A MICROSCOPIC THEORY OF SPIN EXCITATIONS IN A CYLINDRICAL FERROMAGNETIC NANOTUBES

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Spin-waves excitations in a cylindrical ferromagnetic nanotubes are investigated by use of the Green function method. The nano-tube consists of the core and the surface shell and the core is surrounded by the surface shell. The expressions of Green's function for different spins of ferromagnetic nanotubes are obtained. The temperature dependence of magnetization is clarified in the surface shell and core. The results are illustrated numerically for a particular choice of parameters

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1. INTRODUCTION

In the last decade, there has been growing attention to the magnetic properties of materials at the nanoscales, such as nanowires, nanoparticles, nanofilms, nanobelts, nanotubes, nanorods etc [1-3]. The reason is that these materials have potential for applications in magneto-electronic devices. On the other hand, these systems show many new typical, peculiar, and unexpected magnetic properties that cannot be exhibit in bulk systems [4-6]. In the experimental area, the ferromagnetic nano-tubes have been successfully synthesized by various methods and there magnetic properties have been investigated. Magnetic nanotubes have potential applications in ultrahigh-density magnetic storage devices, biotechnology, nanomedicine, information storage devices, and nanoelectronic devices etc [7-9].

In the theoretical area, the magnetic nanomaterials have been investigated within the various theoretical methods, such as effective- field theory (EFT) with correlations, Monte Carlo Simulations (MC_S), mean-field approximation (MFA), Green's function (GF) formalism [10-12].

Spin-wave excitations in ferromagnetic nanotube have recently been studied by a number of authors [5,6]. For example, A.L.Gonzalez, P.Landeros, Alvaro S.Nunes investigate the spin wave spectra associated to a vortex domain wall confined within a ferromagnetic nanotube [2]. Bin-Zhou Mi, Huai-Yu Wang Yun-Song Zhou developed a microscopic theory for magnetic behaviors of single-walled nanotubes use of the many-body Green's function method [6]. A nanotube can be modeled as having a chosen shape and size cross section (in the x-y plane) with a finite number spins arranged. The magnetic properties of nanostructures are strongly dependent on the system shape and size.

2. MODEL AND FORMULATION

The schematic representation of nanotube with core-surface shell structure is displayed in fig.1. The black and white circles are magnetic atoms constituting the core and surface shell, respectively. The lines connecting them represent the nearest-neighbor exchange interaction. On the other hand, each spins is connected to the nearest-neighbor spins on the above and below section.

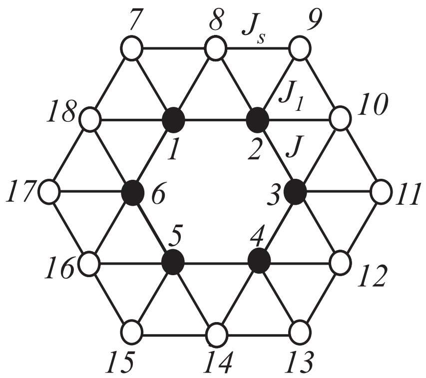

Fig.1. Schematic representation of a cylindrical nanotubes (side view). The nanotubes are infinite in the direction perpendicular to the axes z.

The system will be represented by the Hamiltonian

$$H = -J_s \sum_{i,\delta} S_i S_{i+\delta} - J \sum_{j,\delta} S_j S_{j+\delta} - J_1 \sum_{l,m} S_i S_j - h\left(\sum_i S_i^z + \sum_j S_j^z \right) - D\left(\sum_i \left(S_i^z\right)^2 + \sum_j \left(S_j^z\right)^2 \right) \quad (1)$$

where J_s, J and J_1 are the exchange coupling between two neighboring magnetic atoms at the shell surface, core and shell surface and core, respectively. S_i and S_j are spin operators, the sum δ is over nearest neighbors only at surface and core. The second term of Eq. (1) describes the Zeeman interaction of the spins when an external magnetic field h applied along the z-direction, the last contribution is a single-ion anisotropy term (i.e. crystal field).

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To study the magnetic properties of the nanotube under consideration, we evaluate a retarded GF of the form $\langle\langle S_i^+(t); S_j^-(t')\rangle\rangle$. After time Fourier transformation the retarded GF is denoted as $G_{i,j}(\omega) = \langle\langle S_i^+; S_j^-\rangle\rangle_\omega$, and then employing the equation of motion in the random-phase- approximation (RPA), one obtains the following equations

$$\begin{cases} \left(\omega - h - D - 4J\langle S_c^z\rangle - 3J_1\langle S_s^z\rangle\right)G_{n,m}^{1,\tau} + J\langle S_c^z\rangle\left(G_{n,m}^{2,\tau} + G_{n,m}^{6,\tau} + G_{n+1,m}^{1,\tau} + G_{n-1,m}^{1,\tau}\right) + J_1\langle S_c^z\rangle\left(G_{n,m}^{18,\tau} + G_{n,m}^{8,\tau} + G_{n,m}^{7,\tau}\right) = \delta_{n,m}\delta_{1,\tau} \\ \left(\omega - h - D - 4J_s\langle S_s^z\rangle - J_1\langle S_c^z\rangle\right)G_{n,m}^{7,\tau} + J_s\langle S_s^z\rangle\left(G_{n,m}^{8,\tau} + G_{n,m}^{18,\tau} + G_{n+1,m}^{7,\tau} + G_{n-1,m}^{7,\tau}\right) + J_1\langle S_s^z\rangle G_{n,m}^{1,\tau} = \delta_{n,m}\delta_{7,\tau} \\ \left(\omega - h - D - 4J_s\langle S_s^z\rangle - 2J_1\langle S_c^z\rangle\right)G_{n,m}^{8,\tau} + J_s\langle S_s^z\rangle\left(G_{n,m}^{7,\tau} + G_{n,m}^{9,\tau} + G_{n+1,m}^{8,\tau} + G_{n-1,m}^{8,\tau}\right) + J_1\langle S_s^z\rangle\left(G_{n,m}^{1,\tau} + G_{n,m}^{2,\tau}\right) = \delta_{n,m}\delta_{8,\tau} \end{cases} \qquad (2)$$

here n and m are layer indices, while 1,…,18 and τ label the position of the spins in layers n and m, respectively.

Now the GF is further Fourier transformed along the nanotube axis which periodic boundary condition. The total wave vector has two components $k_{tot} = (k, q)$. The system is periodic in the z direction, which lattice constant is a. According to Bloch's theorem has been employed for plane waves in order to receive the system equations [13,14]

$$G_{n\pm1,m}^{(1,7,8),\tau} = \exp[\pm ika]G_{n,m}^{(1,7,8,),\tau} \qquad (3)$$

As for circumferential direction, the discrete Fourier transformed is taken with periodicity condition. One of wave vector component denoted as q takes the following values [6]:

$$q = \frac{\pi l}{3a} \quad l = 0,1,2,...,5 \qquad (4)$$

Then the Fourier transformation of the GF is written as

$$G_{n,m}^{(6,18),\tau} = \frac{1}{6}\sum_{l=o}^{5} G_{n,m}^{(1,8),\tau} \exp[-iqa] \; ; \; G_{n,m}^{(2,9),\tau} = \frac{1}{6}\sum_{l=o}^{5} G_{n,m}^{(1,7),\tau} \exp[iqa] \qquad (5)$$

Using (3) and (5) the GF can be obtained by solving the equations (2)

$$G_{n,n}^{\tau,\tau} = \sum_{l=1}^{3}\frac{\alpha_1(\omega_{kl})}{\omega - \omega_{kl}} + \sum_{l=4}^{6}\frac{\alpha_4(\omega_{kl})}{\omega - \omega_{kl}} + \sum_{l=7}^{9}\frac{\alpha_7(\omega_{kl})}{\omega - \omega_{kl}} + \sum_{l=10}^{11}\frac{\alpha_{10}(\omega_{kl})}{\omega - \omega_{kl}}; \quad \tau = (1,....,6)$$

$$\alpha_1(\omega_{kl}) = \frac{(\omega_{k,l} - \lambda_s)^2 - J_1\langle S_c^z\rangle(\omega_{k,l} - \lambda_s) - J_s^2\langle S_s^z\rangle^2}{3\prod_{j\neq l}(\omega_{kl} - \omega_{kj})}$$

$$\alpha_4(\omega_{kl}) = \frac{(\omega_{k,l} - \lambda_s)^2 - J_1\langle S_c^z\rangle(\omega_{k,l} - \lambda_s) - 3J_s^2\langle S_s^z\rangle^2}{3\prod_{j\neq l}(\omega_{kl} - \omega_{kj})}$$

$$\alpha_7(\omega_{kl}) = \frac{(\omega_{k,l} - \lambda_s)^2 - J_1\langle S_c^z\rangle(\omega_{k,l} - \lambda_s) - 4J_s^2\langle S_s^z\rangle^2}{6\prod_{j\neq l}(\omega_{kl} - \omega_{kj})}$$

$$\alpha_{10}(\omega_{kl}) = \frac{\omega_{k,l} - \lambda_s}{6(\omega_{k,l} - \omega_{k,j})} \quad (j \neq l) \qquad (6a)$$

$$G_{n,n}^{\tau,\tau} = \sum_{l=1}^{3} \frac{\beta_1(\omega_{kl})}{\omega-\omega_{kl}} + \sum_{l=4}^{6} \frac{\beta_4(\omega_{kl})}{\omega-\omega_{kl}} + \sum_{l=7}^{9} \frac{\beta_7(\omega_{kl})}{\omega-\omega_{kl}} + \sum_{l=10}^{11} \frac{\beta_{10}(\omega_{kl})}{\omega-\omega_{kl}}; \quad \tau = (7, 9, 11, ..., 17)$$

$$\beta_1(\omega_{kl}) = \frac{(\omega_{k,l}-\lambda_c)(\omega_{k,l}-\lambda_s) - J_1\langle S_c^z\rangle(\omega_{k,l}-\lambda_c + J_1\langle S_s^z\rangle) - J\langle S_c^z\rangle(\omega_{k,l}-\lambda_s - J_1\langle S_c^z\rangle)}{3\prod_{j\neq l}(\omega_{kl}-\omega_{kj})}$$

$$\beta_4(\omega_{kl}) = \frac{(\omega_{k,l}-\lambda_c)(\omega_{k,l}-\lambda_s) - J_1\langle S_c^z\rangle(\omega_{k,l}-\lambda_c + 3J_1\langle S_s^z\rangle) + J\langle S_c^z\rangle(\omega_{k,l}-\lambda_s - J_1\langle S_c^z\rangle)}{3\prod_{j\neq l}(\omega_{kl}-\omega_{kj})} \qquad (6b)$$

$$\beta_7(\omega_{kl}) = \frac{(\omega_{k,l}-\lambda_c)(\omega_{k,l}-\lambda_s) - J_1\langle S_c^z\rangle(\omega_{k,l}-\lambda_c + 4J_1\langle S_s^z\rangle) + 2J\langle S_c^z\rangle(\omega_{k,l}-\lambda_s - J_1\langle S_c^z\rangle)}{6\prod_{j\neq l}(\omega_{kl}-\omega_{kj})}$$

$$\beta_{10}(\omega_{kl}) = \frac{\omega_{k,l}-\lambda_c - 2J\langle S_s^z\rangle}{6(\omega_{k,l}-\omega_{k,j})}$$

$$G_{n,n}^{\tau,\tau} = \sum_{l=1}^{3} \frac{\gamma_1(\omega_{kl})}{\omega-\omega_{kl}} + \sum_{l=4}^{6} \frac{\gamma_4(\omega_{kl})}{\omega-\omega_{kl}} + \sum_{l=7}^{9} \frac{\gamma_7(\omega_{kl})}{\omega-\omega_{kl}} + \frac{1}{6(\omega-\omega_{k12})}; \quad \tau = (8, 10, 12, ..., 18)$$

$$\gamma_1(\omega_{kl}) = \frac{J_1^2\langle S_c^z\rangle\langle S_s^z\rangle - (\omega_{k,l}-\lambda_s)(\omega_{k,l}-\lambda_c - J\langle S_c^z\rangle)}{3\prod_{j\neq l}(\omega_{kl}-\omega_{kj})}$$

$$\gamma_4(\omega_{kl}) = \frac{-J_1^2\langle S_c^z\rangle\langle S_s^z\rangle + (\omega_{k,l}-\lambda_s)(\omega_{k,l}-\lambda_c + J\langle S_c^z\rangle)}{3\prod_{j\neq l}(\omega_{kl}-\omega_{kj})} \qquad (6c)$$

$$\gamma_7(\omega_{kl}) = \frac{-J_1^2\langle S_c^z\rangle\langle S_s^z\rangle + (\omega_{k,l}-\lambda_s)(\omega_{k,l}-\lambda_c + 2J\langle S_c^z\rangle)}{6\prod_{j\neq l}(\omega_{kl}-\omega_{kj})}$$

$$\lambda_c = h + D + 3J_1\langle S_s^z\rangle + 2J\langle S_c^z\rangle(2-\cos ka), \quad \lambda_s = h + D + J_1\langle S_c^z\rangle + 2J_s\langle S_s^z\rangle(2-\cos ka)$$

The poles of the Green functions occur at energies, which are the roots of the spin wave dispersion equation for the nanotubes under consideration:

$$\begin{aligned}
&\omega_{ki} = -2r_i \cos(\varphi_i/3) + b_i/3, \quad i = 1,4,7 \\
&\omega_{ki} = 2r_{i-1} \cos((\pi - \varphi_{i-1})/3) + b_{i-1}/3, \quad i = 2,5,8 \\
&\omega_{ki} = 2r_{i-2} \cos((\pi + \varphi_{i-2})/3) + b_{i-2}/3, \quad i = 3,6,9 \\
&\omega_{k10} = 0.5(2J\langle S_c^z\rangle + \lambda_c + \lambda_s) + 0.5\sqrt{(2J\langle S_c^z\rangle + \lambda_c + \lambda_s)^2 + 4(J_1^2\langle S_c^z\rangle\langle S_s^z\rangle - 2J\lambda_c\langle S_c^z\rangle - \lambda_c\lambda_s)} \\
&\omega_{k11} = 0.5(2J\langle S_c^z\rangle + \lambda_c + \lambda_s) - 0.5\sqrt{(2J\langle S_c^z\rangle + \lambda_c + \lambda_s)^2 + 4(J_1^2\langle S_c^z\rangle\langle S_s^z\rangle - 2J\lambda_c\langle S_c^z\rangle - \lambda_c\lambda_s)} \\
&\omega_{k12} = J_1\langle S_c^z\rangle + \lambda_s
\end{aligned} \tag{7}$$

where

$$r_i = \sqrt{\left|3c_i - b_i^2\right|}\Big/3, \quad \varphi_i = \arccos\left(\frac{2b_i^3 - 9b_i c_i + 27d_i}{2\sqrt{(3c_i - b_i^3)^3}}\right) \quad i = 1,4,7$$

$$b_1 = -(J + J_1)\langle S_c^z\rangle - \lambda_c - 2\lambda_s$$

$$c_1 = -2J_1^2\langle S_c^z\rangle\langle S_s^z\rangle - J_s^2\langle S_s^z\rangle^2 + J_1\langle S_c^z\rangle\left(J\langle S_c^z\rangle + \lambda_c + \lambda_s\right) + \lambda_s\left(2J\langle S_c^z\rangle + 2\lambda_c + \lambda_s\right)$$

$$d_1 = J_1^3\langle S_c^z\rangle^2\langle S_s^z\rangle + \left(J\langle S_c^z\rangle + \lambda_c\right)\left(J_s^2\langle S_s^z\rangle^2 - \lambda_s^2 - J_1\langle S_c^z\rangle\lambda_s\right) + 2J_1^2\langle S_c^z\rangle\langle S_s^z\rangle\left(J_s\langle S_s^z\rangle + \lambda_s\right)$$

$$b_4 = (J - J_1)\langle S_c^z\rangle - \lambda_c - 2\lambda_s$$

$$c_4 = -4J_1^2\langle S_c^z\rangle\langle S_s^z\rangle - 3J_s^2\langle S_s^z\rangle^2 + J_1\langle S_c^z\rangle\left(-J\langle S_c^z\rangle + \lambda_c + \lambda_s\right) + \lambda_s\left(-2J\langle S_c^z\rangle + 2\lambda_c + \lambda_s\right)$$

$$d_4 = J_1^3\langle S_c^z\rangle^2\langle S_s^z\rangle - \left(J\langle S_c^z\rangle - \lambda_c\right)\left(3J_s^2\langle S_s^z\rangle^2 - \lambda_s^2 - J_1\langle S_c^z\rangle\lambda_s\right) + 2J_1^2\langle S_c^z\rangle\langle S_s^z\rangle\left(3J_s\langle S_s^z\rangle + 2\lambda_s\right)$$

$$b_7 = (2J - J_1)\langle S_c^z\rangle - \lambda_c - 2\lambda_s$$

$$c_7 = -5J_1^2\langle S_c^z\rangle\langle S_s^z\rangle - 4J_s^2\langle S_s^z\rangle^2 + J_1\langle S_c^z\rangle\left(-2J\langle S_c^z\rangle + \lambda_c + \lambda_s\right) + \lambda_s\left(-4J\langle S_c^z\rangle + 2\lambda_c + \lambda_s\right)$$

$$d_7 = J_1^3\langle S_c^z\rangle^2\langle S_s^z\rangle - \left(2J\langle S_c^z\rangle - \lambda_c\right)\left(4J_s^2\langle S_s^z\rangle^2 - \lambda_s^2 - J_1\langle S_c^z\rangle\lambda_s\right) + J_1^2\langle S_c^z\rangle\langle S_s^z\rangle\left(8J_s\langle S_s^z\rangle + 5\lambda_s\right)$$

Solving the average spin, we derive the correlation function $\langle S^-S^+\rangle$ using the spectrum theorem [14,15]

$$\langle S^-S^+\rangle = -\frac{2S}{N\pi}\sum_k \int_{-\infty}^{\infty} d\omega \frac{\mathrm{Im}G(k,\omega + i\varepsilon)}{e^{\beta\omega} - 1} \tag{8}$$

Here $\beta = 1/k_B T$, k_B is the Boltzmann constant, T is the temperature. Using (5) and the relation $1/(x + i\varepsilon) = \mathrm{P}(1/x) - i\pi\delta(x)$ to obtain the imaginary part of the Green functions, one finally obtains

$$\langle S_{n,\tau}^{-}S_{n,\tau}^{+}\rangle = -\frac{2S}{N}\sum_{k}\left(\sum_{l=1}^{3}\frac{\alpha_1(\omega_{kl})}{e^{\beta\omega_{kl}}-1}+\sum_{l=4}^{6}\frac{\alpha_4(\omega_{kl})}{e^{\beta\omega_{kl}}-1}+\sum_{l=7}^{9}\frac{\alpha_7(\omega_{kl})}{e^{\beta\omega_{kl}}-1}+\sum_{l=10}^{11}\frac{\alpha_{10}(\omega_{kl})}{e^{\beta\omega_{kl}}-1}\right) \quad \tau = 1,2...,6$$

$$\langle S_{n,\tau}^{-}S_{n,\tau}^{+}\rangle = -\frac{2S}{N}\sum_{k}\left(\sum_{l=1}^{3}\frac{\beta_1(\omega_{kl})}{e^{\beta\omega_{kl}}-1}+\sum_{l=4}^{6}\frac{\beta_4(\omega_{kl})}{e^{\beta\omega_{kl}}-1}+\sum_{l=7}^{9}\frac{\beta_7(\omega_{kl})}{e^{\beta\omega_{kl}}-1}+\sum_{l=10}^{11}\frac{\beta_{10}(\omega_{kl})}{e^{\beta\omega_{kl}}-1}\right) \quad \tau = 7,9...,17 \qquad (9)$$

$$\langle S_{n,\tau}^{-}S_{n,\tau}^{+}\rangle = -\frac{2S}{N}\sum_{k}\left(\sum_{l=1}^{3}\frac{\gamma_1(\omega_{kl})}{e^{\beta\omega_{kl}}-1}+\sum_{l=4}^{6}\frac{\gamma_4(\omega_{kl})}{e^{\beta\omega_{kl}}-1}+\sum_{l=7}^{9}\frac{\gamma_7(\omega_{kl})}{e^{\beta\omega_{kl}}-1}+\frac{1}{6\left(e^{\beta\omega_{k12}}-1\right)}\right) \quad \tau = 8,10...,18$$

According to the theory of Callen [16] the average spin can be calculated using the following equation

$$\langle S^{z}\rangle = \frac{(S+1+\Phi)\Phi^{2S+1}+(S-\Phi)(1+\Phi)^{2S+1}}{\Phi^{2S+1}-(1+\Phi)^{2S+1}} \qquad (10)$$

where $\Phi = \dfrac{\langle S^{-}S^{+}\rangle}{2\langle S^{z}\rangle}$

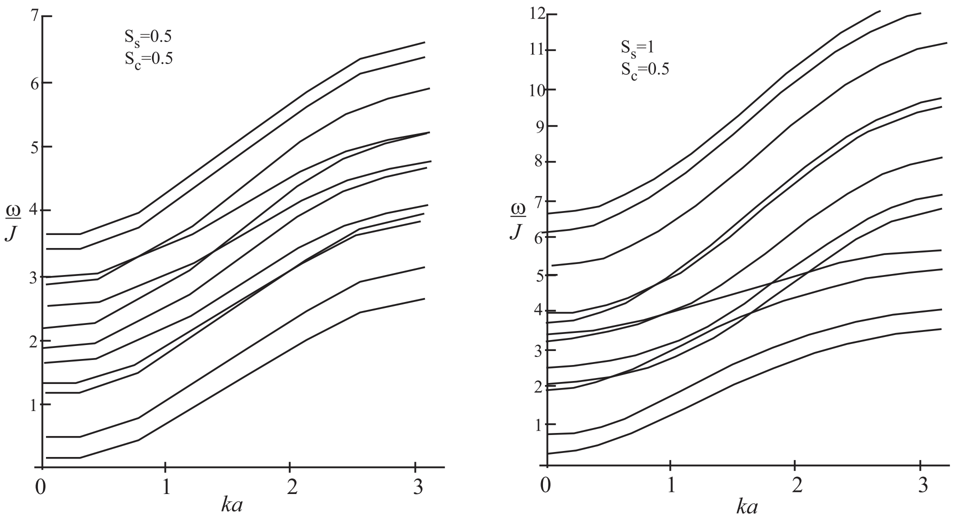

Fig. 2. Spin wave frequency versus wave number *ka* for the nanotubes under consideration with parameters $h/J = 0.2, \quad D/J = 0.1, \; J_1/J = 0.5, \; J_s/J = 1.5$.

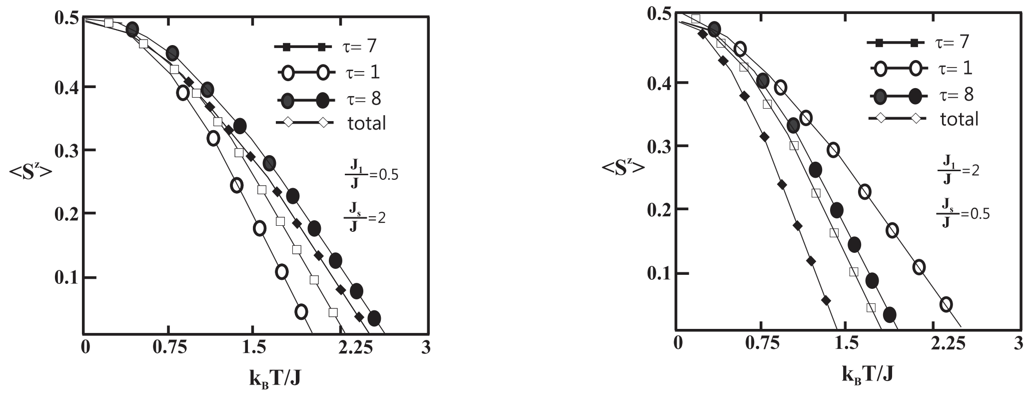

Fig. 3. Temperature dependence of the spin magnetization for the parameters $h/J = 0.2, \quad D/J = 0.1, \quad S_c = S_s = 0.5$

Now the equation (8) and (9) can be solved self consistently to obtain the average spin at any given temperature.

If $S = 1/2 \quad \langle S^{z}\rangle = \frac{1}{2} - \langle S^{-}S^{+}\rangle$.

3. CONCLUSIONS

In this paper, we present the theory of spin-wave excitations of a cylindrical ferromagnetic nanotubes. Dispersion equations of spin waves propagating along the nanotubes, and temperature dependence of magnetizations for nanotube with core/shell structure have been studied. Fig. 2 shows spin-wave spectra for reduced frequency ω/J versus *ka* for nanotubes under consideration. The frequencies for the lowest branches are not zero at $ka = 0$. Easily, it can be explained by applied external magnetic field and single-ion anisotropy. The spin wave frequencies increase with increasing wave vectors and exchange coupling between spins. On the other hand, with increasing value of the spins spin wave frequencies increase. It can be verified from these results that when $J_1 = 0$ for the nanotubes depicted in fig.1 they reduces for the two magnetic single-walled nanotubes.

The temperature dependence of magnetization in the nanotubes under consideration is demonstrated in fig. 3. The spontaneous magnetization of the spins at zero temperature is $\langle S^z \rangle = 0.5$. The magnetizations decrease continuously with increasing values of temperature, and they become zero at critical temperature; therefore a second-order phase transition occurs. We illustrate the magnetization versus reduced temperature for $J_1/J = 0.5$, $J_s/J = 2$ and $J_1/J = 2$, $J_s/J = 0.5$, respectively. In the each case, the total spin magnetization has the middle value. If exchange interaction between magnetic atoms at surface grows weaker, then their magnetizations are weaker than that of core spins. Magnetization of the surface spins labeled $\tau = 7,9,11,13,15,17$ is smaller than that of the spins labeled $\tau = 8,10,12,14,16,18$. This will be able to understand clearly. For example, surface spin labeled $\tau = 7$ exchange interacts with one core spin labeled $\tau = 7$, while spin labeled $\tau = 8$ with two core spins $\tau = 1$ and $\tau = 2$. But in particular case, when $J_1 = 0$ all spins has the same orientation and the curves coincide.

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