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Heisenberg antiferromagnetic properties on the triangular lattice with interlayer coupling

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Abstract. The Heisenberg antiferromagnet on the triangular lattice with interlayer coupling is treated via a double-time Green function. The hierarchy of the equations of motion of the Green functions is decoupled by employing the Kondo–Yamaji methods. The excitation spectrum, the correlation function, the internal energy, the specific heat and the susceptibility are discussed. The results have good agreement with those of the exact diagonalization and the nearest-neighbour virtual bonding state and can be compared with some experiments.

1. Introduction

Recent years have seen a flurry of interest in the properties of frustrated quantum Heisenberg antiferromagnetic models (HAFMs), which have the possibility of non-Néel long-range order. The triangular HAFMs are viable candidates to describe short-range order samples. Indeed, quite some time ago Anderson proposed that the ground state of the triangular HAFM is a resonating-valence-bond (RVB) state, which is a disordered spin liquid [1]. It is well known that the family of high-T_c superconductors have layered structure with a very strong coupling between spins in the plane and very weak coupling between planes. The inter-plane coupling may play an important role in a disordered system.

In this paper, we start from the Heisenberg antiferromagnetic model (HAFM) on a triangular lattice, which has strong intra-plane and weak inter-plane coupling and has no Néel long-range order. We employ the double-time Green function following the Kondo–Yamaji [2] methods to obtain a set of self-consistent equations, from which the spin excitation spectra, the correlation functions, the ground energy, the specific heat and the magnetic susceptibility can be obtained. The plot of specific heat versus temperature agrees very well with the results obtained from the nearest-neighbour virtual bonding state (NNVB) [3]. The ground energy agrees with the RVB and the exact diagonalization results [4], and the susceptibility can be compared with an experiment on Pr_2CuO_4 [5].

2. The self-consistent equations

The spin Hamiltonian appropriate for a strong-intra-plane- and weak-inter-plane-coupling HAFM is

$$H = J_{ab} \sum_{\langle i,j \rangle} \boldsymbol{s}_i \cdot \boldsymbol{s}_j + J_c \sum_{\langle l,j \rangle} \boldsymbol{s}_l \cdot \boldsymbol{s}_j$$

where the first sum is over nearest neighbours in the planes and J_{ab} is the intra-plane coupling parameter; the second sum is over the nearest neighbours out the planes and J_c

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is the inter-plane coupling parameter. We define the ratio $\rho = J_c/J_{ab}$, which determines the strength of intra- and inter-plane interactions. We set $J_{ab} = 1$ (hereafter the Boltzmann constant $K_B = 1$), then

$$H = \sum_{\langle i,j\rangle} \boldsymbol{s}_i \cdot \boldsymbol{s}_j + \rho \sum_{\langle l,j\rangle} \boldsymbol{s}_l \cdot \boldsymbol{s}_j. \tag{1}$$

When $\rho = 0$, the system becomes as a two-dimensional triangular HAFM; and when $\rho \neq 0$, the system is supposed to be a hexagonal space lattice HAFM with the nearest-neighbour distance in planes equal to the inter-layer interval.

The quantum spin operators obey the Pauli spin algebra, and the spin Green function can be defined by

$$G(i-j, t-t') = -\mathrm{i}\theta(t-t')\langle[s_i^z, s_j^z]\rangle = \langle\langle s_i^z(t); s_j^z(t')\rangle\rangle \tag{2}$$

where $\theta(t)$ denotes a step function, and $\langle\cdots\rangle$ denotes the thermal average. The time-Fourier transform of the double-time Green function satisfies the equation

$$\omega\langle\langle s_0^z; s_n^z\rangle\rangle = \langle\langle[s_0^z, H]; s_n^z\rangle\rangle. \tag{3}$$

Because the average $\langle s^z\rangle$ vanishes for the short-range order systems, employing the theory of Kondo and Yamaji, which is a Green function decoupling scheme in the absence of any finite magnetization and can be used to describe a spin-wave-like excitation in short-range order, we introduce the correlation or short-range order C_n, which is defined by

$$C_n = \langle \boldsymbol{s}_0 \cdot \boldsymbol{s}_n\rangle = \tfrac{3}{2}\langle s_0^+ s_n^-\rangle = 3\langle s_0^z s_n^z\rangle. \tag{4}$$

The decoupling approximations are

$$\langle\langle s_\rho^\sigma s_\rho^{-\sigma} s_0^z - s_0^\sigma s_0^{-\sigma} s_\rho^z; s_n^z\rangle\rangle = \langle s_\rho^\sigma s_\rho^{-\sigma}\rangle\langle\langle s_0^z; s_n^z\rangle\rangle - \langle s_0^\sigma s_0^{-\sigma}\rangle\langle\langle s_\rho^z; s_n^z\rangle\rangle \tag{5}$$

$$\begin{aligned}\langle\langle s_{\rho'}^\sigma s_\rho^{-\sigma} s_0^z - s_0^\sigma s_\rho^{-\sigma} s_{\rho'}^z; s_n^z\rangle\rangle &= \langle s_{\rho'}^\sigma s_\rho^{-\sigma} + 2(\alpha-1)s_{\rho'}^z s_\rho^z\rangle\langle\langle s_0^z; s_n^z\rangle\rangle \\ &\quad -\langle s_0^\sigma s_\rho^{-\sigma} + 2(\alpha-1)s_0^z s_\rho^z\rangle\langle\langle s_{\rho'}^z; s_n^z\rangle\rangle\end{aligned} \tag{6}$$

where $\sigma = \pm 1$. The correlation function can be expressed by

$$\langle s_n^z s_0^z\rangle = \mathrm{i}\int_{-\infty}^{+\infty} \frac{\mathrm{d}\omega}{\mathrm{e}^{\beta\omega}-1}\{\langle\langle s_0^z; s_n^z\rangle\rangle_{\omega+\mathrm{i}0^+} - \langle\langle s_0^z; s_n^z\rangle\rangle_{\omega-\mathrm{i}0^+}\}. \tag{7}$$

The space-Fourier transform of $\langle\langle s_0^z; s_n^z\rangle\rangle$ reads

$$G(\boldsymbol{k}, \omega) \equiv \sum_n \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{n}}\langle\langle s_0^z; s_n^z\rangle\rangle. \tag{8}$$

From equation (1), and from (3)–(8) we have the Green function

$$G(\boldsymbol{k}, \omega) = -\frac{C_1}{3\pi}\frac{z_s(1-\gamma_{sk}) + \rho z_c(1-\gamma_{ck})}{\omega^2 - \omega_k^2} \tag{9}$$

the spin wave excitation spectrum

$$\begin{aligned}\omega_k^2 &= \tfrac{2}{3}z_s(1-\gamma_{sk})(\tfrac{3}{4} - \alpha C_1 + \alpha C_2 + \rho\alpha C_3) + \tfrac{2}{3}\rho z_c(1-\gamma_{ck})[\rho(\tfrac{3}{4} - \alpha C_1 + \alpha C_4) + 3\alpha C_3] \\ &\quad -\tfrac{2}{3}\alpha C_1(z_s\gamma_{sk} + \rho z_c\gamma_{ck})[z_s(1-\gamma_{sk}) + \rho z_c(1-\gamma_{ck})]\end{aligned} \tag{10}$$

and the correlation function

$$C_n = \frac{C_1}{N}\sum_k \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{n}}\frac{A(\boldsymbol{k})}{\omega_k}\coth\frac{\omega_k}{2k_BT} \tag{11}$$

where the α [2] is the decoupling parameter, which can be regarded as the vertex correction,

$$C_1 = \langle \boldsymbol{s}_0 \cdot \boldsymbol{s}_\rho\rangle = \frac{3}{2}\langle s_0^+ s_\rho^-\rangle = 3\langle s_0^z s_\rho^z\rangle \qquad C_2 = \sum_{\rho\neq-\rho'} C_{\rho+\rho'} \qquad C_3 = \sum_\delta C_{\rho+\delta}$$

$$C_4 = \sum_{\delta \neq -\delta'} C_{\delta+\delta'} \qquad \gamma_{sk} = \frac{1}{z_s}\sum_{\rho} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\rho} \qquad \gamma_{ck} = \frac{1}{z_c}\sum_{\delta} \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\delta}$$
$$A(\boldsymbol{k}) = -[z_s(1-\gamma_{sk}) + \rho z_c(1-\gamma_{ck})]$$

and ρ and δ are the nearest-neighbour vectors in and out of plane respectively; z_s and z_c are the numbers of nearest-neighbour sites in and out of plane respectively. From equation (11) we can obtain the self-consistent equation group as

$$\frac{3}{4} = \frac{C_1}{N}\sum_k \frac{A(\boldsymbol{k})}{\omega_k}\coth\frac{\omega_k}{2k_BT} \tag{12}$$

$$1 = \frac{1}{N}\sum_k \frac{\gamma_{sk}A(\boldsymbol{k})}{\omega_k}\coth\frac{\omega_k}{2k_BT} \tag{13}$$

$$C_2 = \frac{C_1}{N}\sum_k (z_s\gamma_{sk}^2 - 1)\frac{A(\boldsymbol{k})}{\omega_k}\coth\frac{\omega_k}{2k_BT} \tag{14}$$

$$C_3 = \frac{C_1 z_c}{N}\sum_k \frac{\gamma_{sk}\gamma_{ck}A(\boldsymbol{k})}{\omega_k}\coth\frac{\omega_k}{2k_BT} \tag{15}$$

$$C_4 = \frac{C_1}{N}\sum_k (z_c\gamma_{ck}^2 - 1)\frac{A(\boldsymbol{k})}{\omega_k}\coth\frac{\omega_k}{2k_BT}. \tag{16}$$

The internal energy and the static magnetic susceptibility of the system can be expressed by

$$E = \langle H\rangle = N(z_s + \rho z_c)C_1 \tag{17}$$

$$\chi = \frac{g^2\mu_B^2}{3T}\sum_n C_n = -\frac{2g^2\mu_B^2(z_s+\rho z_c)}{3B} \tag{18}$$

where

$$B = \tfrac{2}{3}\{z_s(\tfrac{3}{4} - \alpha C_1 + \alpha C_2 + \rho\alpha C_3) + \rho z_c[\rho(\tfrac{3}{4} - \alpha C_1 + \alpha C_4) + 3\alpha C_3] \\ -\alpha C_1(z_s\gamma_{sk} + \rho z_c\gamma_{ck})(z_s + \rho z_c)\}/C_1 \tag{19}$$

μ_B is the Bohr magneton, g is the Lande factor and n is any lattice vector.

From the resolutions of the equation group we can plot the correlation, the internal energy, the specific heat and the susceptibility versus T (see figure 1). Figure 1(b) shows that when the ratio $\rho = 10^{-15}$ and 10^{-5}, which means that the system nears a two-dimensional sheet , the ground energy per site is about $E/N = -0.95$. This value is slightly higher than that calculated from the exact diagonalization , -1.1 [4], near to the RVB result, -0.98 [1], lower than that estimated from the variational spin-wave theory, -0.926 [1], and close to that of the $m = 2$ fractional quantum Hall state, -0.94 [6]. When ρ increases from 0.5 to 1.0 the ground energy varies from -1.07 to -1.40. Figure 1(c) shows that the curves of specific heat have peaks around $T = 0.75$. In particular, for small ratio ($\rho = 10^{-15}, 10^{-5}$) the curve quantitatively agrees with the results of NNVB [3]. Finally, figure 1(d) gives some favourable results:the susceptibility peaks occur around $T = 0.75$ for medium ρ; but as the sample approaches the two-dimensional sheet, i.e. the interlayer coupling becomes very weak, the peaks are flattened and finally disappear. This conclusion agrees with some experiments on non-triangular but doped samples, for example, Pr_2CuO_4 [5].

3. Conclusion

It is well known that a susceptibility peak occurs in undoped samples but the peaks are flattened and finally absent with increased doping in the samples. In contrast, when the

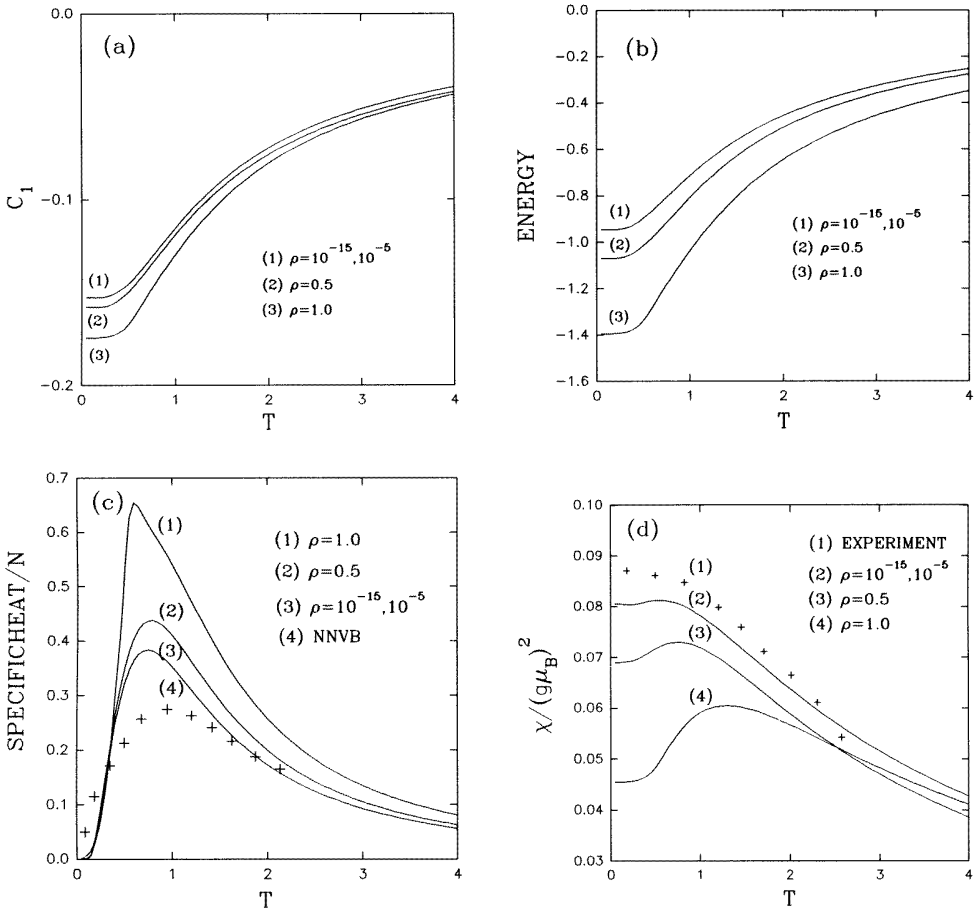

Figure 1. (a) The correlation function C_1 of the 3D triangular HAFM with inter-plane coupling against the temperature T when (1) $\rho = 10^{-15}$ or 10^{-5}, (2) $\rho = 0.5$ and (3) $\rho = 1.0$. (b) The energy of the 3D triangular HAFM with inter-plane coupling against the temperature T when (1) $\rho = 10^{-15}$ or 10^{-5}, (2) $\rho = 0.5$ and (3) $\rho = 1.0$. (c) (1–3) The specific heat of the 3D triangular HAFM with inter-plane coupling against the temperature T when (1) $\rho = 1.0$, (2) $\rho = 0.5$, (3) $\rho = 10^{-15}$ or 10^{-5} and (4) the NNVB results. (d) Plot (1) is the magnetic susceptibility χ from experiment for Pr_2CuO_4 against T. Plots (2)–(4) are the magnetic susceptibility χ of the 3D triangular HAFM with inter-plane coupling when $\rho = 10^{-15}$ or 10^{-4}, $\rho = 0.5$ and $\rho = 1.0$ respectively.

inter-plane interactions are taken into account the susceptibility peak of the undoped sample disappears with the decrease of the inter-plane coupling strength. The conflict between these two cases means that even a very small out-of-plane coupling is enough to destroy the two-dimensional energy balance between the competing structures, thus generating some observed transitions. In conclusion, the disappearance of the susceptibility peak is not a general feature of an isotropic Heisenberg antiferromagnet and rather must be attributed to anisotropies and in- and out-of-plane interaction, for example, the Dzyaloshinski–Moriya interaction [7]. Indeed both doping and inter-plane coupling are causes of increased frustration to the considered samples. Inter-plane coupling plays a doping-like role.

Finally, we should stress that this paper ignores the difference between in-and out-

of-plane correlations. The in-plane correlation can be described by $\langle s_i^x s_j^x \rangle$ or $\langle s_i^y s_j^y \rangle$ and the out-of-plane correlation by $\langle s_i^z s_j^z \rangle$. If $\langle s_i^x s_j^x \rangle = \langle s_i^y s_j^y \rangle = \langle s_i^z s_j^z \rangle$ there is only one spin excitation spectrum. Generally, $\langle s_i^x s_j^x \rangle = \langle s_i^y s_j^y \rangle \neq \langle s_i^z s_j^z \rangle$ and the consideration of this difference will cause the 2D-like spin waves to be split into acoustic and optical branches and will accordingly cause changes of other properties.

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