DYNAMICS OF THREE-WALLED MIXED-SPIN (1/2, 1 AND 3/2) ISING NANOTUBE

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Mean-field approximation and Glauber-type stochastic dynamic approach has been employed to study of three-walled mixed-spin Ising nanotube with an inner hexagonal vacancy. The effects of different exchange couplings, single-ion anisotropies, and temperature on the dynamic behavior of mixed spin (1/2,1, 3/2) Ising system under a time dependent oscillating external magnetic field are attentively discussed. Some different fundamental phases and mixed phases have been observed in the system, which according to the certain values of Hamiltonian parameters. The results are illustrated numerically for a particular choice of parameters.

Keywords: Mixed spin (1/2,1, 3/2) Ising system, Mean-field approximation, Glauber-type stochastic dynamic, Dynamic phase transitions.
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1. INTRODUCTION

In the last two decades, the mixed-spin Ising models belong to the most actively studied lattice-statistical models in the solid-state physics as these systems also supply simple models for the study of nanostructures, which could be potentially useful materials for technological applications [1-6]. On the other hand, these systems have been of interest because they have less translational symmetry than their single-spin counterparts, since they consist of some interpenetrating sublattices.

In particular, Ising systems with spins of different magnitudes are useful models that allow a deeper understanding of the magnetic behavior of certain ferrimagnetic materials. In this regard, the study of the ferrimagnetic behavior of mixed-spin Ising models has become a very active area of research in the last few decades [7-9]. Therefore, the synthesis of new ferrimagnetic material is an active field in material science. However, despite intensive research, there are so far only a few examples of exactly solvable mixed-spin Ising models. Recently, there have been many theoretical studies of mixed-spin Ising ferrimagnetic systems. İn the Ising model, the spins can only lie along one chosen axis which is often taken to be the z-axis. These systems may be relatively easy to deal with when compared with the Heisenberg model, because the spins now have freedom to orient themselves in any three-dimensional space. Many combinations of mixed-spin Ising systems, such as spins (1⁄2, 1), spins (1⁄2, 3⁄2), spins (1, 3⁄2), spins (1, 2), (2, 5⁄2) etc., have been studied [10-13]. Half-integer spin systems are more exciting, because they can show multicritical behavior or a magnetoelastic transition or instability. The most well-known and most studied mixed spin Ising systems are spins (1, 1/2), spins (1/2, 3/2), spins (1, 3/2), and spins (1, 2). Half-integer mixed-spin Ising system (1⁄2, 5⁄2) has been investigated less than spins (1⁄2, 3⁄2). Another possible semi-integer mixed spin Ising system (3/2, 5/2) is the highest mixed spin Ising system and less studied.

The model for different values of spins has been investigated by exact on honey- comb lattice, as well as on Bethe lattice, mean-field approximation, effective-field theory with correlations, cluster variational theory, renormalization-group technique and Monte-Carlo simulation [14-18]. The attention was devoted to the high order two-sublattice mixed spin ferrimagnetic systems, and also three -sublattice mixed -spin Ising sytem in order to constuct their phase diagrams in the temperature -anisotropy plane and to consuder their magnetic properties. Bobak and Dely investigated the effect of single-ion anisotropy on the phase diagram of the mixed spin-3/2 and spin-2 Ising system by the use of a mean-field theory based on the Bogoliubov inequality for the free energy [19]. D. Sabi Takou and others studied thermodynamic properties of the mixed spin-3/2 and spin-1/2 Heisenberg model within the Oguchi approximation in the presence of a random crystal-field [20].

Considerable efforts have been devoted to the magnetic nanostructures and their physical and functional properties [21-26]. Much interest has been paid to the critical investigations of magnetic nanotubes with various structures including single-, and/or multi-walled or core-shell structures. From the theoretical point of view, magnetic properties, for example impact of the applied field and temperature on the magnetic properties counting the magnetization, the susceptibility, the specific heat, and the thermal energy of a transverse Ising nanotube with a core-shell structure are investigated for different cases [27-30].

The present work is motivated by the intense dynamics of research on magnetic nanotubes. We are going to investigate dynamical aspect of the mixed spin-1/2, spin-1 and spin-3/2 Ising system Hamiltonian with a crystal-field interaction in the presence of a time-dependent oscillating external magnetic field. We employ the Glauber transition rates to construct the set of mean-field dynamic equations. We investigate the time variations of average magnetizations to find the phases in the system. The paper will be organized as follows: in Section 2, we briefly outline the model and

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description of the Glauber-type stochastic dynamic and give the mean-field dynamical equations describing the dynamic behavior of the system for the mixed spin that we propose investigating. Finally, numerical results and discussion are given in Section 3.

2. DESCRIPTION OF THE METHOD AND MODEL

Here, we consider a three-wall Ising hexagonal nanotube with mixed spins consisting of a central nanotube that determines the geometry of the other two adjacent walls. The intermediate nanotube has a spin 1, while the central and the outer nanotubes have half-integer 1/2 spin and 3/2 spin, respectively. As shown from figure 1. the system consisting of three sublattices A, B and C. The sublattice B are occupied by integer spin S_j, which take the spin values of $0, \pm 1$ sublattices, while A and C are occupied by half-integer spins σ_i and μ_l, which take the spin values of $\pm 1/2$ and $\pm 1/2, \pm 3/2$, respectively. In B and C site of the lattice, there is a single-ion anisotropy acting in the spin-1 and spin -3/2, respectively.

The Hamiltonian of the mixed spin-1/2, spin-1, and spin-3/2 Ising model with the bilinear (J) nearest-neighbor pair interaction and a single-ion potential or crystal-field interaction (D) in the presence of a time-dependent oscillating external magnetic field is

$$H = H_a + H_b + H_c + H_{int} \tag{1}$$

$$H_a = -J_{aa} \sum_{<i,i'>} \sigma_i \sigma_{i'} - h(t) \sum_{<i>} \sigma_i$$

$$H_b = -J_{bb} \sum_{<j,j'>} S_j S_{j'} - D \sum_{<j>} S_j^2 - h(t) \sum_{<j>} S_j$$

$$H_c = -J_{cc} \sum_{<l,l'>} \mu_l \mu_{l'} - D \sum_{<l>} \mu_l^2 - h(t) \sum_{<l>} \mu_l$$

$$H_{\text{int}} = -J_{ab} \sum_{<i,j>} \sigma_i S_j - J_{bc} \sum_{<j,l>} S_j \mu_l$$

where $< i, i' >, < j, j' >$ and $< l, l' >$ indicates a summation over all pairs of nearest-neighboring at central, intermediate and outer nanotubes, respectively. The J_{ab} and J_{bc} are exchange interaction parameters between the two nearest-neighbor particles at central-intermediate and intermediate-outer nanotubes, respectively, and $h(t) = h_0 cos\omega t$ is an oscillating magnetic field of the form.

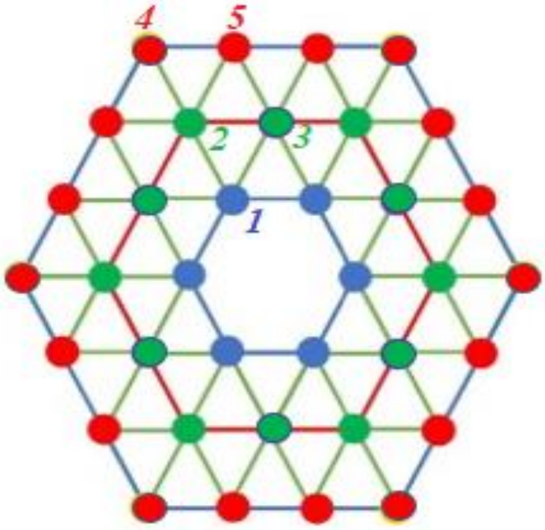

Fig. 1. Schematic representation of a cross section of a mixed-spin Ising hexagonal nanotube model. The green circles denote spin *S*=1 atoms, while the blue and red circles denote the decorating spin σ=1/2 and μ=3/2 atoms, respectively. The nanotubes are infinite in the direction to the axes z.

Now, we apply Glauber-type stochastic dynamics to obtain the mean-field dynamic equation of motion. For the nanotube depicted in fig.1, there exist one magnetization $(m_a = m_1)$ on sublattice A, two magnetizations $(m_b = m_{2,}\ m_b = m_3)$ on sublattice B and two magnetizations $(m_c = m_{5,}\ \ m_c = m_6)$ on sublattice C. Within the framework on Glauber dynamics and benefit from the master equation, we can obtain the mean-field dynamical equations describing the dynamic behavior of the system for these magnetizations

$$\Omega \frac{d}{d\xi} m_1 = -m_1 + \frac{1}{2} \tanh\left[\beta \left(4J_{aa} m_1 + J_{ab} \left(m_2 + 2m_3 \right) + h(\xi) \right) / 2 \right] \tag{2}$$

$$\Omega \frac{d}{d\xi} m_2 = -m_2 + \frac{2sinh\left[\beta \left(J_{ab} m_1 + 2J_{bb} \left(m_2 + m_3 \right) + J_{bc} \left(m_4 + 2m_5 \right) + h(\xi) \right) \right]}{\exp(-\beta D) + 2\cos h\left[\beta \left(J_{ab} m_1 + 2J_{bb} \left(m_2 + m_3 \right) + J_{bc} \left(m_4 + 2m_5 \right) + h(\xi) \right) \right]} \tag{3}$$

$$\Omega \frac{d}{d\xi} m_3 = -m_3 + \frac{2sinh\left[\beta \left(2J_{ab} m_1 + 2J_{bb} \left(m_2 + m_3 \right) + 2J_{bc} m_5 + h(\xi) \right) \right]}{\exp(-\beta D) + 2\cos h\left[\beta \left(2J_{ab} m_1 + 2J_{bb} \left(m_2 + m_3 \right) + 2J_{bc} m_5 + h(\xi) \right) \right]} \tag{4}$$

$$\Omega\frac{d}{d\xi}m_4=-m_4+\frac{3sinh(3\gamma_4)+\exp(-2\beta D)sinh(\gamma_4)}{2\cos h(3\gamma_4)+2\exp(-2\beta D)\cos h(\gamma_4)}$$
$$\gamma_4=\beta\left(2J_{cc}\left(m_4+m_5\right)+J_{bc}m_2+h(\xi)\right)/2 \tag{5}$$

$$\Omega\frac{d}{d\xi}m_5=-m_5+\frac{3sinh(3\gamma_5)+\exp(-2\beta D)sinh(\gamma_5)}{2\cos h(3\gamma_5)+2\exp(-2\beta D)\cos h(\gamma_5)}$$
$$\gamma_5=\beta\left(J_{cc}\left(3m_5+m_4\right)+J_{bc}\left(m_2+m_3\right)+h(\xi)\right)/2 \tag{6}$$

3. NUMERICAL RESULTS AND DISCUSSION

We have analyzed the time variations of the average sublattice magnetizations of the three-walled mixed-spin (1/2, 1 and 3/2) Ising nanotube using Glauber dynamics. In order to investigate the behaviors of time variations of magnetizations, we have to study the stationary solutions of the set of coupled mean-field dynamical equations given in Eqs. (2)-(6) when the parameters T, J_{aa}, J_{bb}, J_{cc}, J_{ab}, J_{bc}, D and h_0 are varied.

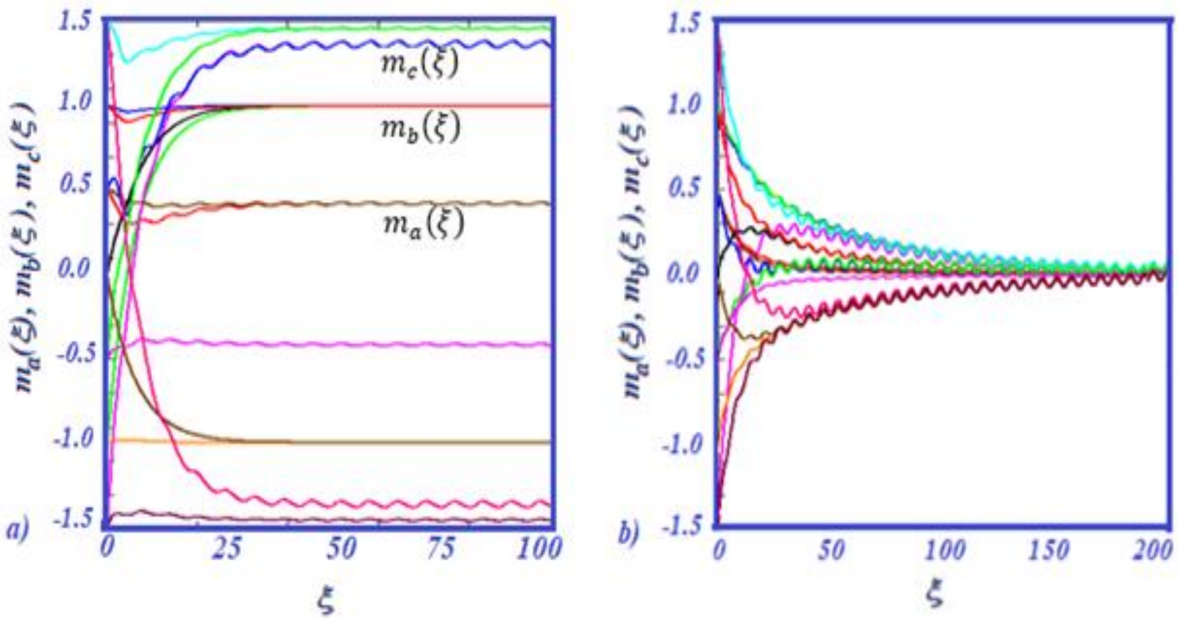

Fig. 2. Time variations of magnetizations of the three-walled mixed-spin (1/2, 1 and 3/2) Ising nanotube:
a) $k_BT/J_{aa}=2.8$, $h_0/J_{aa}=2$, $D/J_{aa}=0.8$, $J_{bb}/J_{aa}=1.5$, $J_{cc}/J_{aa}=0.5$, $J_{ab}/J_{aa}=1.8$, $J_{bc}/J_{aa}=2.5$;
b) $k_BT/J_{aa}=4.8$, $h_0/J_{aa}=0.8$, $D/J_{aa}=-0.4$, $J_{bb}/J_{aa}=1.5$, $J_{cc}/J_{aa}=0.8$, $J_{ab}/J_{aa}=0.5$, $J_{bc}/J_{aa}=0.3$;

The stationary solutions of these equations will be periodic functions of ξ with period 2π; that is, $m_a(\xi)=m_a(\xi+2\pi)$, $m_b(\xi)=m_b(\xi+2\pi)$ and $m_c(\xi)=m_c(\xi+2\pi)$. There are some types of solutions in the system under consideration and corresponding to these phases are shown in fig. 2, 3 and 4. As seen in fig. 2, we have two fundamental solutions in the system:

a) Exhibiting $m_a(\xi)\neq 0$, $m_b(\xi)\neq 0$ and $m_c(\xi)\neq 0$ phase: in this phase, all average sublattice magnetizations have different values. So that, $m_a(\xi)$ oscillate around ±0.5 values, while $m_b(\xi)$ and $m_c(\xi)$ oscillates around ±1 and ±1.5 values, respectively.
b) Paramagnetic phase. It corresponds to a disordered solution. In this solution, the sub-magnetizations $m_a(\xi)$, $m_b(\xi)$ and $m_c(\xi)$ are equal to each other. They oscillate around zero and are delayed with respect to the external magnetic field.

Figure 3 shows some of the phases that may be present in the system, with two sub-magnetizations oscillating around zero and one sub-magnetizing oscillating around a different value from zero:

a) Exhibiting $m_a(\xi)=m_b(\xi)=0$, $m_c(\xi)=\pm1.5\neq 0$ phase: in this solution, average sublattice magnetizations $m_a(\xi)$ and $m_b(\xi)$ are equal to each other and oscillate around zero values, while $m_c(\xi)$ oscillates around ±1.5 values.
b) Exhibiting $m_a(\xi)=m_c(\xi)=0$, $m_b(\xi)=\pm0.5\neq 0$ phase: in this case, average sublattice magnetizations $m_a(\xi)$ and $m_c(\xi)$ oscillate around zero, but $m_b(\xi)$ have different

values from $m_a(\xi)$ and $m_c(\xi)$. So that, $m_b(\xi)$ oscillate around ±0.5 values.

c) Exhibiting $m_b(\xi) = m_c(\xi) = 0$, $m_a(\xi) = \pm 0.5 \neq 0$ phase: in this phase magnetizations $m_b(\xi)$ and $m_c(\xi)$ oscillate around zero values, while $m_a(\xi)$ oscillates around ± 0.5 values, respectively.

The system may also have phases in which one sub-magnetization oscillates around zero and two sub-magnetizations oscillate around a different value from zero. Such phases are depicted in Figure 4.

a) Exhibiting $m_a(\xi) = 0$, $m_b(\xi) = \pm 1 \neq 0$ and $m_c(\xi) = \pm 1.5 \neq 0$ phase: this phase corresponds to $m_b(\xi)$ and $m_c(\xi)$ oscillate around ± 1 and ± 1.5 values, respectively, but magnetizations $m_a(\xi)$ oscillate around zero.

b) Exhibiting $m_a(\xi) = 0$, $m_b(\xi) = \pm 1 \neq 0$ and $m_c(\xi) = \pm 0.5 \neq 0$ phase: the average sublattice magnetizations $m_a(\xi)$ oscillate around zero values, while $m_b(\xi)$ and $m_c(\xi)$ are oscillate around nonzero values. So that, magnetizations $m_b(\xi)$ and $m_c(\xi)$ oscillate around ± 1 and $\pm 1/2$ values, respectively.

c) Exhibiting $m_c(\xi) = 0$, $m_a(\xi) = \pm 0.5 \neq 0$ and $m_b(\xi) = \pm 1 \neq 0$ phase: in this case, the magnetizations $m_c(\xi)$ oscillate around zero. But magnetizations $m_a(\xi)$ and $m_b(\xi)$ are not equal zero, they oscillate around $\pm 1/2$ and ± 1 values, respectively.

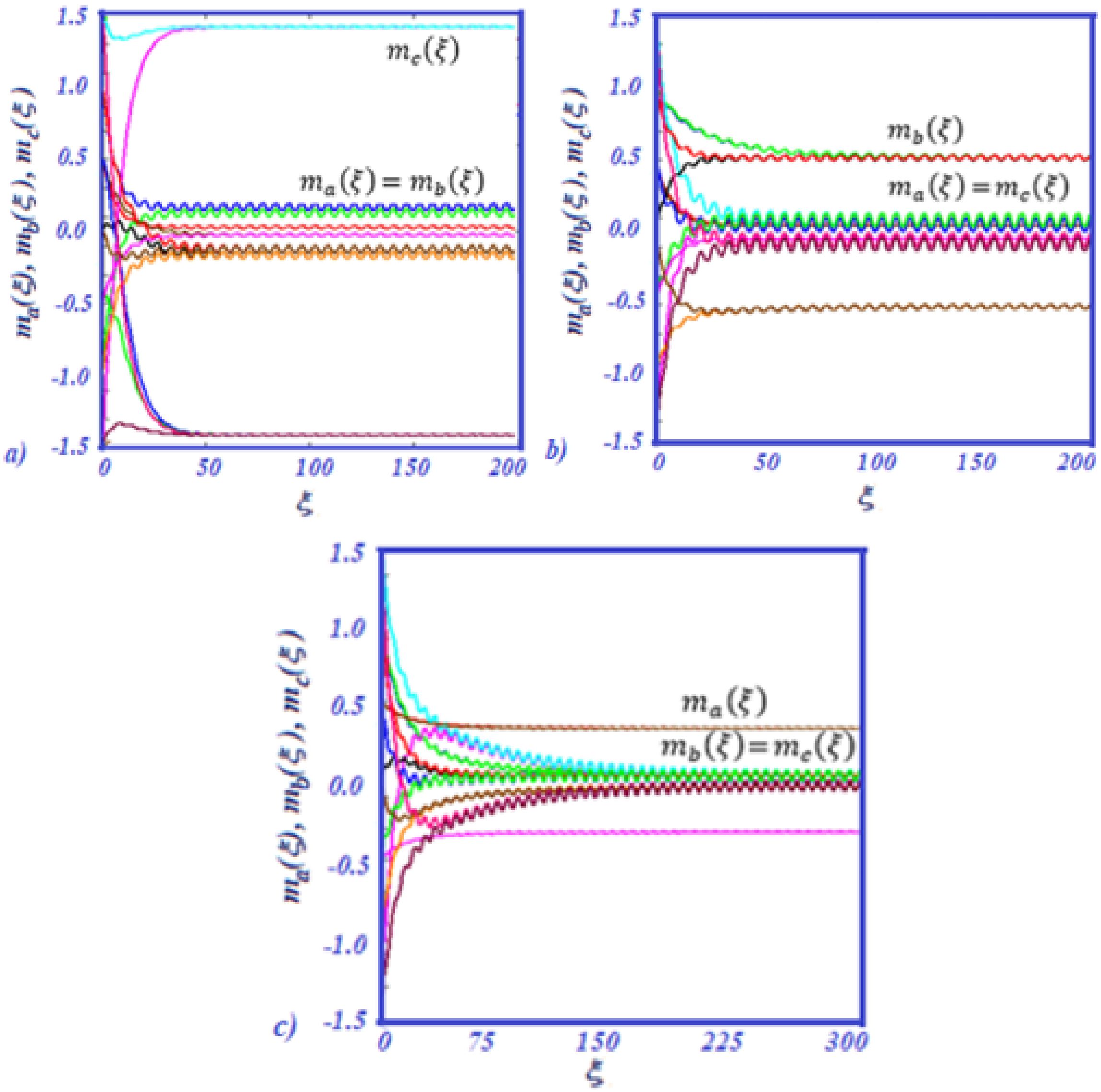

Fig. 3. Time variations of magnetizations of the three-walled mixed-spin (1/2, 1 and 3/2) Ising nanotube:
a) $k_B T / J_{aa} = 8$, $h_0 / J_{aa} = 2$, $D / J_{aa} = 0.4$, $J_{bb} / J_{aa} = 0.5$, $J_{cc} / J_{aa} = 3.5$, $J_{ab} / J_{aa} = 1.8$, $J_{bc} / J_{aa} = 0.4$;
b) $k_B T / J_{aa} = 8.5$, $h_0 / J_{aa} = 2$, $D / J_{aa} = 0.4$, $J_{bb} / J_{aa} = 3.5$, $J_{cc} / J_{aa} = 0.5$, $J_{ab} / J_{aa} = 0.8$, $J_{bc} / J_{aa} = 0.4$;
c) $k_B T / J_{bb} = 5$, $h_0 / J_{bb} = 0.8$, $D / J_{bb} = 0.4$, $J_{aa} / J_{bb} = 6$, $J_{cc} / J_{bb} = 0.8$, $J_{ab} / J_{bb} = 0.2$, $J_{bc} / J_{bb} = 0.3$;

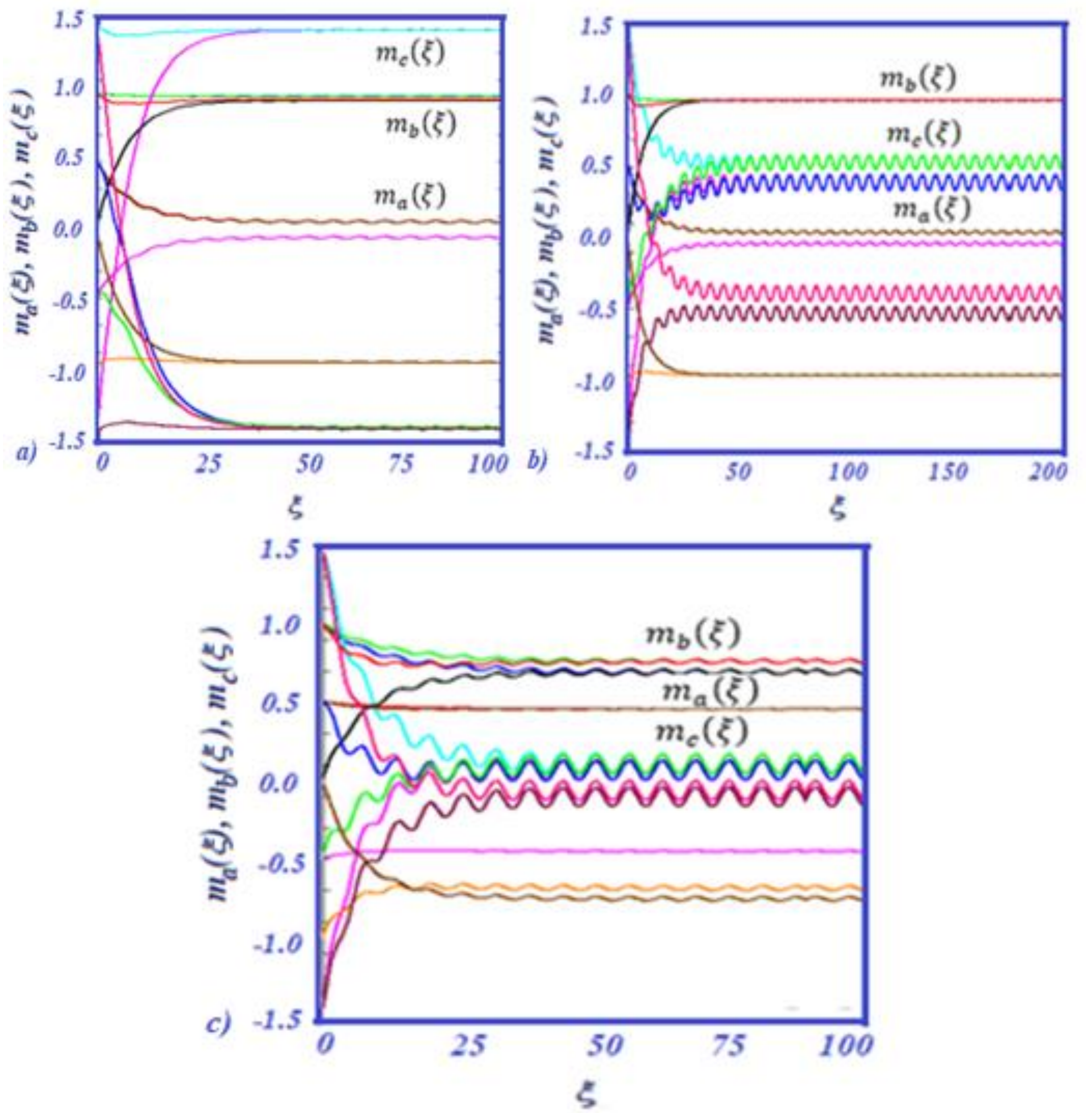

Fig. 4. Time variations of magnetizations of the three-walled mixed-spin (1/2, 1 and 3/2) Ising nanotube:

a) $k_B T/J_{aa} = 3.5$, $h_0/J_{aa} = 0.8$, $D/J_{aa} = 0.4$, $J_{bb}/J_{aa} = 3$, $J_{cc}/J_{aa} = 1.8$, $J_{ab}/J_{aa} = 0.2$, $J_{bc}/J_{aa} = 0.3$;

b) $k_B T/J_{aa} = 2.8$, $h_0/J_{aa} = 0.8$, $D/J_{aa} = 0.4$, $J_{bb}/J_{aa} = 2.5$, $J_{cc}/J_{aa} = 0.3$, $J_{ab}/J_{aa} = 0.1$, $J_{bc}/J_{aa} = 0.3$;

c) $k_B T/J_{bb} = 2.8$, $h_0/J_{bb} = 0.8$, $D/J_{bb} = 0.4$, $J_{aa}/J_{bb} = 3$, $J_{cc}/J_{bb} = 0.2$, $J_{ab}/J_{bb} = 1.4$, $J_{bc}/J_{bb} = 0.1$;

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