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The magnetic properties of a mixed spin-1/2 and spin-1 Heisenberg ferrimagnetic system on a two-dimensional square lattice

Ai-Yuan Hu [a,*], A.-Jie Zhang [b]

[a] School of Physics and Electronic Engineering, Chongqing Normal University, Chongqing 401331, China
[b] Military Operational Research Teaching Division of the 4th Department, PLA Academy of National Defense Information, Wuhan 430000, China

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ABSTRACT

The magnetic properties of a mixed spin-1/2 and spin-1 Heisenberg ferrimagnetic system on a two-dimensional square lattice are investigated by means of the double-time Green's function technique within the random phase decoupling approximation. The role of the nearest-, next-nearest-neighbors interactions and the exchange anisotropy in the Hamiltonian is explored. And their effects on the critical and compensation temperature are discussed in detail. Our investigation indicates that both the next-nearest-neighbor interactions and the anisotropy have a great effect on the phase diagram.

1. Introduction

In physics, a ferrimagnetic material is one that has populations of atoms with opposing magnetic moments, as in antiferromagnetism; however, in ferrimagnetic materials, the opposing moments are unequal. Thus, unlike antiferromagnets, these materials have a net magnetic moment at low temperature that vanishes at a critical temperature T_c. In addition, since the sublattice moments have, in general, a different temperature dependence, there is the possibility that they may exactly cancel at some lower temperature T_{com}, known as a compensation point. Such compensation points have been observed in a number of real materials, and have obvious technological interest [1,2].

In the last years, many theoretical models have been used with different techniques to understand their magnetic properties. For example, Mert has used Green's function for a mixed spin-1 and spin-2 Heisenberg ferrimagnetic system [3]. Oitmaa and Enting have used the high-temperature expansions for a mixed spin-1/2 and spin-1 ferrimagnetic Ising model [4]. Keskin et al. have used the Glauber-type stochastic dynamics for a mixed spin-1/2 and spin-3/2 Ising model [5]. Andrej et al. have studied the magnetic susceptibility of the mixed spin-1 and spin-1/2 anisotropic Heisenberg model based on the Oguchi approximation [6]. Bayram et al. have used the mean field method for a mixed spin-1/2 and spin-3/2 Ising ferrimagnetic model [7]. Buendía and Cardona have used the Monto Carlo technique for a mixed spin-3/2 and spin-1/2 Ising ferrimagnetic model [8]. Silvia and Michal have used the generalized mapping transformation technique for the mixed spin-1/2 and spin-S Ising ferrimagnetic model [9]. Zhang and Yan have used the effective field method for a mixed spin-1/2 and spin-1 Blume–Capel model [10].

One general conclusion emerges from the above work, i.e., in order to obtain a compensation point, single-ion anisotropy terms appear to be necessary. Therefore, the single-ion anisotropy is included in general investigation. Nevertheless, less investigation concerns ferrimagnetic model with an exchange anisotropy. In this paper, we consider an exchange anisotropy for a mixed spin-1/2 and spin-1 Heisenberg ferrimagnetic model on a square lattice. Our investigations show that a compensation point can also emerge in an exchange anisotropy.

The outline of this paper is as follows. In Section 2, the model and fundamental equations are presented. In Section 3, results and discussions are given. Finally, Section 4 contains conclusions.

2. Model and method

The Hamiltonian of a mixed spin-1/2 and spin-1 Heisenberg ferrimagnetic model on a two-dimensional square lattice may be

* Corresponding author.
E-mail address: huaiyuanhuyuanai@126.com (A.-Y. Hu).

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written as

$$H = J_1 \sum_{\langle i,j\rangle} [\frac{\eta_1}{2}(s_i^+ S_j^- + s_i^- S_j^+) + s_i^z S_j^z] - \frac{J_2}{2} \sum_{[i,j]} [\frac{\eta_2}{2}(s_i^+ s_j^- + s_i^- s_j^+) + s_i^z s_j^z] - \frac{J_3}{2} \sum_{[i,j]} [\frac{\eta_3}{2}(S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z]. \quad (1)$$

where $s=1/2$ and $S=1$. The sums $\langle i, j\rangle$ and $[i, j]$ run over the nearest-neighbor (nn) and next-nearest-neighbor (nnn) lattice sites, respectively. J_1 is the antiferromagnetic nn exchange interaction, J_2 and J_3 are the ferromagnetic nnn exchange interaction. η_1, η_2 and η_3 are the exchange anisotropy parameters. The ferrimagnetic lattice can be partitioned into two equivalent sublattices, labeled by s and S, respectively. Therefore, the sublattice magnetization can be defined as $m_s = \langle s_i^z\rangle$, $m_S = \langle S_i^z\rangle$.

In the following, we introduce four kinds of Green's functions to obtain the sublattice magnetization and the energy of the magnetic excitation:

$$G_{ss} = \langle\langle s_i^+; e^{us_j^z} s_j^-\rangle\rangle; \quad G_{Ss} = \langle\langle S_i^+; e^{us_j^z} s_j^-\rangle\rangle; G_{SS} = \langle\langle S_i^+; e^{uS_j^z} S_j^-\rangle\rangle; \quad G_{sS} = \langle\langle s_i^+; e^{uS_j^z} S_j^-\rangle\rangle,$$

where u is the Callen parameter [11]. We derive the equation of motion of Green's function by the standard procedure [12]. In the course of derivation, the higher order Green's functions have to be decoupled. In this paper, we use the random phase approximation (RPA) decoupling [11,12]

$$\langle\langle A_l^z A_i^+; e^{uA_j^z} A_j^-\rangle\rangle = \langle A_l^z\rangle\langle\langle A_i^+; e^{uA_j^z} A_j^-\rangle\rangle; \quad l \neq i, \quad (2)$$

where $A = s, S$. The equal-time correlation function

$$Q(u) = \langle e^{uA_i^z} A_i^- A_i^+\rangle \quad (3)$$

is calculated via the spectral theorem [11,12]. It is expressed by

$$\frac{2}{N} \sum_k \langle e^{uA_i^z} A_i^- A_i^+\rangle(k) = \theta(u)\phi_A, \quad (4)$$

with

$$\theta(u) = \langle [A_i^+, e^{uA_j^z} A_i^-]\rangle, \quad (5)$$

where N is the number of lattice sites. The summation over wavevector k runs over the first Brillouin zone. Green's functions are Fourier-transformed into wavevector space. After that, the equal-time correlation function $\langle e^{uA_i^z} A_i^- A_i^+\rangle(k)$ is calculated via the spectral theorem. For $u=0$, $\theta(u) = 2\langle A^z\rangle$, we obtain

$$\phi_A = \frac{2}{N} \sum_k \frac{1}{2(w_k^+ - w_k^-)} [(w_k^+ + E_A)\coth\frac{\beta w_k^+}{2} - (w_k^- + E_A) \coth\frac{\beta w_k^-}{2}] - \frac{1}{2}, \quad (6)$$

with

$$w_k^\pm = \frac{-(E_s + E_S) \pm \sqrt{(E_s - E_S)^2 + 4E_3E_4}}{2}, \quad (7)$$

$$E_s = 4J_1 m_s + 4J_2 m_S(\eta_3\gamma_{2k} - 1); \quad E_3 = 4J_1 m_s \eta_1\gamma_{1k} E_S = 4J_1 m_S + 4J_2 m_s(\eta_2\gamma_{2k} - 1); \quad E_4 = 4J_1 m_S \eta_1\gamma_{1k} \quad (8)$$

$$\gamma_{1k} = \tfrac{1}{2}(\cos k_x + \cos k_y); \quad \gamma_{2k} = \cos k_x \cos k_y.$$

Using the relations $\langle A_i^- A_i^+\rangle = A(A+1) - \langle A_i^z\rangle - \langle (A_i^z)^2\rangle$, the solution of equation for m_A

$$m_A = \frac{(\phi_A + 1 + A)\phi_s^{2A+1} - (\phi_A - A)(\phi_A + 1)^{2A+1}}{(\phi_A + 1)^{2A+1} - \phi_A^{2A+1}}. \quad (9)$$

Thus, the total magnetization M of system is defined as

$$M = m_s + m_S \quad (10)$$

3. Results and discussions

In Fig. 1, we discuss the effect of J_3 on the magnetization when the nnn interaction in sublattice s is not included. As seen from Fig. 1(a)–(c), they exhibit two types of magnetization behavior according to the Néel classification [13]. For example, for a strong anisotropy (see Fig. 1(a)), the magnetization curves are of Q-type behavior when $J_3=0$, 0.1 and 0.5. For a weak anisotropy (see Fig. 1(b) and Fig. 1(c)), they are of P-type behavior when $J_3=0.8$ and 1. Nevertheless, only the P-type magnetization curves exist for the large value of J_3 (see Fig. 1(d)). Compared with a strong anisotropy case, the total magnetization in a weak anisotropy case is more sensitive to the change of J_3.

Meanwhile, we notice that Fig. 1(a)–(c) show the total magnetization dependence on temperature for some small values of J_3. Fig. 1(d) exhibits the sublattice magnetization and the total magnetization as a function of temperature for some large values of J_3. Our results show that the magnetization simply goes to zero at the critical temperature. The compensation temperature does not appear for arbitrary J_3 value when the J_2 is not included. And one can find from Fig. 1(d) that, the s sublattice magnetization is insensitive to the change of J_3 in the whole temperature range as J_2 is zero, whereas the S sublattice magnetization is sensitive to the change of J_3 in the high temperature. In low temperature, the S sublattice magnetization is also insensitive to J_3. It shows that the case of $m_s = -m_S \neq 0$ will not exist. This also means that the compensation point cannot appear.

In Fig. 2(a) and (b), we discuss the effect of J_2 on the magnetization in a strong and weak anisotropy when the J_3 is not included. One can see that the compensation point appears when the J_2 is considered. For different anisotropies, the J_2 hardly affects the compensation temperature, whereas the critical temperature increases with the increasing of J_2. For a fixed J_2 (see Fig. 2(c)), the T_C and T_{com} increase with increasing J_3. Nevertheless, the T_{com} is more sensitive to the change of J_3 than T_C.

In Figs. 3, 4 and 5, the impact of exchange interaction, anisotropy on the compensation and critical temperature is explored respectively in detail. For fixed J_1 and J_2 (see Fig. 3), the T_C decreases with increasing η (here $\eta = \eta_1 = \eta_2 = \eta_3$). This is because that the anisotropy impedes the quantum fluctuation. It leads to a large T_C. However, the anisotropy hardly affects the T_{com}. Meanwhile, one find that the T_{com} is very sensitive to the change of J_3. It can more easily be seen from Fig. 4. In Fig. 4, we show the T_{com} and T_C as a function of J_3 for $\eta = 0.5$ and $J_1 = 1$ when $J_2=4$, 6 and 8. It clearly exhibits that the T_{com} rapidly increases with increasing J_3. And it also shows that the T_C with larger J_2 and J_3 is larger.

Fig. 5 exhibits the compensation temperature dependence of J_2 for $\eta=0.5$ and $J_1 = 1$ when $J_3=0$, 0.5 and 1. For fixed J_1 and J_3, the values of T_{com} almost unchange with the change of J_2. Note that the compensation point does not always appear when the J_2 is included. But there is a minimum value of J_2 (i.e., J_2^{min}), and only when $J_2 \geq J_2^{min}$, the compensation point can appear. Moreover, the value of J_2^{min} becomes large with the increasing J_3. For example, when $J_3=0$, 0.5 and 1, the corresponding values of J_2^{min} are 1.8,