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The magnetic and thermodynamic properties of a spin-2 Heisenberg ferromagnetic system

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ABSTRACT

The magnetic and thermodynamic properties such as the magnetization, internal energy, specific heat and susceptibility of spin-2 Heisenberg ferromagnetic system on a square lattice are studied by using Green's function technique. Without including the next nearest neighbor interaction, one doesn't observe the second-order phase transitions. We found that only when the next nearest neighbor interaction is greater than the nearest neighbor interaction, the second-order phase transitions exist for the small single-ion anisotropy values. Indeed, in the case of negative anisotropy which corresponds to first-order phase transitions, the energies have discontinuities. At the same time, the specific heat shows two peaks.

1. Introduction

Owing to the exchange interaction, some materials exhibit a spontaneous magnetic moment below a certain critical temperature which is associated with a second-order phase transition from ferromagnetic to paramagnetic. The various magnetic properties of Heisenberg ferromagnetic system can be investigated by the double-time temperature-dependence Green's function theory [1–5]; Tahir-Kheli and ter Haar have calculated the internal energy and specific heat [2,3]. Fröbrich et al. have developed a method to calculate more than one component of the magnetization for ferromagnetic films [6–9]. Junger et al. have found that the specific heat had two maxima and power laws for the position and height of the susceptibility maximum did not support the predictions of Landau theory [10,11]. Wang et al. have very recently presented a very nice formalism which gave the internal energy as the thermal average in terms of z-component of spin operator by using time derivatives of correlation function [12,13].

Indeed, there have been many interesting works dealing with the Heisenberg ferromagnet in one- and two-dimensional systems [14–19]. For some ferromagnetic low dimensional systems, Hamedoun et al. have found that there existed a phase transition from ferromagnetic to paramagnetic state at a finite temperature [20].

In this work, we will apply Green's function technique to investigate the magnetization, internal energy, specific heat, susceptibility of spin-2 Heisenberg ferromagnet on the square lattice. In order to obtain the internal energy, we will follow the above-mentioned formalism of Wang et al. [13], but we introduce the next nearest neighbor interaction. The outline of this paper is as follows. In Section 2, we present the formalism of the Green's function method. In Section 3, the numerical results are discussed for the magnetization, internal energy, specific heat and susceptibility. Finally, Section 4 contributes to conclusions.

2. Model and formalism

Let us consider the spin-2 Heisenberg ferromagnetic model on a square lattice whose lattice constant is a. Hamiltonian which includes nearest neighbor and next nearest neighbor interactions, single-ion anisotropy and an external magnetic field in the z-direction is as follows:

$$H = -\frac{1}{2}J\sum_{ij}\boldsymbol{S}_i \times \boldsymbol{S}_j - \frac{1}{2}J_1\sum_{ii'}\boldsymbol{S}_i \times \boldsymbol{S}_{i'} - D\sum_i (S_i^z)^2 - h\sum_i S_i^z, \quad (1)$$

The first summation runs over pairs of the nearest neighbor sites and the second runs over pairs of the next nearest neighbor sites. J is the exchange coupling constant between the nearest neighboring sites and J_1 between the next nearest neighboring sites. We consider only ferromagnetic cases which have positive exchange parameters (J and $J_1 > 0$). D is the single-ion anisotropy parameter and the magnetic field h is applied along the z-axis.

In order to study magnetic properties of the model, we introduce the Green's function $\langle\langle S_i^+(t); B_l(0)\rangle\rangle$, where $B_l = e^{\eta S_i^z} S_i^-$

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(η is a parameter) and $S_i^+(t)$ and $S_i^-(0)$ are Heisenberg spin operators [4].

We have obtained the following equation of motion for the Green's function:

$$\omega\langle\langle S_i^+; B_l\rangle\rangle = \delta_{il}\langle[S_i^+, B_l]\rangle - J\sum_j \langle\langle (S_i^z S_j^+ - S_i^+ S_j^z); B_l\rangle\rangle - J_1\sum_{i'}\langle\langle (S_i^z S_{i'}^+ - S_i^+ S_{i'}^z); B_l\rangle\rangle \quad (2)$$

where δ is Dirac's delta function and $\langle\ldots\rangle$ denotes the canonical thermal average. We have taken the value of $\hbar$ as unit.

In the equations of motion, the higher order Green's functions will appear. For the decoupling process, we perform the random phase approximation concerning the exchange interaction terms [2,3]

$$\langle\langle S_i^z S_j^+; B_l\rangle\rangle \cong \langle S_i^z\rangle\langle\langle S_j^+; B_l\rangle\rangle, \quad (3)$$

and a generalization of the Anderson–Callen's decoupling schema concerning the single-ion anisotropy term [5]

$$\langle\langle (S_i^+ S_i^z + S_i^z S_i^+); B_l\rangle\rangle \cong \tau\langle\langle S_i^+; B_l\rangle\rangle, \quad (4)$$

where

$$\tau = \{2 - [S_p - 2\langle (S^z)^2\rangle]/S^2\}\langle S^z\rangle. \quad (5)$$

here $S_p = S(S+1)$.

Then we obtain the following Green's function

$$G(\omega, \mathbf{k}) = \frac{\langle [S^+, B]\rangle}{\omega - \omega(\mathbf{k})}, \quad (6)$$

where

$$\omega(\mathbf{k}) = \{D\tau + 4(J + J_1) - 2J\gamma - 4J_1\gamma_1\}\langle S^z\rangle + h, \quad (7)$$

$$\gamma = \cos(k_x a) + \cos(k_y a), \quad (8)$$

$$\gamma_1 = \cos(\sqrt{2}k_x a)\cos(\sqrt{2}k_y a). \quad (9)$$

One has the following expressions for $\langle S^z\rangle$and its other power thermal averages by means of spectral theorem and Callen's technique [4]

$$\langle S^z\rangle = \frac{(S-\Phi)(1+\Phi)^{2S+1} + (S+1+\Phi)\Phi^{2S+1}}{(1+\Phi)^{2S+1} - \Phi^{2S+1}}, \quad (10)$$

$$\langle (S^z)^2\rangle = S_p - (1+2\Phi)\langle S^z\rangle, \quad (11)$$

$$\langle (S^z)^3\rangle = \{(1+2\Phi)[S_p - 3\langle (S^z)^2\rangle] + [2S_p - 1]\langle S^z\rangle\}/2, \quad (12)$$

$$\langle (S^z)^4\rangle = S_p^2 - \langle (S^z)^2\rangle - 2(1+2\Phi)\langle (S^z)^3\rangle, \quad (13)$$

where

$$\Phi = \frac{1}{N}\sum_{\mathbf{k}} \frac{1}{e^{\beta\omega(\mathbf{k})} - 1}, \quad (14)$$

here $\mathbf{k}$ sums over the first Brillouin Zone and N is the total site number in the system.

In order to obtain internal energy, we have followed the formalism developed by Wang et al. [13]. The internal energy is defined as a statistical average of the Hamiltonian per site: $U_{in} = -(\langle H\rangle/N)$. The internal energy is formed from two parts defined as the transverse correlation energy (U_{TC}) and the longitudinal correlation energy (U_{LC}). So, we obtain these terms of the internal energy as follows:

$$U_{TC} = -\langle S^z\rangle\Phi_1, \quad (15)$$

$$U_{LC} = -\frac{1}{2[S_p+1]}\Big\{[S_p - (2S_p+1)\langle S^z\rangle - 3\langle (S^z)^2\rangle + 4\langle (S^z)^3\rangle]\Phi_1 + [-S_p - 3\langle S^z\rangle + 3\langle (S^z)^2\rangle]\Phi_2 + 4(J + J_1)[S_p + \langle (S^z)^3\rangle]\langle S^z\rangle + D[2\langle (S^z)^4\rangle + \langle (S^z)^3\rangle - 2(S_p+1)\langle (S^z)^2\rangle + (S_p+1)\langle S^z\rangle + S_p] + h[S_p - (S_p+1)\langle S^z\rangle + \langle (S^z)^3\rangle]\Big\} \quad (16)$$

where

$$\Phi_1 = \frac{1}{N}\sum_{\mathbf{k}} \frac{J(\mathbf{k})}{e^{\beta\omega(\mathbf{k})} - 1}, \quad (17)$$

$$\Phi_2 = \frac{1}{N}\sum_{\mathbf{k}} \frac{\omega(\mathbf{k})}{e^{\beta\omega(\mathbf{k})} - 1}, \quad (18)$$

where $\omega(\mathbf{k})$ is given by Eq. (7) and $J(\mathbf{k}) = J\sum_m e^{i\mathbf{k}\cdot\mathbf{m}} + J_1\sum_n e^{i\mathbf{k}\cdot\mathbf{n}}$, here the first summation is over nearest neighbors and second is over the next nearest neighbors.

Specific heat C is defined as the derivative of the internal energy with respect to temperature:

$$C = \frac{\partial U(T)}{\partial T}. \quad (19)$$

Parallel susceptibility $\chi_{//}$ is calculated as follows:

$$\chi_{//} = \frac{\langle S^z\rangle_h - \langle S^z\rangle_0}{h}. \quad (20)$$

3. Results and discussions

The coupled Eqs. (10)–(18) can be solved self-consistently for each value of temperature. Thus, the magnetization and internal energy are calculated numerically, depending on the values of the applied magnetic field. Also the specific heat and parallel susceptibility can be found numerically.

We start by demonstrating results for phase diagrams of spin-2 Heisenberg ferromagnet on square lattice. In Fig. 1, we plot phase diagrams in the $(J_1 - T)$ plane at $J=5$ for both positive and negative values of the single-ion anisotropy. The dotted and solid lines represent the first-order and second-order phase transition temperatures, respectively. When the next nearest neighbor interaction is zero, for all value of single-ion anisotropy, the transition becomes the first-order. Only when $J_1 > J$ and for the small values of single-ion anisotropy one observe the second-order phase transition. At the same time, these results are valid for the negative values of the single-ion anisotropy, but another discontinuity exists. This transition also becomes the first-order. We show these with the chain-dotted, chain-double-dotted, short-dashed and long-dashed lines in Fig. 1(b). For $D=-0.01$ and -0.05, it disappears just after the critical temperature appears.

Fig. 2 demonstrates the influence of an external magnetic field on magnetization when the value of the anisotropy is equal to $D=-0.01$ at $J=5$ and $J_1=3$. At this parameters, there is no the second-order phase transition. In the case of negative anisotropy, the magnetization decreases to zero discontinuously with increasing the temperature for both $h=0$ and $h=0.01$. Therefore, the first-order phase transition occurs at $T_D=17.6$ (for $h=0$) and $T_D=13.9$ (for $h=0.01$), whereas the curve for $h=0.05$ shows the typical behavior of ferromagnetic case without discontinuity. At the same time, similar behaviors are seen for the temperature variations of energies and specific heat. For the same values in Fig. 2, we plot the transverse correlation energy, the longitudinal correlation energy and the internal energy in Fig. 3. As seen from the figure, for both $h=0$ and $h=0.01$, the energies have discontinuities at the first-order phase transition temperature at $T_D=17.6$ and $T_D=13.9$, respectively.