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Theoretical simulations of magnetic nanotubes using Monte Carlo method

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ABSTRACT

We present the results of the Monte Carlo simulations of magnetic nanotubes, which are based on the plane structures with the square unit cell at low temperatures. The spin configurations, thermal equilibrium magnetization, magnetic susceptibility and the specific heat are investigated for the nanotubes of different diameters, using armchair or zigzag edges. The dipolar interaction, Heisenberg model interaction and also their combination are considered for both ferromagnetic and anti-ferromagnetic cases. It turns out that the magnetic properties of the nanotubes strongly depend on the form of the rolling up (armchair or zigzag). The effect of dipolar interaction component strongly manifests itself for the small radius nanotubes, while for the larger radius nanotubes the Heisenberg interaction is always dominating. In the thermodynamic part, we have found that the specific heat is always smaller for the nanotubes with smaller radii.

1. Introduction

Since the discovery of carbon nanotubes [1], the electronic, magnetic and mechanical properties of the nanometric scale materials have been attracting considerable attention. During the last few years one could observe a growing interest in the experimental and theoretical investigations of various new structures at nano-scale [2–5]. These structures include different geometric configurations such as fullerenes, nanotubes, nano-particles, nano-cones, nano-rings and so on. The exploration of different properties of these objects opens wide perspectives for applications. One of the potentially interesting aspects of nanophysics is related to magnetic phenomena. In particular, experimental and theoretical investigations of the magnetism in nanostructures stimulates extensive theoretical studies of different materials at the nanometric scale, such as pure and doped different carbon-based materials [6–12] and semiconductor nanoclusters, ferromagnetic and anti-ferromagnetic nanocrystals [13–16] and thin films [17]. The new experimental works which have been done recently in this area opened the way for the creation of nanotubes based on the composite molecules that contain metal atoms [18–20]. In this case, we can consider the nanotube as a tube, composed of rectangular (square, or others) unit cells with spins situated in the vertices of the unit cells.

The magnetic properties of nano-scale materials look promising for applications, and this represents a strong motivation for theoretical investigation. In particular, different types of theoretical techniques have been used for the numerical simulations of magnetic properties such as the spin model with dipolar and nearest-neighbor interactions [17,21,22], the nearest-neighbor tight-binding Hamiltonian [11,23–25], the calculations using the *ab initio* pack with the spin-polarized density functional theory [26] and the Monte Carlo simulations [27].

In the present paper, we start a systematic analysis of the magnetic properties of nanotubes. As a first step, we perform the theoretical simulations of various properties of the model magnetic nanotubes based on the geometrically simplest lattice with the square unit cell. The main target of our study is the dependence of the thermodynamic and magnetic properties on geometry. In particular, we explore the difference between the nanotubes of different diameters and also the dependence on the type of the rolling which affects, in particular, the form of the edge. The results of the analysis look rather natural and one can expect similar dependencies for the more realistic cases of magnetic nanotubes, e.g., similar to those considered in Refs. [18–20].

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2. Method of calculations

The purpose of present work is to investigate the possible influence of the nanotube's diameter and the type of the edge on the magnetic properties of nanotubes, based on the plane structure with the square unit cell. In Fig. 1 one can observe the two-dimensional plane with the square unit cell of the lattice. The rolling up corresponding to the armchair nanotubes is indicated by the vector $(m,0)$ while the rolling up corresponding to the zigzag nanotubes is indicated by the vector (m,m). The value of the integer m defined the size of the nanotubes. In this paper, we are using the terms "armchair" and "zigzag" which are traditional for the carbon nanotubes. However, we use these terms in the opposite order, such that they agree with the actual geometry of the nanotubes under consideration. The geometry here means the form of the edge: for the case of the armchair the rolling up vector is passing through the neighboring vertices of the unit cells; for the case of zigzag this vector is passing through the diagonal vertices of the unit cells. After rolling, any nanotube is defined by the pair of integer parameters (m_1,m_2), which describe its circumference vector on the initial plane, that is $\vec{L} = m_1\vec{a}_1 + m_2\vec{a}_2$, where $\vec{a}_1, \vec{a}_2$ are unit cell's vectors (later we used a as a lattice constant, which we set to unity, $a = 1$). It proves useful to introduce the following terminology. The two spins belong to the same "line" if the vector directed from one of them to another is parallel to the axis of the magnetic nanotube. So, the space position of each spin may be characterized by the line and by the layer.

In what follows, we will explore the spin configurations obtained using the numerical calculations within the Monte Carlo method for the nanotubes of different diameters, with the armchair or zigzag edges, for dipolar interaction, Heisenberg model interaction and the combinations of these two interactions, in the ferromagnetic and anti-ferromagnetic cases. We will be using the nanotubes of the (4,0), (5,0), (6,0), (7,0), (8,0), (12,0), (4,4), (5,5), (6,6), (7,7), (8,8) and (12,12) types. Obviously, these nanotubes have different diameters and chiralities. Table 1 contains the radii of these nanotubes. Furthermore, the investigated nanotubes had finite length; in our case they had 9 or 13 layers along the axis. In order to illustrate the geometry of the structures under consideration, we present a corresponding picture for the (8,0) and (8,8) cases in Fig. 2. We have investigated the spin configurations, the thermal equilibrium magnetization, the susceptibility and the specific heat for these structures. As a result of this study, one can observe how the spin configurations

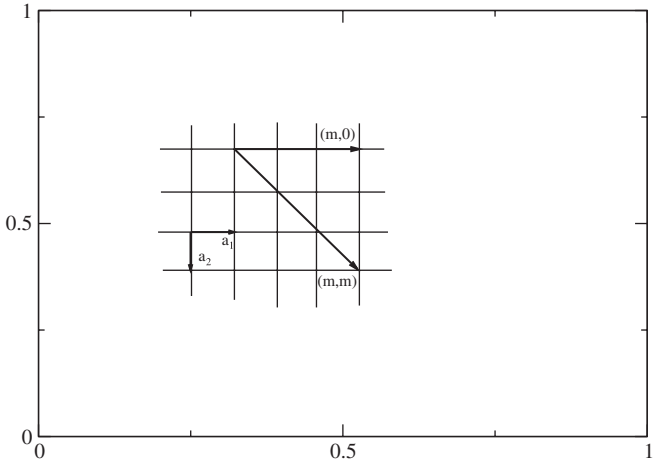

Fig. 1. Two-dimensional square unit cell lattice. The indicated vectors are used for rolling up the armchair and zigzag nanotubes.

Table 1
The radii of the nanotubes expressed in the units of a (unit cell's size)

Structure	Radius (in units of a)
(4,0)	0.6362
(5,0)	0.7958
(6,0)	0.9549
(7,0)	1.1141
(8,0)	1.2732
(12,0)	1.9099
(4,4)	0.9003
(5,5)	1.1254
(6,6)	1.3505
(7,7)	1.5756
(8,8)	1.8006
(12,12)	2.7010

depend on the diameter of the nanotube, on the form of the edge and also on the type of the interactions between spins.

In our simulations we used a Hamiltonian model given by [21]

$$H = -J\sum_{\langle i,j\rangle}\vec{S}_i\vec{S}_j - \vec{B}\cdot\sum_i\vec{S}_i - \omega\sum_{i<j}\frac{3(\vec{S}_i\cdot\vec{e}_{ij})(\vec{e}_{ij}\cdot\vec{S}_j) - \vec{S}_i\vec{S}_j}{r_{ij}^3}$$

In this expression the first sum represents the ferromagnetic (or anti-ferromagnetic) exchange between the nearest-neighbors with a coupling constant J, the second sum stands for the coupling of the spins to an external magnetic field B and the last sum is the dipolar interaction term, where the coupling ω describes the strength of the dipole–dipole interaction. The $\vec{S}_i$ are three-dimensional magnetic moments of unit length, $\vec{e}_{ij}$ are unit vectors pointed from lattice site i to the lattice site j and r_{ij} are the distances between these lattice sites. The correlation between constant values was chosen as $\omega/J = 0.001$, in according to Ref. [21].

For the numerical analysis of the magnetic nanotubes described above, we have used the Monte Carlo simulations with the Metropolis algorithm [28,29]. The Metropolis Monte Carlo algorithm enables one to obtain the macro-state equilibrium for a physical system at the given temperature T. The basic idea of this method consists of the following procedure: we start from some randomly chosen initial micro-state and then proceed by performing a very large number of random transformations of the micro-states, until we arrive at the equilibrium macro-state. In our case, we start simulations with an initial configuration in which all spins have parallel directions. Then the direction of one (randomly chosen) of these spins is randomly changed. In this way, we arrive at the new micro- and macro-states and evaluate the change of the overall energy ΔE compared to the previous configuration. If $\Delta E<0$, the temporary direction of the spin becomes permanent. If $\Delta E>0$, the temporary direction becomes permanent with the probability $\exp(-\Delta E/k_bT)$. We repeat this procedure $n = 10{,}000$ multiplied by the factor equal to the number of sites (spins). The final state corresponds to the stable configuration and is interpreted as equilibrium macro-state. In order to fix the number n, the simulation is firstly performed several times for one particular system. The criterion of the choice of the number n is that the change of the overall energy ΔE in the last steps (at least 20%) must be negligible. These preliminary calculations show that the equilibrium state is really achieved for 10^4 Monte Carlo steps per spin and, therefore, this number of steps is adequate for our calculations. After that, all simulations have been performed for this choice of n.

In the case of dipolar interaction the spin at the site i was allowed to interact with all other spins of the nanotube. In the Heisenberg interaction case the spin at the site i was allowed to interact only with the nearest-neighboring spins. The same