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Local spin excitations in the rectangular ferromagnetic semiconductor nanowires

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A Green function analysis is used to study spin-waves excitations in a ferromagnetic semiconductor nanowires. The expressions of Green function for different spins of ferromagnetic nanowires are derived. The nanowire is modeled as having a cubic cross section. The results are illustrated numerically for a particular choice of parameters

PACS: 75.30.Ds Spin waves;
75.70.Cn Magnetic properties of interfaces.

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Introduction

Materials with magnetic properties periodically modulated at the nanometer scale apart from demonstrating new physical phenomena have potential applications in fields as diverse as optics, electronics, catalysis, magnetism, electrochemistry, information processing and storage. Nowdays preparation of magnetic materials at the nanometer scale can be achieved by different methods, such as electrochemistry, nanoprint techniques, physical deposition combined with micro-fabrication method etc. [1–4].

Both semiconductors and magnetic materials play an important role in modern electronics. Although progress has been made in the understanding magnetic nanostructured materials studies of magnetic semiconductors nanotubes and nanowires (NWs) are still at a nascent stage [5–7]. Ferromagnetic semiconductors NWs can bring interesting applications to future magnetic recording media and electronic devices.

The interplay of magnetism and semiconducting properties has been observed in magnetic semiconductors. However, investigation of nanostructures have shown a noticeable difference in their static magnetic properties as well as the significant advantage of nanosized structures over the bulk state [8–10].

Model and formulation

Theoretically, various nanowires can be modeled as having a chosen shape and size cross section (in the *x*–*y* plane) with a finite number spins arranged [11,12]. These layers are stacked vertically to form a long nanowire extending in the *z* direction from $-\infty$ to ∞.

As indicated in Fig. 1. we consider a simple cubic ferromagnetic semiconductor nanowires. The Hamiltonian describing the local spin of the system is expressed as the sum of two terms:

$$H_M = -\frac{1}{2}\sum_{i,j} J_{i,j} S_i S_j - g\mu_B H_0 \sum_i S_i^z ,$$

$$H_I = -I\sum_i S_i s_i . \tag{1}$$

H_M is the Heisenberg Hamiltonian for the localized spins of *d* or *f* type, the most important term is an *s*–*d* (or *s*–*f*) interaction Hamiltonian H_I. Here J_{ij} is the exchange coupling between sites labeled *i* and *j*, $S_{i(j)}$ and $s_{i(j)}$ are the spins operators of localized spins and conductions electrons, respectively. Also, H_0 is externally applied field in the direction along the nanowires under consideration, I is a contact interaction energy.

To study the spin excitations of the system we introduce two types of Green's functions $G_{i,j}(t) = \langle\langle S_i^+(t) \,|\, S_j^-(0)\rangle\rangle$ and $G'_{i,j}(t) = \langle\langle s_i^+(t) \,|\, S_j^-(0)\rangle\rangle$. The equation of motion for the Fourier transform of the Green function's in the random-phase-approximation (RPA) at $T << T_c$ have the following form:

$$\{\omega - g_i\mu_B H_0 - I\langle s_i^z\rangle - \sum_\delta J_{i,i+\delta}\langle S_{i+\delta}^z\rangle\} G_{i,j}(\omega) +$$

$$+ \langle S_i^z\rangle \sum_\delta J_{i,i+\delta} G_{i,i+\delta}(\omega) = 2\langle S_i^z\rangle\delta_{ij}, \quad (2)$$

$$\{\omega - g_e\mu_B H_0 - I\langle S_i^z\rangle\} G'_{i,j}(\omega) - I\langle s_i^z\rangle G_{i,j}(\omega) = 0. \quad (3)$$

Note that in RPA, local spins are assumed to respond only to the total magnetic field which is the sum of external field and local effective field. For all temperatures below T_c it is a good approximation. Combining Eqs. (7) and (8) we obtain the following equation [13,14]:

$$\left\{\omega - g\mu_B H_0 - I\langle s_i^z\rangle - \frac{I^2\langle S_i^z\rangle\langle s_i^z\rangle}{\omega - g_e\mu_B H_0 - I\langle S_i^z\rangle} - \sum_\delta J_{i,i+\delta}\langle S_{i+\delta}^z\rangle\right\} G_{i,j}(\omega) + \langle S_i^z\rangle \sum_\delta J_{i,i+\delta} G_{i,i+\delta}(\omega) = 2\langle S_i^z\rangle\delta_{ij}. \quad (4)$$

Employing the Eq. (4) for the nanowires under consideration one obtains the following system equations:

$$\begin{cases}
(\Omega - 4J_s\langle S^z\rangle) G_{n,m}^{1,\tau} + J_s\langle S^z\rangle (G_{n,m}^{2,\tau} + G_{n,m}^{8,\tau} + G_{n+1,m}^{1,\tau} + G_{n-1,m}^{1,\tau}) = \delta_{n,m}\delta_{1,r}, \\
(\Omega - 4J_s\langle S^z\rangle - J\langle S^z\rangle) G_{n,m}^{2,\tau} + J_s\langle S^z\rangle (G_{n,m}^{1,\tau} + G_{n,m}^{3,\tau} + G_{n+1,m}^{2,\tau} + G_{n-1,m}^{2,\tau}) + J\langle S^z\rangle G_{n,m}^{9,\tau} = \delta_{n,m}\delta_{2,r}, \\
(\Omega - 4J_s\langle S^z\rangle) G_{n,m}^{3,\tau} + J_s\langle S^z\rangle (G_{n,m}^{2,\tau} + G_{n,m}^{4,\tau} + G_{n+1,m}^{3,\tau} + G_{n-1,m}^{3,\tau}) = \delta_{n,m}\delta_{3,r}, \\
(\Omega - 4J_s\langle S^z\rangle - J\langle S^z\rangle) G_{n,m}^{4,\tau} + J_s\langle S^z\rangle (G_{n,m}^{3,\tau} + G_{n,m}^{5,\tau} + G_{n+1,m}^{4,\tau} + G_{n-1,m}^{4,\tau}) + J\langle S^z\rangle G_{n,m}^{9,\tau} = \delta_{n,m}\delta_{4,r}, \\
(\Omega - 4J_s\langle S^z\rangle) G_{n,m}^{5,\tau} + J_s\langle S^z\rangle (G_{n,m}^{4,\tau} + G_{n,m}^{6,\tau} + G_{n+1,m}^{5,\tau} + G_{n-1,m}^{5,\tau}) = \delta_{n,m}\delta_{5,r}, \\
(\Omega - 4J_s\langle S^z\rangle - J\langle S^z\rangle) G_{n,m}^{6,\tau} + J_s\langle S^z\rangle (G_{n,m}^{5,\tau} + G_{n,m}^{7,\tau} + G_{n+1,m}^{6,\tau} + G_{n-1,m}^{6,\tau}) + J\langle S^z\rangle G_{n,m}^{9,\tau} = \delta_{n,m}\delta_{6,r}, \\
(\Omega - 4J_s\langle S^z\rangle) G_{n,m}^{7,\tau} + J_s\langle S^z\rangle (G_{n,m}^{6,\tau} + G_{n,m}^{8,\tau} + G_{n+1,m}^{7,\tau} + G_{n-1,m}^{7,\tau}) = \delta_{n,m}\delta_{7,r}, \\
(\Omega - 4J_s\langle S^z\rangle - J\langle S^z\rangle) G_{n,m}^{8,\tau} + J_s\langle S^z\rangle (G_{n,m}^{7,\tau} + G_{n,m}^{1,\tau} + G_{n+1,m}^{8,\tau} + G_{n-1,m}^{8,\tau}) + J\langle S^z\rangle G_{n,m}^{9,\tau} = \delta_{n,m}\delta_{8,r}, \\
(\Omega - 6J\langle S^z\rangle) G_{n,m}^{9,\tau} + J\langle S^z\rangle (G_{n,m}^{2,\tau} + G_{n,m}^{4,\tau} + G_{n,m}^{6,\tau} + G_{n,m}^{8,\tau} + G_{n+1,m}^{9,\tau} + G_{n-1,m}^{9,\tau}) = \delta_{n,m}\delta_{9,r}.
\end{cases} \quad (5)$$

Here $\Omega = \omega - g\mu H_0 - I\langle s^z\rangle - I^2\langle S^z\rangle\langle s^z\rangle/(\omega - g_e\mu H_0 - I\langle S^z\rangle)$, also n and m are layer indices, while 1, …, 9 and τ label the position of the spins in layers n and m, respectively. As shown in Fig. 1. J is the exchange coupling between spins labeled 1 and its nearest neigbours, and J_s is that between surface spins.

The system is also 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 [14,15]

$$G_{n\pm1,m}^{(1,2,3,4,5,6,7,8,9),\tau} = \exp[\pm ika] G_{n,m}^{(1,2,3,4,5,6,7,8,9),\tau}. \quad (6)$$

Using (6) the Green functions were obtained by solving the Eq. (5):

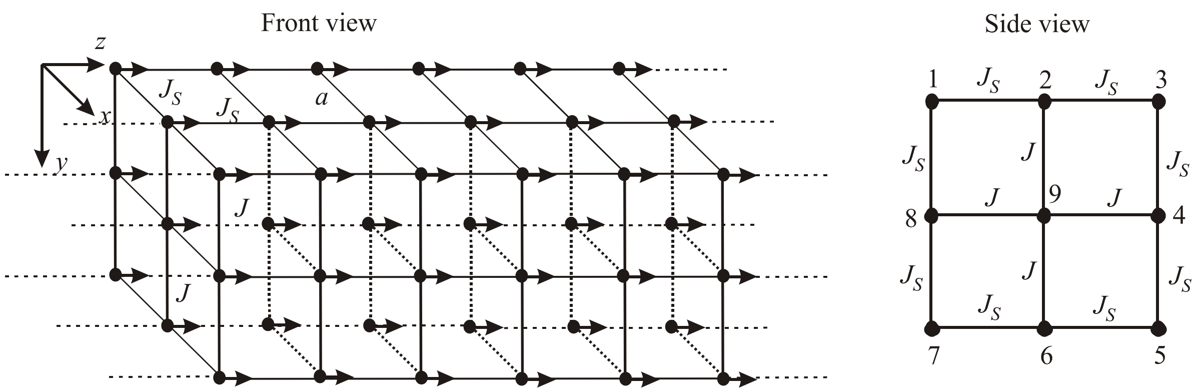

Fig. 1. Model of simple cubic ferromagnetic semiconductor nanowires. The nanowires are infinite in the direction to the axes *z*.

$$G_{n,n}^{\tau,\tau}(\omega)=\sum_{\substack{l=1\\l\neq4}}^{7}\left(\frac{a(\omega_{kl}^{+})}{\omega-\omega_{kl}^{+}}+\frac{a(\omega_{kl}^{-})}{\omega-\omega_{kl}^{-}}\right),\qquad \tau=(1,\,3,\,5,\,7)\,,$$

$$a(\omega_{kl}^{\pm})=\frac{2J_s^4\langle S^z\rangle^4(\Omega_{kl}-\Omega_b)+4J_s^2\langle S^z\rangle^2(\Omega_{kl}-\Omega_t)[J^2\langle S^z\rangle^2+\alpha(\Omega_{kl})]+[4J^2\langle S^z\rangle^2+\alpha(\Omega_{kl})](\Omega_{kl}-\Omega_t)^2(J\langle S^z\rangle-\Omega_{kl}+\Omega_t)}{(\omega_{kl}^{\pm}-\omega_{kl}^{\mp})/(\omega_{kl}^{\pm}-g_e\mu H_0-I\langle S^z\rangle)\prod\limits_{\substack{j\neq l\\j\neq4}}(\Omega_{kl}-\Omega_{kj})},$$

$$\alpha(\Omega_{kl})=(\Omega_{kl}-\Omega_b)(J\langle S^z\rangle-\Omega_{kl}+\Omega_t),\quad G_{n,n}^{\tau,\tau}=\sum_{\substack{l=1\\l\neq5}}^{7}\left(\frac{b(\omega_{kl}^{+})}{\omega-\omega_{kl}^{+}}+\frac{b(\omega_{kl}^{-})}{\omega-\omega_{kl}^{-}}\right),\quad \tau=(2,\,4,\,6,\,8)\,,$$

$$b(\omega_{kl}^{\pm})=\frac{2J_s^4\langle S^z\rangle^4(\Omega_{kl}-\Omega_b)+2J_s^2\langle S^z\rangle^2(\Omega_{kl}-\Omega_t)[J^2\langle S^z\rangle^2+2\alpha(\Omega_{kl})]+[3J^2\langle S^z\rangle^2+\alpha(\Omega_{kl})](\Omega_{kl}-\Omega_t)^2(J\langle S^z\rangle-\Omega_{kl}+\Omega_t)}{(\omega_{kl}^{\pm}-\omega_{kj}^{\mp})/(\omega_{kl}^{\pm}-g_e\mu H_0-I\langle S^z\rangle)\prod\limits_{\substack{j\neq l\\j\neq5}}(\Omega_{kl}-\Omega_{kj})},$$

$$G_{n,n}^{9,9}=\sum_{l=1}^{3}\left(\frac{c(\omega_{kl}^{+})}{\omega-\omega_{kl}^{+}}+\frac{c(\omega_{kl}^{-})}{\omega-\omega_{kl}^{-}}\right);\qquad c(\omega_{kl}^{\pm})=-\frac{4J_s^2\langle S^z\rangle^2+(\Omega_{kl}-\Omega_t)(JS+\Omega_{kl}+\Omega_t)}{(\omega_{kl}^{\pm}-\omega_{kj}^{\mp})/(\omega_{kl}^{\pm}-g_e\mu H_0-I\langle S^z\rangle)\cdot\prod\limits_{\substack{l=1\\j\neq l}}(\Omega_{kl}-\Omega_{kj})}\,. \tag{7}$$

The poles of the Green functions occur at energies, which are the roots of the spin wave dispersion equation for the nanowires under consideration. Note that it was expected to obtain eighteen frequencies in this system. But in fact the expressions for fourteen different frequencies were obtained, because of degenerate in four frequencies.

$$\omega_{kl}^{\pm}=0.5\big(\mu H_0(g_e+g)+I(\langle S^z\rangle+\langle s^z\rangle)+\Omega_{kl}\pm$$
$$\pm\sqrt{[\mu H_0(g_e-g)+I(\langle S^z\rangle-\langle s^z\rangle)-\Omega_{kl}]^2+4I^2\langle S^z\rangle\langle s^z\rangle}\big), \tag{8}$$

$$\Omega_{k1}=-2r\cos(\varphi/3)+(J\langle S^z\rangle+2\Omega_t+\Omega_b)/3,$$
$$\Omega_{k2}=2r\cos((\pi-\varphi)/3)+(J\langle S^z\rangle+2\Omega_t+\Omega_b)/3,$$
$$\Omega_{k3}=2r\cos((\pi+\varphi)/3)+(J\langle S^z\rangle+2\Omega_t+\Omega_b)/3,$$
$$\Omega_{k4}=\Omega_t+J\langle S^z\rangle,$$
$$\Omega_{k5}=\Omega_t,$$
$$\Omega_{k6}=0.5(J\langle S^z\rangle+2\Omega_t)+0.5\langle S^z\rangle\sqrt{J^2+8J_s^2},$$
$$\Omega_{k7}=0.5(J\langle S^z\rangle+2\Omega_t)-0.5\langle S^z\rangle\sqrt{J^2+8J_s^2},$$

where

$$r=\sqrt{|\,3\psi-(J\langle S^z\rangle+2\Omega_t+\Omega_b)^2\,|/3},\qquad \varphi=\arccos\left(\frac{q}{r^3}\right),$$

$$q=(J\langle S^z\rangle+2\Omega_t+\Omega_b)^3/27-\psi(J\langle S^z\rangle+2\Omega_t+\Omega_b)/6-$$
$$-2S^2(J_s^2\Omega_b+J^2\Omega_t)+\Omega_t\Omega_b(J\langle S^z\rangle+\Omega_t)/2\,,$$

$$\psi=-4\langle S^z\rangle^2(J_s^2+J^2)+J\langle S^z\rangle(\Omega_b+\Omega_t)+2\Omega_t\Omega_b+\Omega_t{}^2,$$

$$\Omega_t=2J_s\langle S^z\rangle(2-\cos ka),\quad \Omega_b=2J\langle S^z\rangle(3-\cos ka)\,.$$

To find the average spin, we derive the correlation function $\langle S^-S^+\rangle$ using the spectrum theorem [15,16]

$$\langle S^-S^+\rangle=-\frac{2S}{N\pi}\sum_k\int_{-\infty}^{\infty}d\omega\,\frac{\operatorname{Im}G(k,\omega+i\varepsilon)}{e^{\beta\omega}-1}\,. \tag{9}$$

Here $\beta=1/k_BT$, k_B is the Boltzmann constant, T is the temperature. Using (7) and the relation $1/(x+i\varepsilon)=$ $=P(1/x)-i\pi\delta(x)$ to obtain the imaginary part of the Green functions, we finally found [15]

$$\langle S_{n,9}^-S_{n,9}^+\rangle=-\frac{2S}{N}\sum_k\sum_{l=1}^{3}\left(\frac{c(\omega_{kl}^{+})}{\exp(\beta\omega_{kl}^{+})-1}+\frac{c(\omega_{kl}^{-})}{\exp(\beta\omega_{kl}^{-})-1}\right),$$

$$\langle S_{n,\tau}^-S_{n,\tau}^+\rangle=-\frac{2S}{N}\sum_k\sum_{\substack{l=1\\l\neq4}}^{7}\left(\frac{a(\omega_{kl}^{+})}{\exp(\beta\omega_{kl}^{+})-1}+\frac{a(\omega_{kl}^{-})}{\exp(\beta\omega_{kl}^{+})-1}\right),$$
$$\tau=1,\,3,\,5,\,7, \tag{10}$$

$$\langle S_{n,\tau}^-S_{n,\tau}^+\rangle=-\frac{2S}{N}\sum_k\sum_{\substack{l=1\\l\neq5}}^{7}\left(\frac{b(\omega_{kl}^{+})}{\exp(\beta\omega_{kl}^{+})-1}+\frac{b(\omega_{kl}^{-})}{\exp(\beta\omega_{kl}^{-})-1}\right),$$

$\tau=2,\,4,\,6,\,8.$

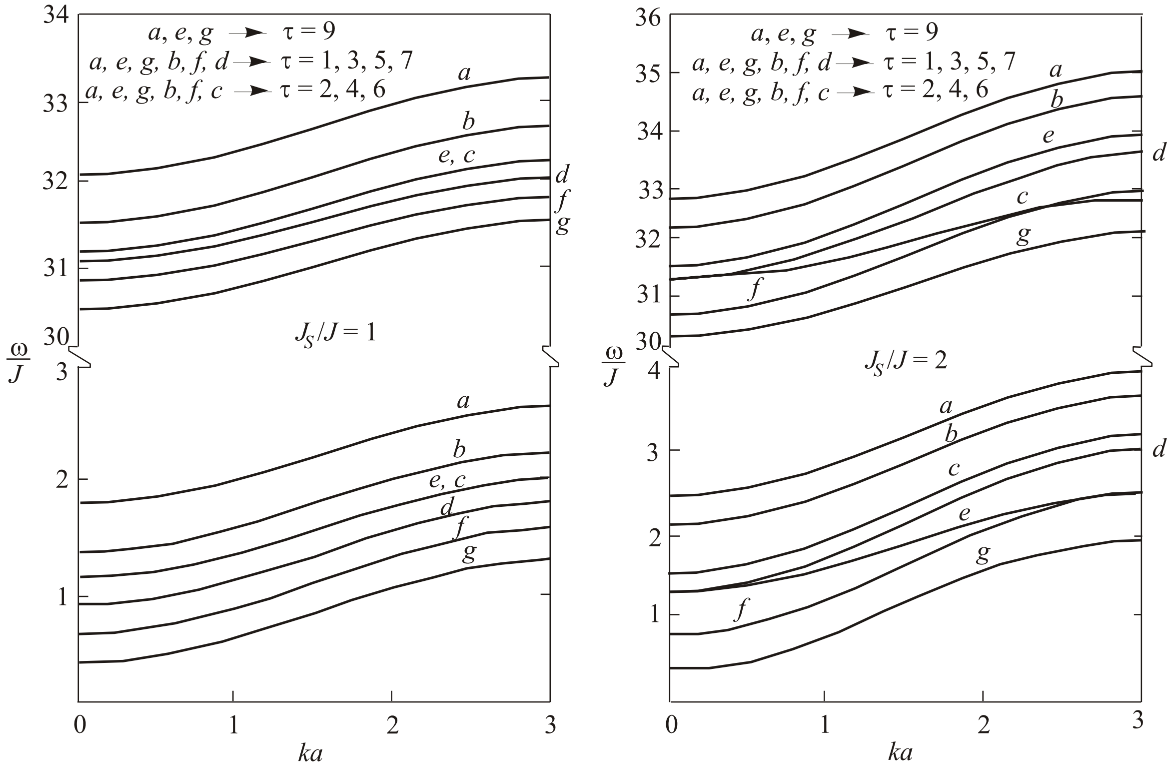

Fig. 2. The frequencies of the spin-wave branches plotted versus ka for nanowires under consideration. The parameters are $g\mu_B H_0/J$ = = 0.3, $g_e\mu_B H_0/J$ = 0.2, $\langle S^z\rangle$ = 0.5, $\langle s^z\rangle$ = 0.5, I/J = 30.

According to the theory of Callen [17] the average spin can be calculated using the following equation:

$$\langle S^z\rangle = \frac{(S+1+\Phi)\Phi^{2S+1}+(S-\Phi)(1+\Phi)^{2S+1}}{\Phi^{2S+1}-(1+\Phi)^{2S+1}}, \quad (11)$$

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

The total average spins of per site of the nanowire under concentration can be calculated as

$$\langle S^z\rangle = \frac{\langle S_9^z\rangle + 4\langle S_1^z\rangle + 4\langle S_2^z\rangle}{9}.$$

Now the Eqs. (10) and (11) can be solved self consistently to obtain the average spin at any given temperature.

If $S = \dfrac{1}{2}$, $\langle S^z\rangle = \dfrac{1}{2} - \langle S^- S^+\rangle$

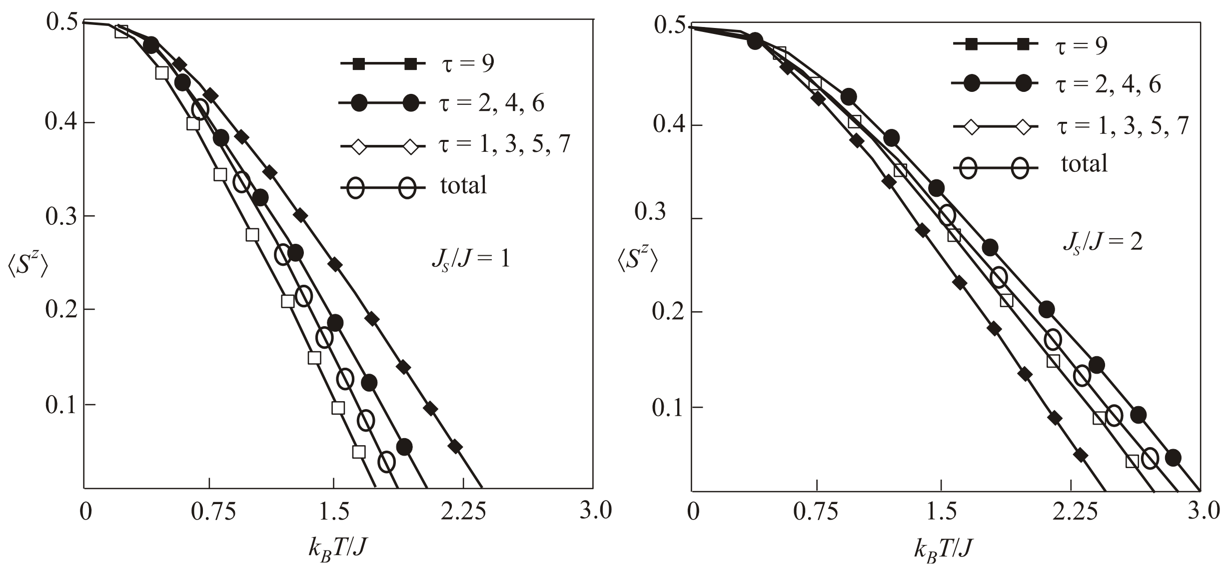

Fig. 3. The temperature dependence of magnetization in the nanowires under consideration. The spontaneous magnetization of the spins at zero temperature is $\langle S^z\rangle$ = 0.5. The parameters are $g\mu_B H_0/J$ = 0.3, $g_e\mu_B H_0/J$ = 0.2, $\langle s^z\rangle$ = 0.5, I/J =30.

Numerical results and discussions

In this section we present numerical calculations of the theoretical results. Figure 2 shows the frequencies of the spin-wave branches plotted versus *ka* for nanowires under consideration. As one can see, spin-wave branches appears in two ranges of low and high frequencies. Both the low and high frequencies have minimum at zero wave vector. The spin wave frequencies increase with increasing wave vectors, exchange coupling between localized spins and also (*sd*) or (*sf*) exchange interaction of the conduction electrons spins.

The temperature dependence of magnetization in the nanowires under consideration is demonstrated in Fig. 3. The spontaneous magnetization of the spins at zero temperature is $\langle S^z \rangle = 0.5$. In the case $J_S = J$ magnetization of the surface spins labeled $\tau = 1, 3, 5, 7$ is smaller than that of the spins labeled $\tau = 2, 4, 6, 8,$ and the bulk spin $(\tau = 9)$ magnetization is stronger than that of the surface spins. With the increase of the exchange interaction between surface localized spins magnetization is stronger than that of bulk localized spins. Besides, the weakening *sd* (*sf*) interaction also decreases the local magnetization and tends to zero at lower temperatures.

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