Vol 18 No 8, August 2009
1674-1056/2009/18(08)/3547-04

Chinese Physics B

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Quantum fluctuations of the antiferro-antiferromagnetic double-layer*

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(Received 12 April 2009; revised manuscript received 20 April 2008)

This paper stuides the magnetization and quantum fluctuations of an antiferro-antiferromagnetic (AF-AF) double-layer at zero temperature. It is found that the exchanges and anisotropy constants affect the quantum fluctuations of spins. If the anisotropy exists, there will be no acoustic energy branch in the system. The anisotropy constant, antiferromagnetic intralayer and interlayer coupling have important roles in a balance of the quantum competition.

Keywords: quantum fluctuations, antiferromagnetic double-layer, magnetization
PACC: 7510H, 7550E,7530D

1. Introduction

Because the ground state of the antiferromagnets has not been confirmed, the study on the ground state of AF-AF double-layer has more importance and complexity, which mainly originates from the quantum fluctuations. The anisotropic Heisenberg antiferromagnet (AF) model is believed to describe the magnetic properties of the cupric oxide materials.[1−3] Many results of previous works have been obtained by using numerical calculation and various methods to study the magnetic properties of AF systems.[4] The ground-state property of the anisotropic Heisenberg AF, which is defined as a three-dimensional simple cubic lattice, is studied by using spin-wave theory.[5] The Green-function Monte Carlo (GFMC) method is used to study the ground-state correlations of quantum AFs.[6] Within the Tyablikov's theoretical framework, the ground-state property of the two-dimensional antiferromagnetic Heisenberg model has been studied.[7] Moschel *et al* have investigated a ferromagnetic-antiferromagnetic double-layer system in which frustrated spins exist without an applied magnetic field by using a spin-Green function method.[8] Very recently, a new class of high-temperature superconductors has been discovered in layered iron arsenic compounds, which has a striped antiferromagnetic pattern.[9] Layered magnetic materials show many unique characteristics which are distinctly different from those for their bulk counterparts. In our recent works,[10,11] we calculated the spinwave spectra and physical properties of F-AF doublelayer and superlattices. In the present work, we shall carry out a detailed study of the magnetization and quantum fluctuations of an AF-AF double-layer at zero temperature. Emphasis will be put on the effects of the antiferromagnetic exchange and the anisotropy constants on the quantum fluctuations.

2. Theory

The Hamiltonian of the AF-AF double layers is

$$H = \sum_{i,j} J_{ij} S_i S_j - \sum_{i,j} D_{ij} S_i^z S_j^z, \qquad (1)$$

where the summation is over all the nearest-neighbor spins. The $J_{ij}(D_{ij})$ is equal to $J_1 < 0$ ($D_1 < 0$) in the first layer, equal to $J_2 < 0$ ($D_2 < 0$) in the second layer, and equal to $J_z < 0$ ($D_z < 0$) between the first and the second layer. It is convenient to divide the system into four sublattices A, B, C and D, among which A and B (up and down spins) have spin values of S_a and S_b, C and D (down and up spins) have spin values of S_c and S_d, respectively. There are N sites on each sublattice, and a total of $4N$ sites for the system.

*Project supported by the Natural Science Foundation of the Educational Department of Liaoning Province, China (Grant Nos 20060638 and 2008533).

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Using the method of Refs.[10] and [11], we obtain the equation of the Green's function

$$G(k,\omega)=\frac{1}{\det(D(\omega))}[M_{i,j}]_{4\times4}[N_{i,j}]_{4\times4}. \quad (2)$$

The matrix elements in the four-order matrix M are $M_{i,j}$ $(i,j=1,2,3,4)$. $N_{i,j}$ $(i,j=1,2,3,4)$ is the unit matrix ($N_{11}=1$, $N_{22}=-1$, $N_{33}=-1$, $N_{44}=1$). In the above equation

$$D(\omega)=[H_{i,j}]_{4\times4}+[\omega_{i,i}]_{4\times4} \quad (3)$$

with

$$\begin{aligned}
H_{11}&=-8(J_1+D_1)S_b-2(J_z+D_z)S_c,\\
H_{22}&=8(J_1+D_1)S_a+2(J_z+D_z)S_d,\\
H_{33}&=8(J_2+D_2)S_d+2(J_z+D_z)S_a,\\
H_{44}&=-8(J_2+D_2)S_c-2(J_z+D_z)S_b,\\
H_{12}&=2J_1\sqrt{S_aS_b}\gamma_k,\\
H_{13}&=2J_z\sqrt{S_aS_c},\\
H_{34}&=2J_2\sqrt{S_dS_c}\gamma_k,\\
H_{24}&=2J_z\sqrt{S_dS_b}\gamma_k,\\
\gamma_k&=2(\cos k_x+\cos k_y).
\end{aligned}$$

Equation (3) $\det(D(\omega))=0$ has four real roots ω_l ($l=1,2,3,4$, $\omega_1>0$, $\omega_2>0$, $\omega_3<0$, $\omega_4<0$) corresponding to four branches of the spin-wave spectrum which are equal to the number of sublattices. The magnetization per site (the unit is taken to be $g\mu_{\rm B}$, being a normalized unit) of each sublattice at zero temperature is

$$M_{a(d)}=S_{a(d)}+\frac{1}{\pi^2}\int\int_0^\pi\left[\frac{M_{11(44)}(\omega_3)}{\omega_a}+\frac{M_{11(44)}(\omega_4)}{\omega_b}\right]{\rm d}k_x{\rm d}k_y, \quad (4)$$

$$M_{b(c)}=-1-S_{b(c)}+\frac{1}{\pi^2}\int\int_0^\pi\left[\frac{M_{22(33)}(\omega_3)}{\omega_a}+\frac{M_{22(33)}(\omega_4)}{\omega_b}\right]{\rm d}k_x{\rm d}k_y. \quad (5)$$

Here

$$\begin{aligned}
\omega_a&=(\omega_3-\omega_1)(\omega_3-\omega_2)(\omega_3-\omega_4),\\
\omega_b&=(\omega_4-\omega_1)(\omega_4-\omega_2)(\omega_4-\omega_3).
\end{aligned}$$

3. Numerical results and discussion

In the AF-AF double-layer spin configuration, J_1 is negative, therefore in the following discussion, we shall take $|J_1|$=1 as unit and treat other parameters as relative to $|J_1|$, $S_a=S_c=0.5$. From equation $\det(D(\omega)=0)$, we obtain numerical solutions of the spin-wave spectra for the system. Figure 1 represents the k_x dependence of the energy spectra ω of the AF-AF double-layer with $J_2=-0.8$, $J_z=-0.4$, $D_z=0.0$, and $k_y=0$. Here, the solid lines and dashed lines are for the case $D_1=D_2=0.0$ and $D_1=D_2=-0.1$, respectively. The spin-wave spectra have two branches with positive and two with negative energies, one for each sublattice. The positive and negative branches of the system are symmetric, which reflects the magnetically structural symmetry of the AF-AF double-layer. As shown in Fig.1, ω_1 and ω_4 are two optical branches, while ω_2 and ω_3 are two acoustic branches since $k_x\to0$, $\omega_2\to0$, $\omega_3\to0$ for the case $D_1=D_2=0.0$. However, when the anisotropy constants are not zero ($D_1=D_2=-0.1$), ω_1, ω_2, ω_3 and ω_4 are all optical branches. The absolute values of four spin-wave spectra are bigger for the case $D_1=D_2=0.0$ than those for $D_1=D_2=-0.1$.

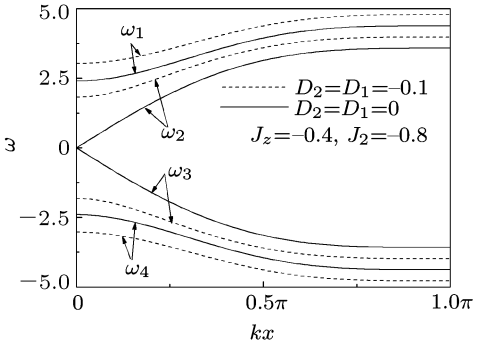


Fig.1. k_x dependence of the energy spectra ω of the system with $J_2=-0.8$, $J_z=-0.4$, $D_z=0.0$, $k_y=0$. Here, the solid lines and dashed lines are for the case $D_1=D_2=0.0$ and $D_1=D_2=-0.1$, respectively.

The dependence of interlayer exchange coupling J_z on the four-sublattice magnetizations of the AF-AF double-layer with $J_1=-1.0$, $D_z=0.0$, $D_1=D_2=-0.05$ is plotted in Fig.2. The solid lines and dashed lines are for the case $J_2=-1.2$ and $J_2=-0.8$, respectively. In the figure M_a and M_b are magnetizations of sublattices A and B in the first antiferromagnetic layer, M_c and M_d of C and D in the second antiferromagnetic layer, respectively. All of the absolute values of the sublattice magnetizations are smaller than their spin values at zero temperature. The deviation of the four-sublattice magnetizations $\Delta M(\Delta M_{i(j)}=S_{i(j)}-|M_{i(j)}|,\ i(j)=a,d(b,c))$ originated from the quantum fluctuations of spins, which

influences the magnetization of the AF-AF double-layer.

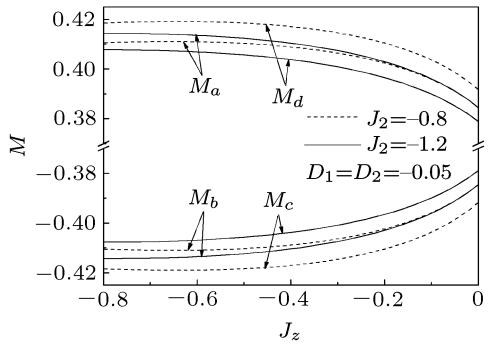


Fig.2. The dependence of J_z on the four-sublattice magnetizations of the system with $D_z = 0.0$, $D_1 = D_2 = -0.05$. Here, the solid lines and dashed lines are for the case $J_2 = -1.2$ and $J_2 = -0.8$, respectively.

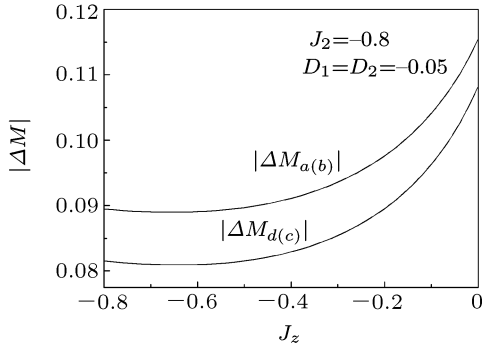


Fig.3. The dependence of J_z on the four-sublattice quantum fluctuations of the AF-AF double-layer with $D_z = 0.0$, $D_1 = D_2 = -0.05$ and $J_2 = -0.8$.

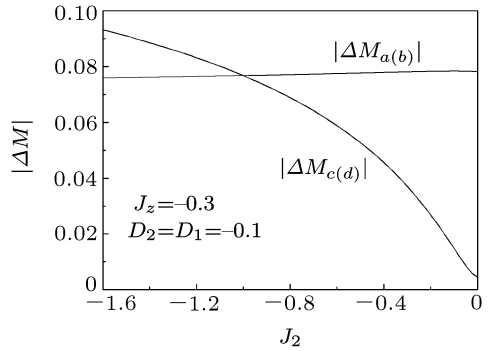


Fig.4. The dependence of J_2 on the four-sublattice quantum fluctuations of the AF-AF double-layer with $D_z = 0.0$, $D_1 = D_2 = -0.1$ and $J_z = -0.3$.

The effects of the interlayer exchange coupling J_z, the antiferromagnetic intralayer exchange coupling J_2 and the anisotropy constant D_2 on the quantum fluctuations of spins for four-sublattice magnetizations at zero temperature are given in Figs.3–5. The dependence of J_z on the four-sublattice quantum fluctuations of the AF-AF double-layer at zero temperature with $D_z = 0.0$, $D_1 = D_2 = -0.05$ and $J_2 = -0.8$ is plotted in Fig.3.

The quantum fluctuations $|\Delta M_{a(b)}|$ and $|\Delta M_{c(d)}|$ all decrease with the increase of the absolute value of J_z when the J_2 and D_2 are fixed. As shown in Fig.4, the quantum fluctuation of the A(B) sublattice $|\Delta M_{a(b)}|$ is always stronger than that of the C(D) sublattice $|\Delta M_{c(d)}|$ if $|J_1| > |J_2|$ and, correspondingly, the magnetization at 0 K of the former is always weaker than that of the latter. However, $|\Delta M_{a(b)}|$ is bigger than $|\Delta M_{c(d)}|$ if $|J_2| > |J_1|$. In order to investigate carefully the effects of the J_2 and D_2 on the quantum fluctuation of the system, we calculate the $|\Delta M_{a(b)}|$ and $|\Delta M_{c(d)}|$ as functions of the J_2 and D_2 for a fixed J_z=–0.4. The resulting quantum fluctuations in the three-dimensional parameter space ($|\Delta M_{a(b)}|(|\Delta M_{c(d)}|)$, D_2, J_2) for the AF-AF double-layer are plotted in Figs.5(a) and 5(b). From these figures, we can know that the antiferromagnetic exchange coupling J_2 and anisotropy constant D_2 play important roles in a balance of the quantum competition in the AF-AF double-layer.

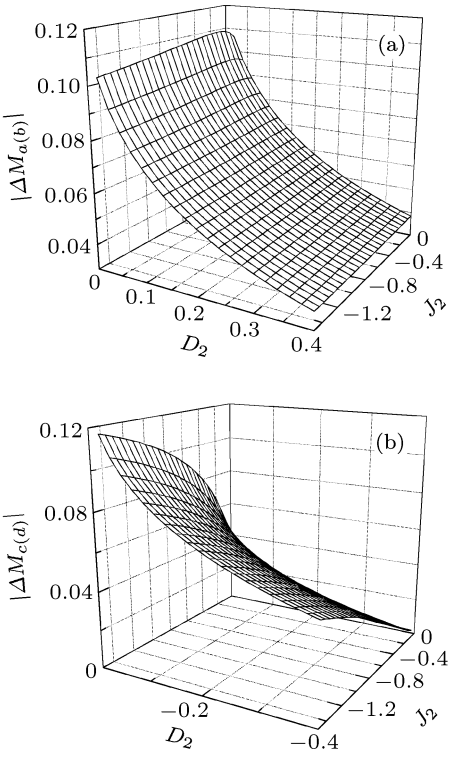


Fig.5. Quantum fluctuations of the AF-AF double-layer with $D_z = 0.0$, $D_1 = D_2$ and $J_z = -0.4$ in the three-dimensional space (a) $|\Delta M_{a(b)}|$, D_2, J_2; (b) $|\Delta M_{c(d)}|$, D_2, J_2.

4. Conclusion

In conclusion, we have studied the magnetic properties of the AF-AF double-layer at zero temperature within the spin-wave theory. The anisotropic four-sublattice AF-AF Heisenberg model is used to describe the magnetic properties of high-temperature superconductivity in layered iron-based compounds. Numerical results have shown that the system has two optical branches and two acoustic branches without anisotropy, and four optical branches with anisotropy. The values of the quantum fluctuations for the A and B sublattices are the same, and for C and D sublattices are also the same. The quantum fluctuation $|\Delta M_{a(b)}|$ is always stronger than that of $|\Delta M_{c(d)}|$ if $|J_1| > |J_2|$ and, correspondingly, the magnetization at 0 K of the former is always weaker than that of the latter. The $|\Delta M_{a(b)}|$ is bigger than $|\Delta M_{c(d)}|$ if $|J_2| > |J_1|$. The antiferromagnetic exchange coupling J_2 and anisotropy constant D_2 play important roles in a balance of the quantum competition in the AF-AF double-layer. The results in this work may be helpful to better understand the magnetic properties of the new class of high-temperature superconductivity in layered iron-based compounds.

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