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Internal energy and specific heat in a ferromagnetic-antiferromagnetic double layers*

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The internal energy and specific heat of a Heisenberg ferro- antiferromagnetic double-layer system are studied by using spin-wave theory and the retarded Green function method at low temperatures. Numerical results show that the antiferromagnetic intralayer coupling J_2 has an important influence on internal energy and specific heat for a four-sublattice system with antiferromagnetic (or ferrimagnetic) interlayer couplings.

Keywords: spin-wave theory, ferromagnetic-antiferromagnetic double layers, internal energy, specific heat

PACC: 7510D, 7510H, 7550G

1. Introduction

The rare-earth (R) and transition-metal (T) intermetallics spin exchange coupling is an antiferromagnetic character and leads to an antiparallel 3d and 4f moment configuration for the heavy rare-earth matters and a parallel moment configuration for the light rare-earth matters. The two-sublattice Heisenberg model can be usually applied to explaining the R and T intermetallics $(R'_xR_{1-x})_2\mathrm{Fe}_{14}\mathrm{B}$ and $(R'_xR_{1-x})\mathrm{Co}_5$ which have outstanding permanent properties.[1−3] Heisenberg model has been applied successfully to various magnetic problems.[4−6] Magnetic systems with a spin current have been studied.[7−9] However, the existence of different R and T sites in some compounds results in the development of a multi-sublattice model. The multi-sublattice model involving different sites in a unit cell, has been applied to describing the properties of $R-T$ materials and explaining the phenomena in magnetic layer and superlattice systems. Usually some magnetic properties, such as spontaneous magnetization and Curie temperature, are of significance in their applications. Studies of these materials may lead to a better understanding of the magnetic properties of the 3d and 4f elements. In this paper, we consider a four-sublattice Heisenberg double-layer system that has been described in our previous work.[10] The Hamiltonian for four-sublattice double layers with a square lattice structure is

$$\begin{aligned} H = &-2\sum_{il}\left[(J_1+D_1)S_i^zS_l^z+\frac{1}{2}J_1(S_i^+S_l^-+S_i^-S_l^+)\right] \\ &-2\sum_{jm}\left[(J_2+D_2)S_j^zS_m^z+\frac{1}{2}J_2(S_j^+S_m^-+S_j^-S_m^+)\right] \\ &-2\sum_{ij}\left[(J_z+D_z)S_i^zS_j^z+\frac{1}{2}J_z(S_i^+S_j^-+S_i^-S_j^+)\right] \\ &-2\sum_{lm}\left[(J_z+D_z)S_l^zS_m^z+\frac{1}{2}J_z(S_l^+S_m^-+S_l^-S_m^+)\right], \end{aligned} \quad (1)$$

where the summation is over all the nearest-neighbour spin; J_1 and D_1 are the exchange integral and anisotropy between S_i and S_l at the lattice sites i and l, respectively, and they are both positive in the ferromagnetic layer; J_2 and D_2 are the exchange integral and anisotropy between S_j and S_m at the lattice sites j and m, respectively, and they are both negative in the antiferromagnetic layer; J_z and D_z are interlayer exchange integral and anisotropy if one spin is in a ferromagnetic layer and the other spin in a antiferromagnetic layer, and they are both negative for antiferromagnetic (or ferrimagnetic) interlayer coupling. It is convenient to divide the system into four sublattices A, B, C and D, among which sublattices A and B (both up spins) have a spin value of S_a, sublattices C and D (down and up spins) with the spin value of S_b. There are N sites on each sublattice, and a total

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of $4N$ sites for the system.

2. Theory

In order to calculate the internal energy, we use the Holstein–Primakoff transform[11] and the linear spin-wave approximation,[12] and introduce the spin-wave operators $a_k(a_k^+)$, $b_k(b_k^+)$, $c_k(c_k^+)$ and d_k (d_k^+). The forth-order matrix retarded Green function can be defined as[10]

$$G(k,\omega)=\begin{pmatrix} \langle\langle a_k;a_k^+\rangle\rangle & \langle\langle a_k;b_k^+\rangle\rangle & \langle\langle a_k;c_k\rangle\rangle & \langle\langle a_k;d_k^+\rangle\rangle \\ \langle\langle b_k;a_k^+\rangle\rangle & \langle\langle b_k;b_k^+\rangle\rangle & \langle\langle b_k;c_k\rangle\rangle & \langle\langle b_k;d_k^+\rangle\rangle \\ \langle\langle c_k^+;a_k^+\rangle\rangle & \langle\langle c_k^+;b_k^+\rangle\rangle & \langle\langle c_k^+;c_k\rangle\rangle & \langle\langle c_k^+;d_k^+\rangle\rangle \\ \langle\langle d_k;a_k^+\rangle\rangle & \langle\langle d_k;b_k^+\rangle\rangle & \langle\langle d_k;c_k\rangle\rangle & \langle\langle d_k;d_k^+\rangle\rangle \end{pmatrix}. \tag{2}$$

Using the equation- of- motion technique for the Green function, we obtain

$$MG=I, \tag{3}$$

where I is the unit matrix and

$$M=\begin{pmatrix} \omega-E_{11} & E_{12} & E_{13} & 0 \\ E_{12} & \omega-E_{22} & 0 & E_{13} \\ -E_{13} & 0 & \omega-E_{33} & -E_{34} \\ 0 & E_{13} & E_{34} & \omega-E_{44} \end{pmatrix} \tag{4}$$

with

$$\begin{aligned} E_{11}&=8(J_1+D_1)S_a-2(J_z+D_z)S_b,\\ E_{22}&=8(J_1+D_1)S_a+2(J_z+D_z)S_b,\\ E_{33}&=8(J_2+D_2)S_b+2(J_z+D_z)S_a,\\ E_{44}&=-8(J_2+D_2)S_b+2(J_z+D_z)S_a,\\ E_{12}&=2J_1S_ap_k,\quad E_{13}=2J_z\sqrt{S_aS_b},\\ E_{34}&=2J_2S_bp_k,\quad p_k=2(\cos k_x+\cos k_y). \end{aligned}$$

The spin-wave spectrum of the four-sublattice model is easily obtained by solving

$$\det(M)=0, \tag{5}$$

where $\det(M)$ is the determinant of the matrix M.

Equation (5) is a quartic equation in ω, it has four real roots ω_l $(l=1,2,3,4)$ corresponding to four branches of the spin-wave spectrum.

Using the spectral theorem, the internal energy per site is obtained as follows:

$$\begin{aligned} U=\frac{1}{4N}\langle H\rangle&=-2[(J_1+D_1)S_a^2-(J_2+D_2)S_b^2]+2(J_2+D_2)S_b+\frac{1}{2}(J_z+D_z)S_a\\ &+\Big[2(J_1+D_1)S_a-\frac{1}{2}(J_z+D_z)S_b\Big]\Big[\frac{1}{\pi^2}\iint_0^\pi F_1\mathrm{d}k_x\mathrm{d}k_y\Big]\\ &+\Big[2(J_1+D_1)S_a+\frac{1}{2}(J_z+D_z)S_b\Big]\Big[\frac{1}{\pi^2}\iint_0^\pi F_2\mathrm{d}k_x\mathrm{d}k_y\Big]\\ &+\Big[2(J_2+D_2)S_b+\frac{1}{2}(J_z+D_z)S_a\Big]\Big[\frac{1}{\pi^2}\iint_0^\pi F_3\mathrm{d}k_x\mathrm{d}k_y\Big]\\ &-\Big[2(J_2+D_2)S_b-\frac{1}{2}(J_z+D_z)S_a\Big]\Big[\frac{1}{\pi^2}\iint_0^\pi F_4\mathrm{d}k_x\mathrm{d}k_y\Big]\\ &-J_z\sqrt{S_aS_b}\frac{1}{\pi^2}\iint_0^\pi F_5\mathrm{d}k_x\mathrm{d}k_y-J_z\sqrt{S_aS_b}\frac{1}{\pi^2}\iint_0^\pi F_6\mathrm{d}k_x\mathrm{d}k_y \end{aligned}$$

$$- J_1 S_a \frac{1}{\pi^2} \iint_0^\pi F_7 p_k \mathrm{d}k_x \mathrm{d}k_y - J_2 S_b \frac{1}{\pi^2} \iint_0^\pi F_8 p_k \mathrm{d}k_x \mathrm{d}k_y, \tag{6}$$

where

$$F_k = \sum_{l=1}^{4} \frac{N_{ij}(\omega_l)}{[\exp(\beta\omega_l) - 1] \prod_{m \neq l} (\omega_l - \omega_m)} \tag{7}$$

with $N_{ij} (i = j;\ i, j = 1, 2;\ i, j = 1, 3;\ i, j = 2, 4;\ i, j = 4, 3)$ being the cofactors of the elements in the matrix M for $\omega = \omega_l$, $k = 1, 2, 3, 4, 5, 6, 7, 8$.

The specific heat at low temperatures for the system is derived as follows:

$$\begin{aligned} C_v = \partial U / \partial T = & \Big[2(J_1 + D_1)S_a - \frac{1}{2}(J_z + D_z)S_b\Big]\Big[\frac{1}{\pi^2} \iint_0^\pi F_1' \mathrm{d}k_x \mathrm{d}k_y\Big] \\ & + \Big[2(J_1 + D_1)S_a + \frac{1}{2}(J_z + D_z)S_b\Big]\Big[\frac{1}{\pi^2} \iint_0^\pi F_2' \mathrm{d}k_x \mathrm{d}k_y\Big] \\ & + \Big[2(J_2 + D_2)S_b + \frac{1}{2}(J_z + D_z)S_a\Big]\Big[\frac{1}{\pi^2} \iint_0^\pi F_3' \mathrm{d}k_x \mathrm{d}k_y\Big] \\ & - \Big[2(J_2 + D_2)S_b - \frac{1}{2}(J_z + D_z)S_a\Big]\Big[\frac{1}{\pi^2} \iint_0^\pi F_4' \mathrm{d}k_x \mathrm{d}k_y\Big] \\ & - J_z \sqrt{S_a S_b} \frac{1}{\pi^2} \iint_0^\pi F_5' \mathrm{d}k_x \mathrm{d}k_y - J_z \sqrt{S_a S_b} \frac{1}{\pi^2} \iint_0^\pi F_6' \mathrm{d}k_x \mathrm{d}k_y \\ & - J_1 S_a \frac{1}{\pi^2} \iint_0^\pi F_7' p_k \mathrm{d}k_x \mathrm{d}k_y - J_2 S_b \frac{1}{\pi^2} \iint_0^\pi F_8' p_k \mathrm{d}k_x \mathrm{d}k_y, \end{aligned} \tag{8}$$

where

$$F_k' = \sum_{l=1}^{4} \frac{N_{ij}(\omega_l) \cdot \omega_l \cdot \exp(\beta\omega_l) \cdot \beta^2}{[\exp(\beta\omega_l) - 1]^2 \prod_{m \neq l} (\omega_l - \omega_m)}. \tag{9}$$

3. Numerical results and discussion

Taking $J_1 = 1.0$, $D_1 = -D_2 = 0.2$, $J_z = -0.5$ and $D_z = 0.0$, we numerically derive the temperature dependence of the internal energy from Eqs.(6) and (7). The results are shown in Figs.1–3. The curves a, b, c, d and e correspond to $J_2 = -0.5, -0.8, -1.0 - 1.2$ and -1.5, respectively. For both the antiferromagnet in Figs.1 and 2 and the ferromagnet in Fig.3, the internal energy U increases with increasing temperature T, with values of S_a, S_b and J_2 fixed, and it decreases with increasing the absolute value J_2, with values of S_a, S_b and T fixed. Comparing Fig.1 with Fig.2, one can see that the internal energy for $S_a = S_b = 0.5$ is bigger than that for $S_a = S_b = 1.0$ at the same values of J_2 and T. In Fig.3, the solid curves represent the case of $S_a = 1.0$ and $S_b = 0.5$, while dashed curves refer to the case of $S_a = 0.5$ and $S_b = 1.0$. For the weaker region of the antiferromagnetic coupling $|J_2| \leq 1$, the internal energy curves a and b (dashed curves) for the case of $S_a = 0.5$ and $S_b = 1.0$ are bigger than those for the case of $S_a = 1.0$ and $S_b = 0.5$ (solid curves). For the stronger region of the antiferromagnetic coupling $|J_2| > 1$, the internal energy curves c, d and e (dashed curves) for the case of $S_a = 0.5$ and $S_b = 1.0$ are smaller than those for the case of $S_a = 1.0$ and $S_b = 0.5$ (solid curves). From Eqs.(8) and (9), the temperature dependence of the specific heat is calculated numerically for various values of J_2 and spins. The results for the cases of $S_a = S_b = 0.5$ and $S_a = S_b = 1.0$ are plotted in Figs.4 and 5, respectively, showing that the specific heat increases with

increasing temperature T, with values of S_a, S_b and J_2 fixed. The specific heat increases with decreasing the absolute value J_2, with the values of S_a, S_b and T fixed. Comparing Figs.4 and 5, one can see that the specific heat for the case of $S_a = S_b = 0.5$ is bigger than that for the case of $S_a = S_b = 1.0$ at the same values of J_2 and T.

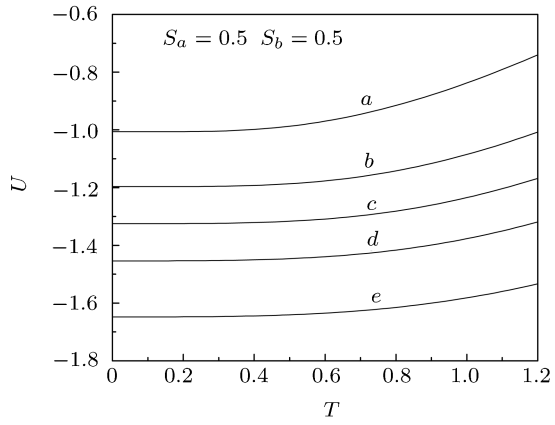


Fig.1. The temperature dependences of internal energy for four-sublattice double layers with $S_a = S_b = 0.5$.

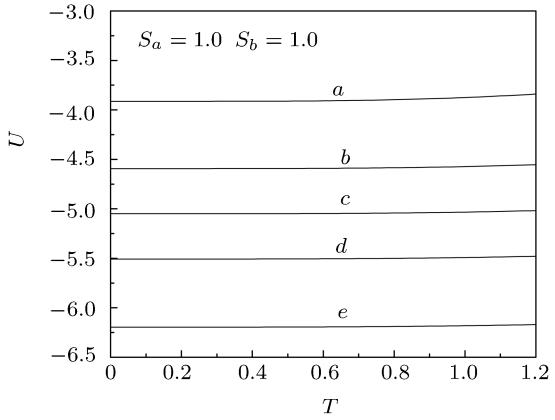


Fig.2. The temperature dependences of internal energy for four-sublattice double layers with $S_a = S_b = 1.0$.

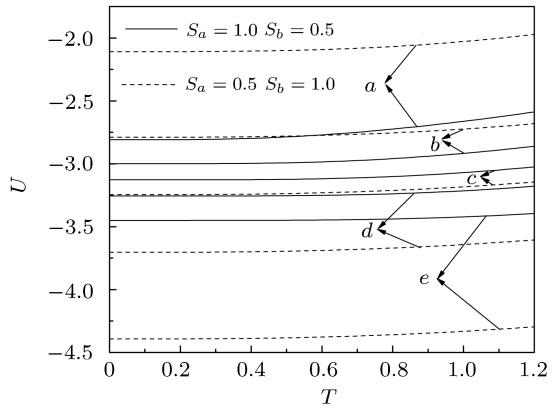


Fig.3. The temperature dependences of internal energy for four-sublattice double layers. The solid curves represent the case of $S_a = 1.0$ and $S_b = 0.5$, while dashed curves refer to the case of $S_a = 0.5$ and $S_b = 1.0$.

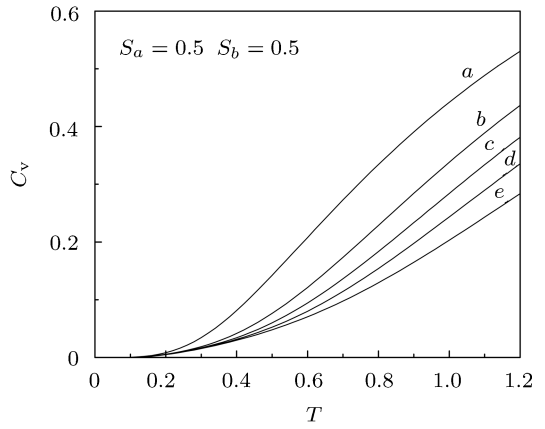


Fig.4. The temperature dependences of specific heat for four-sublattice double layers with $S_a = S_b = 0.5$.

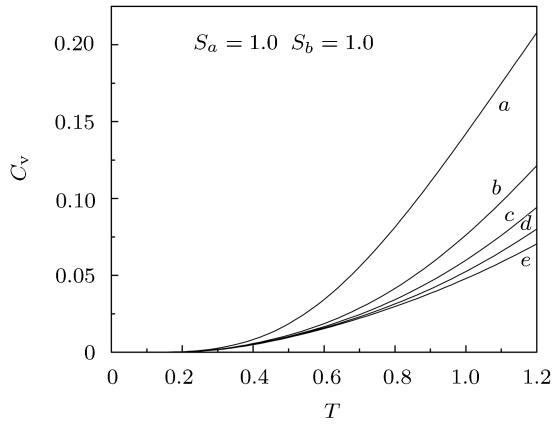


Fig.5. The temperature dependences of specific heat for four-sublattice double layers with $S_a = S_b = 1.0$.

4. Summary

Within the framework of the linear spin wave theory, by employing retard Green function, we have studied the internal energy and the specific heat of the ferromagnetic and antiferromagnetic double layers at low temperatures. Numerical results show that the antiferromagnetic coupling J_2 in the second layer has an important influence on the four-sublattice system. If the antiferromagnetic coupling is$|J_2| \leq 1$, the internal energy for the case of $S_a = 0.5$ and $S_b = 1.0$ is bigger than that for the case of $S_a = 1.0$ and $S_b = 0.5$. If the antiferromagnetic coupling is $|J_2| > 1$, the internal energy for the case of $S_a = 0.5$ and $S_b = 1.0$ is smaller than that for the case of $S_a = 1.0$ and $S_b = 0.5$. The internal energy U and specific heat C_v increase with increasing temperature T. The internal energy U and specific heat C_v decrease with the increase of the antiferromagnetic coupling $|J_2|$ in the second layer.

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