Physics Letters A ••• (••••) •••–•••

Contents lists available at ScienceDirect

Physics Letters A

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Nano-graphene monolayer with higher-order exchange couplings: Monte Carlo study

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ARTICLE INFO

Article history:
Received 30 July 2017
Received in revised form 24 September 2017
Accepted 19 October 2017
Available online xxxx
Communicated by M. Wu

Keywords:
Graphene
Monte Carlo simulation
Magnetic properties
Phase diagrams

ABSTRACT

We have used the Monte Carlo simulation to study the phase diagrams and the magnetic properties of a single nano-graphene layer with next-nearest neighbors coupling J_2 and four-spin interaction J_4. Interesting behaviors have been found. In particular, the nanographene can present tricritical and triple points for appropriate system parameters.

1. Introduction

Graphene has attracted considerable attention given to its potential applications on electronic devices, sensors, nanocomposites and energy storage [1–3]. Graphene has also been used for conductive switching and bioimaging [4,5]. Some relevant experimental and theoretical techniques have been devoted to investigate the physical and the chemical properties of the graphene, especially, since the occurrence of the room temperature ferromagnetism in graphite-like carbon based materials. To explain such ferromagnetism, Norio et al. [6,7] give first a model of $C_{48}H_{24}$ graphene molecule. Both molecular orbital calculation and density function theory based analysis indicate that the highest spin state ($S = 3/2$) is more stable. While in the nitrogen substituted ($-NH$) molecule such as $C_{45}N_3H_{21}$, $C_{59}N_5H_{22}$, $C_{52}N_4H_{20}$ and $C_{61}N_3H_{22}$, the lowest spin state ($S = 1/2$) is more stable than the highest one ($S = 3/2$). Theoretically, some approach technics have been devoted to study the nanographene structure and its physical properties. Using the effective-field theory with correlations [8], an Ising antiferromagnetic–ferromagnetic nanographene bilayer system has been examined. It was found that, the single-ion anisotropy, the external magnetic field and the exchange coupling have a significant effect on the blocking temperature and magnetization of the nanographene. Based on the density functional theory [9], magnetic ordering of single cobalt layer added on graphene has been studied. It was remarked that with a perpendicular alignment to the graphene sheet, the single layer added on the graphene displays ferromagnetic ordering. In Ref. [10], the authors have studied an Ising antiferromagnetic nanographene lattice with spin-3/2 ($S = \pm 3/2, \pm 1/2$) based on Monte Carlo simulation. It was shown that with increasing the temperature, the magnetization of the system increases firstly and then decreases and that the blocking temperature decreases with increasing the external magnetic field. In another work, a bilayer nanographene structure-like with two bloc sizes has been studied [11]. It was found that the magnetization and the blocking temperature decrease with increasing the crystal field. By means of Monte Carlo simulations [12], the magnetic properties of a mixed spin-3/2 and spin-5/2 Ising ferrimagnetic system in a graphene layer has been studied, a compensation behavior has been found. Applying the Monte Carlo simulations [13], a bi-layer decorated graphene structure has been studied. It is remarked that the critical temperature increases as increasing the reduced exchange interaction values. The magnetic properties of some nanographene have also been studied [14–16].

On the other hand, intense interest has been directed to study the Ising model with multi-spin interactions. In particular, the Ising model with four spin interactions is one of the most studied models which have attracted considerable attention. These models are

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https://doi.org/10.1016/j.physleta.2017.10.040
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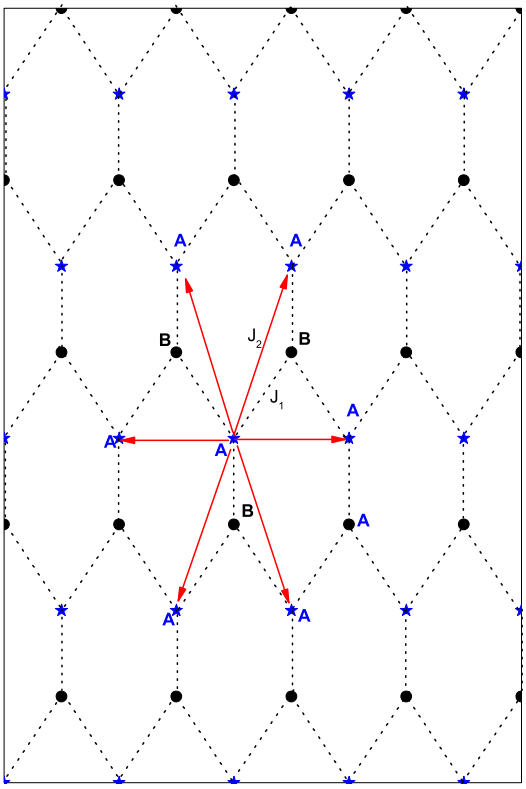

Fig. 1. The schematic representation of a nanographene monolayer. J_1 is the exchange coupling between nearest neighbor spins. J_2 denotes the exchange coupling between next nearest neighbor spins.

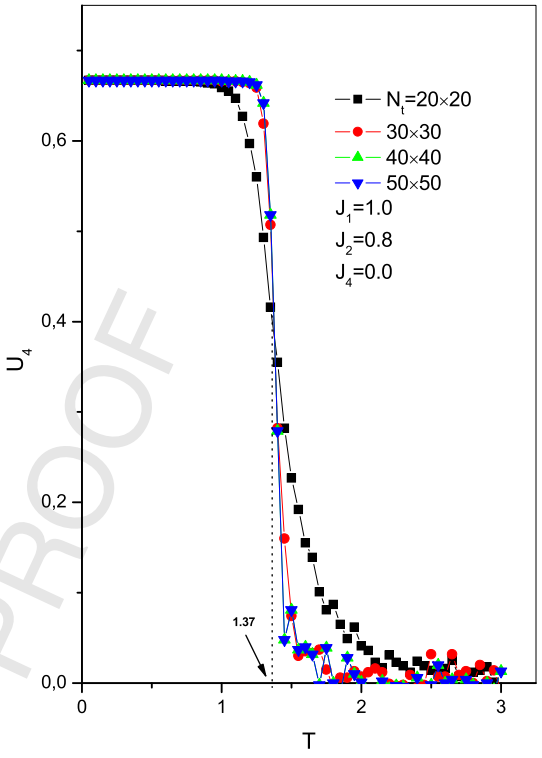

Fig. 2. The behavior of the fourth-order cumulant U_4 as a function temperature for $J_1 = 1.0$, $J_2 = 0.8$, $J_4 = 0.0$ and for selected values of N ($N = 20, 30, 40$ and 50).

interesting because they found their explanation in the theories of the superexchange interaction, the magnetoelastic effect and the phonon coupling [17]. However, it was shown that the Ising model with four spin interaction can exhibits a rich critical phenomena which are not observed in the usual spin systems. Theoretically, the four spin interaction has been investigated [18,19]. Experimentally, the models with multispin interactions can be used to describe various interesting physical systems such as solid ^3He [20], binary alloys [21], classical Fluid [22], metamagnets [23] and rare gases [24].

According to our knowledge, the effects of the multi-spin interactions on the magnetic properties of a single layer Ising in a graphene layer of spin-1/2 has not been investigated. So our paper considers an interesting and timely problem of possible magnetic orderings of spins occupying the honeycomb lattice. The presented article is devoted to study the effects of the next-nearest neighbors coupling and the four-spin interaction on the magnetic properties and the phase diagrams of a ferromagnetic Ising nanographene by means of Monte Carlo simulation. The paper is organized as follows. In Section 2, we give the model and the formalism. In Section 3, we present the results and discussions, finally Section 4 is devoted to a conclusion.

2. Model and Monte Carlo simulation

The system studied in the presented work is a ferromagnetic Ising system in a graphene layer (i.e. a honeycomb lattice). The sites are occupied by spin-1/2. In order to explore the prospective existence of an antiferromagnetic behavior, the system can be devised into two sublattices A and B. Each central atom A (B) is surrounded by three nearest-neighbors atoms B (A) and six next nearest-neighbors atoms A (B) (see Fig. 1).

The Hamiltonian of the system is given by:

$$\mathcal{H} = -J_1 \sum_{\langle nn \rangle} S_i S_j - J_2 \sum_{\langle nnn \rangle} S_i S_j - J_4 \sum_{\langle nn \rangle} S_i S_j S_k S_l \qquad (1)$$

where $S_i = \pm 1/2$ denote the usual Ising variable. The summation index $< nn >$ and $< nnn >$ denote a summation over all pairs of nearest and next nearest-neighbors atoms, respectively. The first exchange interaction parameter J_1 stands over nearest-neighbor pair of spins. The second parameter J_2 represents the next nearest neighbor couplings and the third parameter J_4 refers to the four-spin interaction. In order to compute the magnetic properties of the system, we use Monte Carlo technique and the flips of spins are accepted or rejected by the Metropolis algorithm [25]. One Monte Carlo step (MCS) was defined as all spins are swept. To obtain each point in the system, 4×10^4 MCs were performed after discarding the first 2×10^4 steps. To choose the optimal size of the nanographene, simulations have been performed by changing the total number $N \times N$ of spins in the honeycomb lattice from 20^2 to 50^2. Since for $N \geq 40$, no significant differences were found (see Fig. 2), we have fixed $N = 40$ in the present paper. We apply the periodic boundary conditions in both x and y directions. Our program calculates the following parameters, namely:

- The sublattices magnetizations per spin:

$$M_A = \frac{2}{N_t}\left\langle \sum_i S_{iA} \right\rangle \text{ and } M_B = \frac{2}{N_t}\left\langle \sum_i S_{iB} \right\rangle \qquad (2)$$

- The total magnetization per spin:

$$M = M_A + M_B \qquad (3)$$

– The magnetic susceptibility:

$$\chi = \frac{1}{N_t}\beta(\langle M^2 \rangle - \langle M \rangle^2) \qquad (4)$$

Please cite this article in press as: A. Feraoun, M. Kerouad, Nano-graphene monolayer with higher-order exchange couplings: Monte Carlo study, Phys. Lett. A (2017), https://doi.org/10.1016/j.physleta.2017.10.040