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Monte Carlo study of internal energy and specific heat of a nano-graphene bilayer in a longitudinal magnetic field

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ABSTRACT

The thermodynamic properties of a nano-graphene bilayer, consisting of the upper layer A of spin-3/2 with antiferromagnetic intralayer exchange coupling and the bottom layer B of spin-5/2 with ferromagnetic intralayer exchange coupling, have been studied by the use of Monte Carlo simulation. We find a number of characteristic phenomena. The effects of the exchange coupling, the single-ion anisotropy and the longitudinal magnetic field on the internal energy, the specific heat and the blocking temperature of the mixed-spin bilayer system have been investigated in detail. The internal energy and the specific heat profiles are clarified. In particular, we have found that the specific heat curve may show two peaks phenomenon for appropriate values of the system parameters.

1. Introduction

Since graphene was successfully found in 2004 [1], it has been extensively studied owing to its fascinating physical and chemical properties, such as high mechanical stability, gapless semiconductivity, low-intensity etc. Graphene consists of a honeycomb lattice, which was discovered to be one of the thinnest and lightest two-dimensional materials. With the development of the preparation technology of nano materials, the nano-graphene has been manufactured by various techniques [2–4]. It shows numerous potential applications in biosensors [5], field-effect transistors [6], linear magneto resistance [7], solar cells [8], chemical engineering [9], and environmental science [10] and so on.

On the other hand, in theory many works have been done to investigate the magnetic and thermodynamic properties of the nano-graphene. It is an interesting phenomenon that removing randomly single *C* atoms may induce magnetism of a macroscopic ferrimagnetic state in the multilayered grapheme [11]. The problem of a nonmagnetic impurity in graphene has been studied by the mean field theory [12]. Within the density functional theory, magnetic ordering of single cobalt layer added on grapheme has been examined. It is found that the single Co layer added on graphene displays ferromagnetic ordering with perpendicular alignment to the graphene sheet [13]. The exchange interaction of the nano-graphene has been investigated by computing the lattice Green's function for the tight-binding band structure [14]. Harigaya et al. have studied the antiferromagnetism in the stacked nanographite by using Hubbard-type models. For the A–B stacking, magnetic moments show a tendency to exist at the edge sites in each layer as a result of the large amplitude of wave-functions at these sites [15]. Recent theoretical efforts also have been devoted to the study of the magnetic nano-graphene bilayer system applied to a longitudinal magnetic field. Thanks to the nano-graphene bilayer system rather well described by a mixed spin-3/2 and spin-5/2 bilayer Ising model, these researches emphasize the importance of the longitudinal magnetic field in determining magnetic properties of the nano-graphene bilayer system. Using Monte Carlo simulation, Masrour et al. have analyzed the size effect on the magnetic properties of a nano-graphene bilayer structure. It is pointed out that the blocking temperature decreases on increasing the crystal field and the external magnetic field for a fixed system size [16]. The effect of the defects on the magnetization and hysteresis loops of an Ising antiferromagnetic–ferromagnetic nano-graphene bilayer system has been studied by Monte Carlo simulations [17]. Similar nano-graphene bilayer structure has also described by a transverse Ising model with single-ion anisotropy and exchange coupling [18]. They revealed that the exchange coupling, single-ion anisotropy and the external magnetic field have a significant influence on the blocking temperature and magnetization of the nano-graphene bilayer with the effective-field theory with correlations.

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Recently, a number of theoretical studies have been contributed to the physical properties of various mixed-spin Ising bilayer systems in a longitudinal magnetic field by different methods, such as spins (1/2, 1) [19], spins (1/2, 3/2) [20], spins (1, 3/2) [21], spins (2, 1/2) [22], spins (1, 2) [23], and spins (3/2, 2) [24]. Despite these intensive studies, only few theoretical attempts have been concentrated on the thermodynamic properties of the mixed spin-3/2 and spin-5/2 bilayer system by taking into account the longitudinal magnetic field. In particular, until now the internal energy and the specific heat of the nano-graphene bilayer in a longitudinal magnetic field have been rarely studied by Monte Carlo simulation. Boumali et al. have studied the thermodynamic quantities of the graphene, such as the free energy, the mean energy, the entropy and the specific heat by using an approach based on the zeta function. They found the existence of the quantum phase transition of the grapheme [25]. In our previous works, the magnetic and thermal properties of four sublattice ferromagnetic–antiferromagnetic double-layer superlattices have been investigated by Monte Carlo simulation [26]. Although considerable advances have been made in understanding the magnetic properties of the nano-graphene bilayer, it is necessary and meaningful to study the thermodynamic properties of the mixed spin-3/2 and spin-5/2 bilayer system by Monte Carlo simulation. Therefore, in this paper, emphasis will be put on the effects of the exchange coupling, the anisotropy and the longitudinal magnetic field on the internal energy and the specific heat of the nano-graphene bilayer. The outline of the paper is organized as follows. In Section 2, we briefly describe our model and the method used. In Section 3, typical numerical results for the internal energy, the specific heat of the system are present. Finally, Section 4 is devoted to our conclusion.

2. Model and Monte Carlo simulation

We consider a nano-graphene bilayer which consists of spin $\sigma=3/2$ with antiferromagnetic exchange coupling in the upper layer A ($\uparrow\downarrow$) and spin $S=5/2$ with ferromagnetic exchange coupling in the bottom layer B ($\uparrow\uparrow$). The sketch of the present model is illustrated in Fig. 1. The Hamiltonian of the system can be described by

$$H = -J_A\sum_{i,j}\sigma_{iA}^z\sigma_{jA}^z - J_B\sum_{i,j}S_{iB}^zS_{jB}^z - J_{AB}\sum_{i,j}\sigma_{iA}^zS_{jB}^z - D_A\sum_i\left(\sigma_{iA}^z\right)^2 - D_B\sum_j\left(S_{jB}^z\right)^2 - h\left(\sum_i\sigma_{iA}^z + \sum_j S_{jB}^z\right) \quad (1)$$

Where $\sigma_{iA}^z = \pm 3/2, \pm 1/2$ and $S_{jB}^z = \pm 5/2, \pm 3/2, \pm 1/2$ denote the spin variables of the spin-3/2 and spin-5/2 ions on sublattice of the upper layer A and sublattice of the bottom layer B, respectively. The first three sums involve nearest-neighbours coupling only. J_A (<0) and J_B (>0) are the intralayer exchange coupling constants within sublattices in the upper layer A and sublattices in the bottom layer B, respectively. J_{AB} is the interlayer exchange coupling constant between layers. D_A and D_B are the anisotropy constants for the sublattices in the upper layer A and the bottom layer B, respectively. h represents the longitudinal magnetic field.

In order to simulate the system, we employed the standard single-spin-flip importance sampling method based on the Metropolis algorithm [27] on a $2N^2L$ three-dimensional honeycomb lattice. $2N^2$ is the number of spins in each layer, and $L(=2)$ denotes the layer thickness. Additional simulations have been launched for choosing the size of system. Changing the number of spins in each layer $2N^2$ from 2×40^2 to 2×100^2, no significant differences were discovered. Accordingly, we set 2×40^2 for the simulation. We

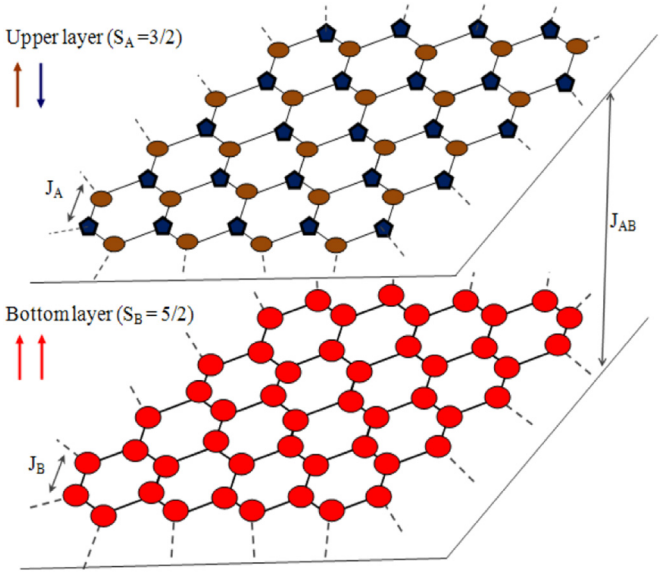

Fig. 1. The sketch of a nano-graphene bilayer with a honeycomb structure. J_A is the antiferromagnetic intralayer exchange coupling between spins $\sigma=3/2$ in the upper layer A ($\uparrow\downarrow$) and J_B is the ferromagnetic intralayer exchange coupling between spins $S=5/2$ in the bottom layer B ($\uparrow\uparrow$). J_{AB} is the interlayer exchange coupling between the upper and the bottom layer.

apply the periodic boundary condition in xy directions and the free boundary condition in the z-direction which is of finite thickness. To equilibrate the system, at least 10,000 Monte Carlo steps (MCS) per site were excluded before averaging thermal quantities over the next 20,000 MCS. In this work, the internal energy per site is calculated by

$$U = \frac{1}{2N^2L}\langle H\rangle \quad (2)$$

and the specific heat per site is

$$\frac{C}{k_B} = \frac{\beta^2}{2N^2L}\left(\left\langle H^2\right\rangle - \langle H\rangle^2\right) \quad (3)$$

The upper layer sublattice magnetizations M_A and the bottom layer sublattice magnetizations M_B are as follows:

$$M_A = \frac{1}{2N^2}\left\langle\sum_i S_{iA}^Z\right\rangle \quad (4)$$

$$M_B = \frac{1}{2N^2}\left\langle\sum_j S_{jB}^Z\right\rangle \quad (5)$$

and the total magnetization M per site

$$M = \frac{1}{2}\left(M_A + M_B\right) \quad (6)$$

Furthermore, the two sublattice magnetic susceptibilities χ_A and χ_B per site are calculated by

$$\chi_A = 2N^2\beta\left(\left\langle M_A{}^2\right\rangle - \langle M_A\rangle^2\right) \quad (7)$$

$$\chi_B = 2N^2\beta\left(\left\langle M_B{}^2\right\rangle - \langle M_B\rangle^2\right) \quad (8)$$

and the total magnetic susceptibility per site χ