrix} + \begin{pmatrix} 2\delta_{n+l,m}\delta_{1,\tau}\left\{1/Y_b - \left(\omega - \lambda'_b\right)/YY_b\langle S^z\rangle\right\} \\ 2\delta_{n+l+1,m}\delta_{1,\tau}/Y \end{pmatrix}. \qquad (5)$$

The matrix T'_a and the power of matrix T_a have the form:

$$T'_a = \begin{pmatrix} \left(\omega - \lambda'_a\right)\left(\omega - \lambda'_b\right)/YY_b\langle S^z\rangle^2 - Y/Y_b & Y_a\left(\omega - \lambda'_b\right)/YY_b\langle S^z\rangle \\ -\left(\omega - \lambda'_a\right)/Y\langle S^z\rangle & -Y_a/Y \end{pmatrix}, \qquad (6a)$$

$$T_a^{l-1} = \frac{1}{\sin(k_a d)} \begin{pmatrix} \sin\{lk_a d\} & -\sin\{(l-1)k_a d\} \\ \sin\{(l-1)k_a d\} & -\sin\{(l-2)k_a d\} \end{pmatrix}, \qquad (6b)$$

$k_a d$ is defined by the expression

$$\cos(k_a d) \equiv \gamma_a = \left(\lambda_a - \omega\right)/2Y_a\langle S^z\rangle . \qquad (6c)$$

For $|\gamma_a| > 1$, $\gamma_a = \cosh(k_a d)$, and one replaces $\sin(nk_a d)$ by $\sinh(nk_a d)$ for $\gamma_a > 1$ and $(-1)^n \sinh(nk_a d)$ for $\gamma_a < -1$.

Using (5) we can easily determine the matrix of transfer, which relates the GFs of spins in the left first

and second atomic layers of a neighboring unit cell

$$\begin{pmatrix} G_{n+l+r+2,m}^{1,\tau} \\ G_{n+l+r+1,m}^{1,\tau} \end{pmatrix} = T \begin{pmatrix} G_{n+1,m}^{1,\tau} \\ G_{n,m}^{1,\tau} \end{pmatrix} + \begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix}, \qquad (7)$$

where $T = T''_b T_b^{r-1} T''_a T_a^{l-1}$ and

$$
\begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix} = \begin{cases} T_b''T_b^{r-1}T_a'T_a^{l+n-m-1}\begin{pmatrix} 2/Y_a \\ 0 \end{pmatrix} & n+1 \le m \le n+l-1 \\[12pt] T_b''T_b^{r-1}\begin{pmatrix} 2/Y_b - 2(\omega - \lambda_b')/YY_b\langle S^z\rangle \\ 0 \end{pmatrix} & m = n+l \\[12pt] T_b''T_b^{r-1}\begin{pmatrix} 0 \\ 2/Y \end{pmatrix} & m = n+l+1 \\[12pt] T_b''T_a^{r+l+n-m}\begin{pmatrix} 2/Y_b \\ 0 \end{pmatrix} & n+l+2 \le m \le n+l+r-1 \\[12pt] \begin{pmatrix} 2/Y_a - 2(\omega - \lambda_a')/YY_a\langle S^z\rangle \\ 0 \end{pmatrix} & m = n+l+r \\[12pt] \begin{pmatrix} 0 \\ 2/Y \end{pmatrix} & m = n+l+r+1 \end{cases} \quad (8)
$$

The matrix elements T_b' and T_b are obtained by replacing all subscripts a by b, and all b by a in the matrix elements T_a' and T_a, respectively. The matrix elements T fulfill the following conditions:

$$
\det T = 1, \quad Tr(T) = Tr(T^{-1}), \quad (9)
$$

where $Tr(T)$ and $Tr(T^{-1})$ are the sum of diagonal elements of T and that of inverse matrix, respectively.

Due to the fact that the system is periodic in the z direction, according to Bloch's theorem we can write

$$
\begin{pmatrix} G_{n+l+r+2,m}^{1,\tau} \\ G_{n+l+r+1,m}^{1,\tau} \end{pmatrix} = \exp[iKD]\begin{pmatrix} G_{n+1,m}^{1,\tau} \\ G_{n,m}^{1,\tau} \end{pmatrix}. \quad (10)
$$

The expression of GF $G_{n+1,m}^{1,\tau}$ and $G_{n,m}^{1,\tau}$ are obtained by using equations (7-9) and (10):

$$
G_{n+1,m}^{1,\tau} = \frac{(\Delta_2 T_{12} - \Delta_1 T_{22})\exp[-iKD] + \Delta_1}{2\cos(KD) - T_{11} - T_{22}}, \quad (11a)
$$

$$
G_{n,m}^{1,\tau} = \frac{(\Delta_1 T_{21} - \Delta_2 T_{11})\exp[-iKD] + \Delta_2}{2\cos(KD) - T_{11} - T_{22}}. \quad (11b)
$$

The GFs for all layers of elementary unit of SLNTs are related to $G_{n,m}^{1,\tau}$ and $G_{n+1,m}^{1,\tau}$ by recurrence relation technique. As known, the spin-wave dispersion spectrum is obtained from the poles of the GFs:

$$
\cos(KD) = 0,5(T_{11} + T_{22}). \quad (12)
$$

3. RESULTS AND DISCUSSION

In this section, as numerical illustration dispersion equation of spin waves propagating along the SLNTs has been studied. The wave vector k characterizing these spin waves depends on k_a and k_b and the latter two quantities are related to ω by the expression (6c). Consequently, dispersion law for SLNTs is related to the dispersion law for components. It is known that there are four spin-wave branches for component nanotubes a and b. Fig. 2a, c, e, g show these spin-wave dispersion curves for a particular choice of parameters, while Fig. 2b, d, f, h show the spin-wave dispersion curves of the SLNTs. The SLNTs dispersion curve exhibits
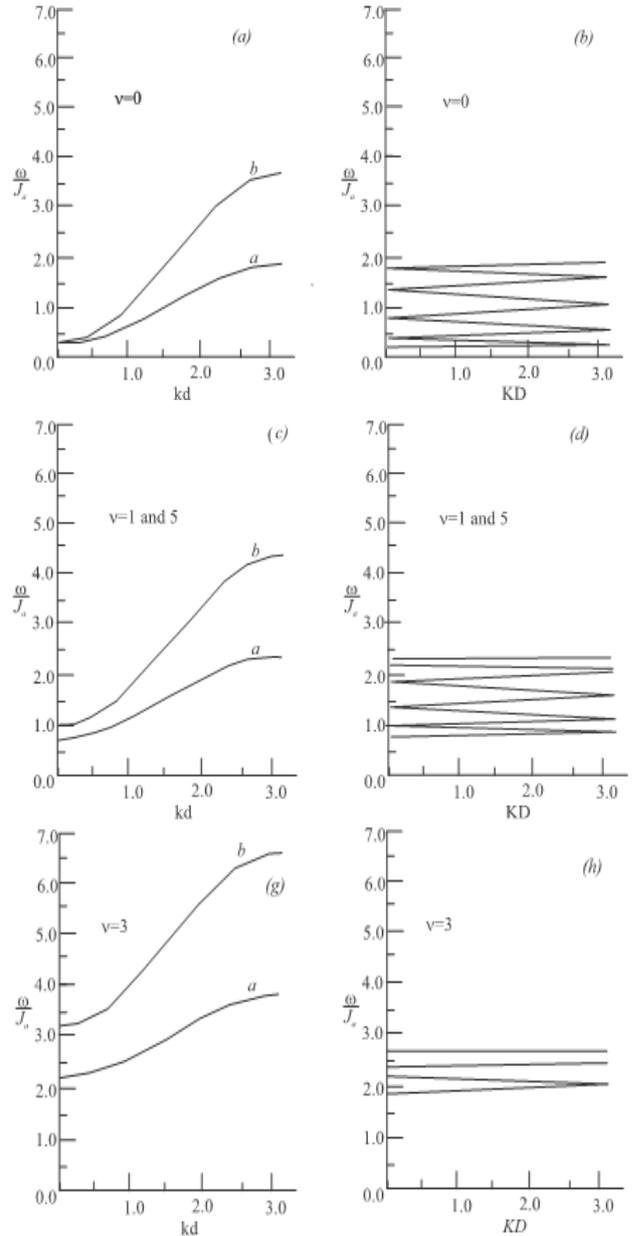

Fig. 2 – The spin-wave dispersion graphs with parameters: $h = 0.2$, $l = 5$, $r = 5$, $\langle S^z\rangle = 0.5$, $Y_a/J_a = 0.8$, $J_b/J_a = 1.5$, $Y_b/J_a = 1.7$, $Y/J_a = 1$

brood pass bands and narrow frequency bands in the frequency range where both component nanotubes a and b have bulk spin waves. This frequency range (in the unit of J_a) corresponds to that, both k_a and k_b are real and $|\cos k_{a(b)}d| \leq 1$. The number of frequency gaps increases with increasing number of atomic layers l

and r in the elementary unit cell of the SLNTs. The forbidden bands appear in the region of frequencies where at least one of both k_a and k_b is complex. The frequencies for the lowest branches are not zero at $kd = 0$ (or $KD = 0$). Easily, it can be explained by the applied external magnetic field.

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Метод функцій Гріна для феромагнітних нанотрубок з надрешіткою

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Збудження спінових хвиль, що поширюються вздовж нанотрубок з надрешіткою, досліджується за допомогою методу функцій Гріна для багатьох тіл у квантовій статистичній теорії. Елементарна комірка нанотрубок з надрешіткою побудована з l атомних шарів феромагнітного матеріалу a та r атомних шарів іншого феромагнітного матеріалу b. Обмінний зв'язок між двома сусідніми магнітними атомами матеріалу a (або b) всередині шарів та між шарами дорівнює відповідно $J_a(J_b)$ та $Y_a(Y_b)$. Обмінна взаємодія між сусідніми спінами двох суміжних матеріалів a і b складає Y. Зовнішнє магнітне поле h прикладене уздовж z-напрямку. Безперервні та дискретні компоненти сумарного хвильового вектора використовуються для врахування періодичності нанотрубок уздовж осі z та напрямку по колу. В рамках наближення випадкової фази вирази функцій Гріна для різних спінів нанотрубок, які моделюються як такі, що мають гексагональний переріз, отримані методом рекурентних співвідношень. Результати проілюстровано чисельно для певного вибору параметрів. Продемонстровано спектри спінової хвилі для зменшеної частоти ω/J_a від компоненти хвильового вектора, який характеризує періодичність у напрямку z для розглянутої системи. Крім того, для уточнення впливу обмінної взаємодії та кількості атомних шарів l і r у елементарній комірці на закон дисперсії, представлено результати для різних значень дискретних компонентів хвильового вектора. Встановлено, що для спінових хвиль, що поширюються у напрямку z, існує чотири діапазони енергії. Коли обидві k_a та k_b є справжніми надрешітками, крива дисперсії демонструє зародкову смугу проходження і вузькі смуги затримки.

Ключові слова: Нанотрубки, Надрешітка, Спінові хвилі, Функція Гріна, Міжшарова обмінна взаємодія.