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Magnetic and thermodynamic properties of a simple-well hexagonal spin nanotube

Z. ElMaddahi, A. Farchakh, M.Y. El Hafidi, M. El Hafidi*

Condensed Matter Physics Laboratory, Faculty of Science Ben M'sik, Hassan II University of Casablanca, B. P 7955, Av. D. El Harty, 20663 Casablanca, Morocco

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ABSTRACT

A hexagonal spin nanotube is studied using the Effective Field Theory with correlations (EFT) and the differential operator technique (DOT). Each spin is connected to the nearest-neighbors through exchange couplings both along the chains ($J_{//}$) and adjacent chains ($J_{\perp}$). The effects of the exchange, the single-ion anisotropy and the magnetic field on the phase diagram and the magnetic properties have been examined. It is shown that the longitudinal and transverse exchange parameters have strong effect on the shape of the phase diagram. Some original behaviors have been emerged. In particular, when the two exchange parameters are opposite, strong frustrations occur, atypical magnetization plateaus and jumps appear.

1. Introduction

Spin nanotube is an assembly of magnetically linked chains. According to the number of related strings, the tube can take various basic forms. Thus, three, four, or six runs, correspond respectively to triangular, square or hexagonal tube, and so on. Taking into account recent advances in the design of atomic and molecular edifices, these new structures are actually realizable in many laboratories. These nanotubes are interesting both on the fundamental and experimental heights: in fact, they offer to theoreticians the possibility to test their models. From the view point of magnetism, the spins are located on chain sites and interact each one to the other via exchange coupling both along the chains ($J_{//}$) and transversely ($J_{\perp}$) between neighboring chains. Thus, according to the strength and the sign of exchange constants $J_{//}$ and $J_{\perp}$, we can achieve systems of controllable dimensionalities: in particular, for the extreme case $\left|\frac{J_{//}}{J_{\perp}}\right| \gg 1$, we obtain a quasi-one-dimensional system, while for $\left|\frac{J_{//}}{J_{\perp}}\right| \ll 1$, a two-dimensional system is realized, whereas for the intermediate cases $\left|\frac{J_{//}}{J_{\perp}}\right| \sim 1$, we will have a three-dimensional system. On the other hand, the existence of conflicting exchange interactions could give rise to frustration. This approves their importance for fundamental magnetism. Experimentally, these nano-materials open up new potential perspectives with various and aspiring technological applications. Different chemical compositions of the nanotubes have been successfully synthesized by various methods [1–3] inaugurating a large spectrum of promising applications such as ultrahigh-density magnetic storage devices, biomagnetic sensors, nanomedicine, molecular devices, nanofilters, nanocatalysts, and nanospintronic devices, etc. Nowadays, there have been intense experimental and theoretical studies to apprehend the physical phenomena of spin tubes. We can mention here the example of the equilateral triangular spin tube in $CsCrF_4$ compounds which exhibit in their ground state a frustrated behavior [4], or the four-leg spin tube such as the new compound $Cu_2Cl_4{\cdot}D_8C_4SO_2$ with spin ½ showing magnetization plateaus [5].

From the theoretical point of view, several methods for the magnetic and thermodynamic properties of spin tubes have been used, such as micromagnetic simulation [6–11], continuum theory of ferromagnetism [12–15], Monte Carlo simulations [16–21], ab initio density functional theory calculations [22], effective-field theory [23–26], and many body Green's function method (MBGFM) of quantum statistical theory [27,28].

However, as far as we know, the magnetic correlation (MC) effect of ferromagnetic single-walled nanotubes (FM-SWNTs) has not yet been fully investigated. This paper is devoted to this point.

In our work, we aim to study hexagonal spin tube in the Effective field Theory with correlations (EFTC) framework and by using the differential operator technique (DOT) [29,30]. The EFTC corresponds to the Zernike approximation [31] and it is admitted that it provides more rigorous results than those given by the mean-field approximation (MFA), since it includes automatically correlations between a number of spins and their near-neighbors.

* Corresponding author.
E-mail address: mohamed.elhafidi@univh2c.ma (M. El Hafidi).

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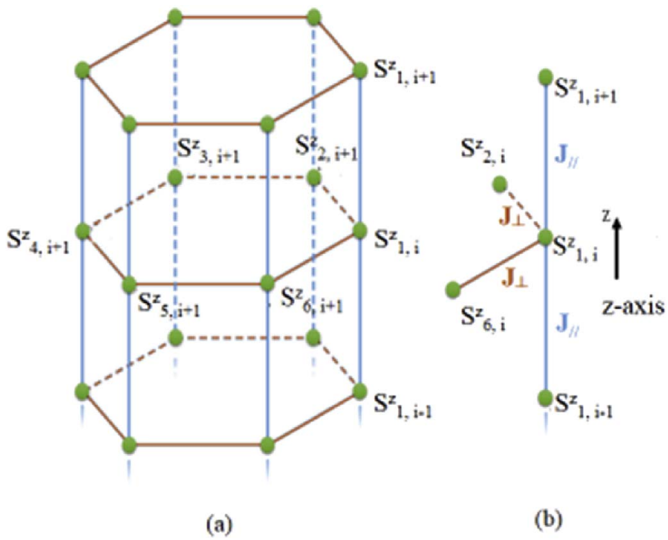

Fig. 1. Schematic structure of the hexagonal spin ½ tube (a). The longitudinal ($J_{//}$) and the transverse ($J_\perp$) exchange couplings are indicated (b).

The paper is organized as follows: In Section 2, we present our model and put down the spin Hamiltonian. Then, we briefly outline the analytical calculations to obtain spontaneous magnetization, critical temperature and other pertinent quantities in the EFTC and DOT approaches. In Section 3, numerical computation is carried out and the role of temperature, exchange, single-ion anisotropy and applied field are carefully analyzed. Finally, Section 4 summarizes the main results.

2. Model and analytical calculations

We consider a hexagonal spin tube. In this model, the spins, localized on the sites of a single honeycomb lattice wall, were assumed to interact via a Heisenberg exchange coupling restricted to their nearest neighbor (nn) sites. The distance between two adjacent chains is a (see Fig. 1). A given spin (i, α) on the chain α (α = 1–6) interacts with its two adjacent neighbors (i ± 1, α) along the chain via the longitudinal exchange $J_{//}$ but also with its two in-plan nearest-neighbors (i, α ± 1) via the transverse component $J_\perp$.

The tube model is governed by the following spin Hamiltonian:

$$H = -J_{//}\sum_i \sum_{\alpha=1..6} \vec{S}_{\alpha,i}\,.\,\vec{S}_{\alpha,i+1} - J_\perp \sum_i \sum_{\alpha=1..6} \vec{S}_{\alpha,i}\,.\,\vec{S}_{\alpha+1,i} - g\mu_B B \sum_{\alpha=1}^{6}\sum_{i=1}^{N} S^z_{\alpha,i} \qquad (1)$$

In Eq. (1), the first term denotes the longitudinal exchange part along the chains, where $J_{//} > 0$ (respectively $J_{//} < 0$) for ferromagnetic, FM (respectively Antiferromagnetic, AFM). The second term describes the transverse exchange part which acts between adjacent chains with the same convention for $J_\perp$.The last term corresponds to Zeeman part. In this paper, we set Boltzmann constant $k_B = 1$. In calculation, all parameters are taken as dimensionless quantities such as the reduced magnetic field h ($h = \frac{g\mu_B BS}{J_{//}}$ where g = 2, S = ½ and the Bohr magnetron is in the same way seated at unity, leading thus to the simple expression $h = \frac{B}{J_{//}}$). There are 6 chains including N sites along each one. The EFTC used here is considered as powerful means [32] to deal with magnetic systems, since this method takes into account the spin correlations, and is useable in the whole temperature range. Furthermore, the EFTC gives good agreement with quantum Monte Carlo simulations in a wide temperature range of the ordered systems [30].

In order to apply the EFTC and the TOD for the considered spin-½ system, we rewrite the above Hamiltonian in the following form:

$$H = -\sum_i^N \sum_{\alpha=1}^{6} H_{i,\alpha} \qquad (2)$$

where

$$H_{i\alpha} = S_{i,\alpha}\left(J_\perp \sum_n S_{i,\sigma} + J_{//}\sum_m S_{m,\alpha} + h\right) \qquad (3)$$

Thus, the statistical average of spin $S_{i,\alpha}$ at the thermodynamic equilibrium is given in the EFTC by:

$$S_{i,a} = \frac{1}{Z} Tr\left(\frac{Tr(S_{i,\alpha}e^{-\beta H_{i\alpha}})}{Tr(e^{-\beta H_{i\alpha}})}\right) \qquad (4)$$

which is simplified as

$$S_{i,\alpha} = \frac{1}{2}\frac{1}{Z} Tr\left(\tanh\left(\frac{\beta E_{i\alpha}}{2}\right)\right) = \frac{1}{2}\tanh\left(\frac{\beta E_{i\alpha}}{2}\right) \qquad (5)$$

for spin ½.

Thus, we can write the magnetization per site as

$$m_{i\alpha} = \left[\prod_\delta \left(cosh\left(\frac{\beta}{4}\nabla J_\perp\right) + 2S_{i,j+\delta} sinh\left(\frac{\beta}{4}\nabla J_\perp\right)\right)\prod_{\delta'}\left(cosh\left(\frac{\beta}{4}\nabla J_{//}\right) + 2S_{i+\delta',j} sinh\left(\frac{\beta}{4}\nabla J_{//}\right)\right)\right] tanh\left(x + \frac{\beta h}{2}\right)\Big|_{x=0} \qquad (6)$$

where $\delta = \pm 1$ *and* $\delta' = \pm 1$ design the nearest neighbors of considered spin

$$m_{i\alpha} = \left[\left(cosh\left(\frac{\beta}{4}\nabla J_\perp\right) + 2S_{in} sinh\left(\frac{\beta}{4}\nabla J_\perp\right)\right)^2 \left(cosh\left(\frac{\beta}{4}\nabla J_{//}\right) + 2S_{mj} sinh\left(\frac{\beta}{4}\nabla J_{//}\right)\right)^2\right] tanh\left(x + \frac{\beta h}{2}\right)\Big|_{x=0} \qquad (7)$$

Since spins are identical (S = ½), their statistically average is the same, ie $m_{in} = m_{mj} = m$, leading to the last magnetization expression

$$m = \left[\left(cosh\left(\frac{\beta}{4}\nabla J_\perp\right) + m\ sinh\left(\frac{\beta}{4}\nabla J_\perp\right)\right)^2 \left(cosh\left(\frac{\beta}{4}\nabla J_{//}\right) + m\ sinh\left(\frac{\beta}{4}\nabla J_{//}\right)\right)^2\right] tanh\left(x + \frac{\beta h}{2}\right)\Big|_{x=0} \qquad (8)$$

whose the expansion is finally given by:

$$m = \frac{1}{16}[P + 4P'm + 2Qm^2 + 4Q'm^3 + Rm^4] \qquad (9)$$

where the introduced parameters are defined as follows:

$$P = \tanh(2(A+B)+C) + \tanh(-2(A+B)+C) + \tanh(2(A-B)+C) + \tanh(-2(A-B)+C) + 2\tanh(2A+C) + 2\tanh(-2A+C) + 2\tanh(2B+C) + 2\tanh(-2B+C) + 4\tanh(C) \qquad (10)$$

$$P' = \tanh(2(A+B)+C) - \tanh(-2(A+B)+C) + \tanh(2A+C) - \tanh(-2A+C) + \tanh(2B+C) - \tanh(-2B+C) \qquad (11)$$

$$Q = 3\tanh(2(A+B)+C) - \tanh(-2(A+B)+C) + 3\tanh(2(A-B)+C) - \tanh(-2(A-B)+C) - 4\tanh(2A+C) + 4\tanh(-2A+C) - 8\tanh(C) \qquad (12)$$

$$Q' = \tanh(2(A+B)+C) - \tanh(-2(A+B)+C) - \tanh(2A+C) + \tanh(-2A+C) - 2\tanh(2B+C) + 2\tanh(-2B+C) \qquad (13)$$