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Spin wave dynamics in Heisenberg ferromagnetic/antiferromagnetic single-walled nanotubes

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ABSTRACT

The spin wave dynamics, including the magnetization, spin wave dispersion relation, and energy level splitting, of Heisenberg ferromagnetic/antiferromagnetic single-walled nanotubes are systematically calculated by use of the double-time Green's function method within the random phase approximation. The role of temperature, diameter of the tube, and wave vector on spin wave energy spectrum and energy level splitting are carefully analyzed. There are two categories of spin wave modes, which are quantized and degenerate, and the total number of independent magnon branches is dependent on diameter of the tube, caused by the physical symmetry of nanotubes. Moreover, the number of flat spin wave modes increases with diameter of the tube rising. The spin wave energy and the energy level splitting decrease with temperature rising, and become zero as temperature reaches the critical point. At any temperature, the energy level splitting varies with wave vector, and for a larger wave vector it is smaller. When $pb=\pi$, the boundary of first Brillouin zone, spin wave energies are degenerate, and the energy level splittings are zero.

1. Introduction

The concept of spin waves as elementary excitations in magnetically ordered materials was presented by Bloch [1] in the early 1930s. Following the discovery, spin wave excitations have attracted great interest in experimental [2–24] and theoretical [24–38] studies due to their essential role for explaining magnetic ordering [1,39] and spin dynamics [40]. Experimentally, the spin wave can be conveniently probed by ferromagnetic resonance [5–9], Raman and Brillouin light scattering [10–14], and inelastic neutron scattering [15–22]. Seen from the perspective of the theory, the semi-classical picture of spin waves was thoroughly explored [39,41,42] and the quantum picture was studied by means of the many-body Green's function method (MBGFM) of quantum statistical theory [25–27]. As low dimensionality and quantum fluctuations on curved surfaces of nano-systems are highly interesting, spin waves propagating on the surface of the nonferromagnetic nanotube in a magnetic field were studied in Refs. [43–47]. In these studies the spectrum of spin waves on the surface of a semiconductor nanotube in magnetic field was calculated using the random phase approximation (RPA) within the framework of short-range electron interaction model in Hartree–Fock approximation (HFA). More recently, there has been intense interest in the spin wave excitations of ferromagnetic (FM) and antiferromagnetic (AFM) nanotubes, nanowires and nanorings [48–60], where the spin wave mode coupling is more complex. Geometrically, magnetic nanotubes (MNTs) are characterized by their external and internal radii, R and r, respectively, and longitudinal length L. It is convenient to define the ratio $\beta_0 \equiv r/R$, so that $\beta_0=0$ represents a solid cylinder (nanowire) and β_0 close to 1 corresponds to a tube with very thin walls. Here we adopt a simplified description of the MNTs, the limit of infinite longitudinal length, i.e. $L\to\infty$, and $\beta_0=1$ corresponds to the magnetic single-walled nanotubes [61–64]. The magnetic properties of single-walled nanotubes can be very easily described by the well-known Heisenberg model.

As far as we know, the physical picture of the spin wave dynamics in the magnetic single-walled nanotubes has not yet been systematically investigated. In this work we study the quantized spin wave modes in Heisenberg ferromagnetic/antiferromagnetic single-walled nanotubes (HFM/HAFM-SWNTs) using the MBGFM within the RPA. In Section 2 we present our model and put down the Hamiltonian of HFM/HAFM-SWNTs. Then we briefly outline the formulas of spontaneous magnetization, critical temperature and spin wave dispersion relation derived by the MBGFM. In Section 3, numerical computation is carried out and the role of temperature, diameter of the tube, and wave vector on spin wave

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energy spectrum and energy level splitting are carefully analyzed. At last, Section 4 summarizes the main results.

2. Model and formulas

We consider a HFM/HAFM-SWNTs of zigzag type [61,62]. In this model, the spins, localized on the sites of a centered quadratic lattice wall, were assumed to interact via a Heisenberg exchange coupling limited to nearest neighbor (nn) sites. The distance between the nn sites is a. The centered quadratic lattice has to be divided into two sublattices and the lattice constant should be $b = \sqrt{2}a$. Moreover, a single-ion anisotropy was assumed to favor the nanotube axis. According to the Mermin–Wagner theorem [65], for one- or two-dimensional (2D) isotropic Heisenberg magnetic systems, there is no spontaneous magnetization at finite temperatures. However, the spontaneous magnetization can occur when a single-ion anisotropy is introduced no matter how small it is [66,67]. It was indeed possible for the single-ion anisotropy to appear in real nanotube materials [68–70]. Some nanotube materials exhibit obvious magnetic anisotropy, and the easy axis is parallel to the nanotube axis.

The Hamiltonian of the HFM/HAFM-SWNTs with two sublattice is given as follows:

$$H = -J\sum_{[1i,2j]}\mathbf{S}_{1i}\cdot\mathbf{S}_{2j} - D\sum_{1i}(S_{1i}^z)^2 - D\sum_{2j}(S_{2j}^z)^2. \tag{1}$$

In Eq. (1), the first term represents the Heisenberg FM exchange energy ($J>0$) or AFM exchange energy ($J<0$), with exchange parameter J. The subscripts $1i$ and $2j$ denote the sublattice 1 and 2 sites, respectively, and $[1i, 2j]$ mean that the nn exchanges are involved. The second and the third term describe the single-ion anisotropy of sublattice 1 and 2, respectively, which causes the uniaxial anisotropy of the system and thus is responsible for appearance of spontaneous magnetization. Note that z-axis labels the directions of tube axis. The anisotropy strength of D is usually believed to be less than the absolute value of J by two orders of magnitude. In this paper, we set Boltzman constant $k_B=1$. In calculation, we fix $|J|=100$, $D=1$, and all parameters are taken as dimensionless quantities. There are N and m sites along the axis and circumference of the tube for each sublattice, respectively.

The MBGFM is a powerful means [71–76] to deal with magnetic systems [77–83] since this method takes into account the spin fluctuation, and is valid in the whole temperature range. Furthermore, the MBGFM gives good agreement with quantum Monte Carlo simulations in a wide temperature range of the ordered phase [75]. In order to study spin waves of the HFM/HAFM-SWNTs, we introduce the retarded Green's function

$$G(t-t') = \left\langle\left\langle \boldsymbol{A}^{\mathrm{T}}; \boldsymbol{B}\right\rangle\right\rangle = -i\theta(t-t')\left\langle \boldsymbol{A}^{\mathrm{T}}\boldsymbol{B} - \boldsymbol{B}\boldsymbol{A}^{\mathrm{T}}\right\rangle, \tag{2}$$

where the operators $\boldsymbol{A}$ and $\boldsymbol{B}$ are actually operator vectors in the following form:

$$\mathbf{A} = \left(S_1^+, S_2^+\right),$$
$$\mathbf{B} = \left(\exp(uS_1^z)S_1^-, \exp(uS_2^z)S_2^-\right), \tag{3}$$

and u is a parameter. Here the Green's function is in fact an 2×2 matrix, and its Fourier component is denoted as $\mathbf{g}(\omega)$. The higher order Green's function appearing in the equation of motion is decoupled by the RPA. As for the term concerning single-ion anisotropy term in Eq. (1), we adopt the Anderson and Callen's (ACs) decoupling [73,74]. The application of the equation of motion of Green's function leads to a linear equations

$$\left[\omega\boldsymbol{I} - \boldsymbol{P}\right]\mathbf{g} = \boldsymbol{F}_{-1}, \tag{4}$$

where $\boldsymbol{I}$ is the unit vector, and $\boldsymbol{F}_{-1}$ is the commutator matrix of operators defined: $\boldsymbol{F}_{-1} = \left[\boldsymbol{A}, \boldsymbol{B}\right]$. The Hamiltonian matrix $\boldsymbol{P}$ is the following:

$$\mathbf{P} = \begin{pmatrix} J(0)\langle S_2^z\rangle + 2DC_1\langle S_1^z\rangle & -J(p,q)\langle S_1^z\rangle \\ -J(p,q)\langle S_2^z\rangle & J(0)\langle S_1^z\rangle + 2DC_2\langle S_2^z\rangle \end{pmatrix}. \tag{5}$$

where

$$J(0) = 4|J|, \tag{6}$$

$$J(\boldsymbol{k}) = J(p,q) = 4|J|\cos\left(\frac{pb}{2}\right)\cos\left(\frac{qb}{2}\right), \tag{7}$$

and

$$C_\mu = 1 - \frac{1}{2S^2}[S(S+1) - \langle S_\mu^z S_\mu^z\rangle],\ \mu = 1, 2. \tag{8}$$

The perimeter of the tube is mb, and the radius R of the tube is determined by $2\pi R=mb$. Hereafter we simply refer m as the diameter. In the Eq. (7), the quantity p is the wave vector along the tube axis z direction that takes the values within the first Brillouin zone (FBZ). The value of q is determined by

$$q = \frac{2\pi n}{mb},\ (n = 0, 1, 2, \ldots, m-1). \tag{9}$$

As m tends to infinity, the nanotube tends to be a 2D monolayer, and all the physical quantities will tend to those of a 2D monolayer [62]. In this sense we can regard p and q in $\omega_\tau(p, q)$ as two components of a wave vector $\boldsymbol{k}$:$\boldsymbol{k}$ = (p,q). One only needs to keep in mind that one of the vector components, q, takes the values determined by Eq. (9).

Note that we use $\langle S_\mu^z\rangle$, ($\mu = 1, 2$) to denote the magnetization of the sublattice 1 and 2, and S to denote spin nominal value. For the FM lattice, the exchange parameter J is positive, $\langle S_1^z\rangle = \langle S_2^z\rangle = \langle S^z\rangle$. For the AFM lattice, the exchange parameter J is negative, and when the external field is absent, $\langle S_1^z\rangle = -\langle S_2^z\rangle = \langle S^z\rangle$. The Hamiltonian matrix $\boldsymbol{P}$ eigenvalues $\omega_\tau(p, q)$, $\tau = 1, 2$ can be solved, which are just the spin wave elementary excitations spectra (EES) of the system. Since the lattice is divided into two sublattices, there are two branches of dispersion relationships. For the HFM-SWNTs,

$$\omega_1 = [J(0) + 2DC_1 + J(\mathbf{k})]\langle S_1^z\rangle,$$
$$\omega_2 = [J(0) + 2DC_2 - J(\mathbf{k})]\langle S_2^z\rangle. \tag{10}$$

For the HAFM-SWNTs,

$$\omega_\mu = \sqrt{\left[J(0) + 2DC_\mu\right]^2 - \left[J(\mathbf{k})\right]^2}\,\langle S_\mu^z\rangle,\ (\mu = 1, 2). \tag{11}$$

Following the Callen's method proposed in Ref. [71], the sublattice magnetization of arbitrary S is expressed [75,76] as follows,

$$\left\langle S_\mu^z\right\rangle = \frac{(\Phi_\mu + 1 + S)\Phi_\mu^{2S+1} - (\Phi_\mu - S)(\Phi_\mu + 1)^{2S+1}}{(\Phi_\mu + 1)^{2S+1} - \Phi_\mu^{2S+1}},\ \mu = 1, 2 \tag{12}$$

and

$$\left\langle S_\mu^z S_\mu^z\right\rangle = S(S+1) - (1 + 2\Phi_\mu)\left\langle S_\mu^z\right\rangle, \tag{13}$$

where

$$\Phi_\mu = \frac{1}{Nm}\sum_k\sum_\tau \frac{U_{\mu\tau}U_{\tau\mu}^{-1}}{e^{\beta\omega_\tau} - 1},\ \tau = 1, 2. \tag{14}$$

The eigenvector matrix $\boldsymbol{U}$ and its inverse $\boldsymbol{U}^{-1}$ of $\boldsymbol{P}$ can be solved, and $\beta = 1/T$, the inverse of temperature.

The RPA solution of the MBGFM [75] obeys the Mermin–