Volume 7, Number 5
1004-423X/98/07050348-06

ACTA PHYSICA SINICA
(Overseas Edition)

May, 1998
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THEORETICAL STUDY OF THE GROUND-STATE PROPERTY OF THE TWO-DIMENSIONAL HEISENBERG ANTIFERROMAGNET ON A TRIANGULAR LATTICE*

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(Received 4 April 1997)

Within the Tyablikov's theoretical framework, the ground-state property of the two-dimensional antiferromagnetic Heisenberg model on a triangular lattice is studied. Our results show that the sublattice magnetization is $M = 0.241$ and the ground-state energy per bond is $E_g/NZJ = -0.166$, which are in agreement with the numerical simulations.

PACC: 7510J; 7530G; 7550M

Since the discovery of copper oxide superconductors, there has been increasing interest in studying magnetic properties of the two-dimensional (2D) quantum antiferromagnetic (AF) systems.[1] This followed from the experiments that the copper oxide sheets in the high-T_c superconductors show strong AF spin correlations. The undoped copper oxide materials are layered AF Mott insulators.[2] When the hole doping concentration exceeds some critical value, the AF long-range-order (AFLRO) disappears and the materials are converted into nonmagnetic metals. Attempting to understand the strong AF correlations and spin fluctuations, Anderson[3] suggested that the ground-state of the copper oxide materials at the half-filling should be the spin resonating-valence-bond state without AFLRO, i. e., the disordered spin liquid state. The resonating-valence-bond state was proposed first by Anderson and Fazekas[4] for studying the 2D Heisenberg antiferromagnet on a triangular lattice. However, much research[5] has shown that there is AFLRO in Heisenberg antiferromagnet on a square lattice, and the sublattice magmetization is equal to about 60% of the classical value due to the spin fluctuations. For the 2D Heisenberg antiferromagnet on a triangular lattice, which is a system with geometric frustration, the nature of the ground-state is still controversial, although the numerical and theoretical analyses[6] have shown that the frustration effect can reduce AFLRO. Using the large-N expanding technique, it is found that there is no AFLRO in the ground-state of the 2D Heisenberg antiferromagnet on a triangular lattice.[7] However, the results obtained from the Monte-Carlo simulation and exact diagonalization show that there is AFLRO in the ground-state, and the sublattice magnetization is equal to about 50% of the classical value.[8]

* Project supported by the National Natural Science Foundation of China and by the Trans-Century Training Programme Foundation for the Talents by the State Education Commission of China.

A popular method to study the quantum spin problem is the spin-wave theory[9,10], where the quantum spin is mapped onto the boson representation in terms of the Holstein-Primakoff transformation. However, this naive spin-wave theory, an expansion and the linear approximation in Holstein-Primakoff bosons, leads to violation of the commutation rule of the quantum spin (the quantum spins obey the Pauli algebra, i. e., the spin one-half raising and lowering operators S_i^+ and S_i^- behave as fermions on the same site and as bosons on different sites). In this paper, we study the ground-state property of the 2D AF Heisenberg model on a triangular lattice within the Tyablikov's decoupling scheme[11], where the commutation rule of the quantum spin is exactly satisfied. Our results show that the sublattice magnetization is $M=0.241$ and the ground-state energy per bond is $E_g/NZJ=-0.166$, which are consistent with the numerical simulations.[8,12-15]

The standard quantum AF Heisenberg model is described by the Hamiltonian,

$$H = J\sum_{i\eta} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+\eta} = J\sum_{i\eta}\left[\frac{1}{2}(S_i^+S_{i+\eta}^- + S_i^-S_{i+\eta}^+) + S_i^zS_{i+\eta}^z\right], \tag{1}$$

with $J>0$, and $\hat{\eta}=\hat{x},\hat{y}$, $\boldsymbol{S}_i=(S_i^x,S_i^y,S_i^z)$ is the spin operator, S_i^+ and S_i^- are the raising and lowering operators of S_i^x, respectively. In the triangular lattice system, there are three sublattices, A, B and C. The spins for each sublattice have an angle difference of $2\pi/3$ to the others, and the nearest-neighbor pairs of spins are on different sublattices. Thus the triangular lattice is more complicated than the square lattice. For convenience, we choose a particular classical ground-state with the spin oriented along the z axis on the A sublattice. The B and C sublattices are rotated by angles $2\pi/3$ and $-2\pi/3$, respectively, to the A sublattice. Then the question will be discussed under the coordinate of the sublattice A.[10]

By a rotation of angle $2\pi/3$, the spin operators of the sublattice B can be written as

$$(S_j^{B+})_{\text{before rotation}} \to \left(\frac{1}{4}S_j^{B-} - \frac{3}{4}S_j^{B-} + \frac{\sqrt{3}}{2}S_j^{Bz}\right)_{\text{after rotation}}, \tag{2a}$$

$$(S_j^{B-})_{\text{before rotation}} \to \left(-\frac{3}{4}S_j^{B+} + \frac{1}{4}S_j^{B-} + \frac{\sqrt{3}}{2}S_j^{Bz}\right)_{\text{after rotation}}, \tag{2b}$$

$$(S_j^{Bz})_{\text{before rotation}} \to \left(-\frac{\sqrt{3}}{4}S_j^{B+} - \frac{\sqrt{3}}{4}S_j^{B-} - \frac{1}{2}S_j^{Bz}\right)_{\text{after rotation}}. \tag{2c}$$

On the C sublattice, having a rotation of angle $-2\pi/3$, the Heisenberg model (1) can be expressed as

$$\begin{aligned} H = {} & J\sum_{\eta_1,i\in A}\Big\{-\frac{3}{4}(S_i^{A+}S_{i+\eta_1}^{B-} + S_i^{A-}S_{i-\eta_1}^{B-}) + \Big[\frac{1}{4}(S_i^{A+}S_{i+\eta_1}^{B-} + S_i^{A-}S_{i+\eta_1}^{B+}) - S_i^{Az}S_{i+\eta_1}^{Bz}\Big] \\ & + \frac{\sqrt{3}}{4}\Big[(S_i^{A+} + S_i^{A-})S_{i+\eta_1}^{Bz} - S_i^{Az}(S_{i+\eta_1}^{B+} + S_{i+\eta_1}^{B-})\Big]\Big\} \\ & + J\sum_{\eta_2,j\in B}\Big\{-\frac{3}{4}(S_j^{B+}S_{j+\eta_2}^{C+} + S_j^{B-}S_{j+\eta_2}^{C+}) + \Big[\frac{1}{4}(S_j^{B-}S_{j+\eta_2}^{C-} + S_j^{B-}S_{j+\eta_2}^{C+}) - S_j^{Bz}S_{j+\eta_2}^{Cz}\Big] \end{aligned}$$

$$+\frac{\sqrt{3}}{4}\left[(S_j^{B+}+S_j^{C-})S_{j+\eta_2}^{Cz}-S_j^{Bz}(S_{j+\eta_2}^{C+}+S_{j+\eta_2}^{C-})\right]\Big\}$$

$$+J\sum_{\eta_3,\,l\in C}\Big\{-\frac{3}{4}(S_l^{C+}S_{l+\eta_3}^{A+}+S_l^{C-}S_{l+\eta_3}^{A-})+\left[\frac{1}{4}(S_l^{C+}S_{l+\eta_3}^{A-}+S_l^{C-}S_{l+\eta_3}^{A+})-S_l^{Cz}S_{l+\eta_3}^{Az}\right]$$

$$+\frac{\sqrt{3}}{4}\left[(S_l^{C+}+S_l^{C-})S_{l+\eta_3}^{Az}-S_l^{Cz}(S_{l+\eta_3}^{A-}+S_{l+\eta_3}^{A-})\right]\Big\}. \tag{3}$$

Since the quantum spin obeys the Pauli spin algebra, this problem can be discussed in terms of the two-time spin Green's function within the Tyablikov's scheme. Six spin Green's functions are difined as follows:

$$G^{AA}(R_i-R_n,t-t')=-i\theta(t-t')<[S_i^{A+}(t),S_n^{A-}(t')]>$$
$$\equiv<<S_i^{A+}(t);S_n^{A-}(t')>>, \tag{4a}$$

$$G^{BA}(R_j-R_n,t-t')=<<S_j^{B+}(t);S_n^{A-}(t')>>, \tag{4b}$$

$$G^{CA}(R_l-R_n,t-t')=<<S_l^{C+}(t);S_n^{A-}(t')>>, \tag{4c}$$

$$g^{AA}(R_i-R_n,t-t')=<<S_i^{A-}(t);S_n^{A-}(t')>>, \tag{4d}$$

$$g^{BA}(R_j-R_n,t-t')=<<S_j^{B-}(t);S_n^{A-}(t')>>, \tag{4e}$$

$$g^{CA}(R_l-R_n,t-t')=<<S_l^{C-}(t);S_n^{A-}(t')>>, \tag{4f}$$

where $\theta(t)$ is a step function and is defined as $\theta(t)=1$ for $t>0$ and $\theta(t)=0$ for $t<0$. The time-Fourier transform of the two-time Green's function satisfies the equation[11]

$$\omega<<A;B>>=\frac{1}{2\pi}<[A,B]>+<<[A,H];B>>_{\omega}. \tag{5}$$

The Green's function can be obtained by applying the Tyablikov's decoupling technique, and the correlation functions can be obtained by the spectral representation[11]

$$<B(t')A(t)>=i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{<<A;B>>_{\omega+i0^+}-<<A;B>>_{\omega-i0^+}}{e^{\beta\omega}-1}e^{-i\omega(t-t')}. \tag{6}$$

According to the Pauli spin algebra and Eq. (5), the equations of motion of the spin Green's function (4) can be obtained as

$$i\frac{d}{dt}G^{AA}(R_i-R_n,t-t')=2<S_i^{Az}>\delta_{in}\delta_{tt'}+<<[S_i^{A+}(t),H(t)];S_n^{A-}(t')>>. \tag{7}$$

Since there are three operators appearing in the second term on the right hand side of Eq. (7), it can be decoupled by Tyablikov's decoupling technique,

$$<<S_i^{Az}(t)S_{i+\eta_1}^{B-};S_n^{A-}(t')>>\rightarrow<S_i^{Az}>g^{BA}(i+\eta_1-n,t-t'), \tag{8a}$$

$$<<S_{i+\eta_3}^{Cz}(t)S_i^{A+};S_n^{A-}(t')>>\rightarrow<S_{i+\eta_3}^{Cz}>G^{AA}(i+\eta_3-n,t-t'). \tag{8b}$$

We define the sublattice magnetization $M=<S_i^{Az}>=<S_j^{Bz}>=<S_l^{Cz}>$ since the B and C sublattices have been rotated by angles $2\pi/3$ and $-2\pi/3$, respectively. With the help of Eq. (8), the Green's function (4) can be evaluated. Although the analysis is quite tedious, the calculation is straightforward, and the energy spectra are

obtained as

$$E_1(k) = \pm \left[144 + 2(\gamma_k + \gamma_k^*) - 8(\gamma_k^2 + \gamma_k^{*2}) - 16\gamma_k\gamma_k^*\right]^{1/2}, \tag{9a}$$

$$E_2(k) = \pm \left[\frac{1}{2}\left(p_k + \sqrt{p_k^2 - 4q_k}\right)\right]^{1/2}, \tag{9b}$$

$$E_3(k) = \pm \left[\frac{1}{2}\left(p_k - \sqrt{p_k^2 - 4q_k}\right)\right]^{1/2}, \tag{9c}$$

with

$$\begin{aligned}
p_k &= 288 + 8(\gamma_k^2 + \gamma_k^{*2}) - 2(\gamma_k + \gamma_k^*) - 32\gamma_k\gamma_k^*, \\
q_k &= 64(\gamma_k^4 + \gamma_k^{*4}) - 128(\gamma_k^*\gamma_k^3 + \gamma_k^{*3}\gamma_k) \\
&\quad + 16E_0(\gamma_k^3 + \gamma_k^{*3}) + 12E_0(\gamma_k^2 + \gamma_k^{*2}) \\
&\quad - 2E_0^3(\gamma_k + \gamma_k^*) + 192\gamma_k^{*2}\gamma_k^2 - 36E_0^2\gamma_k\gamma_k^* + E_0^4, \\
\gamma_k &= \sum_{\eta} e^{ik\cdot\eta},
\end{aligned}$$

and the Green's functions

$$G^{AA}(k, \omega) = -4\sum_{i=1}^{3}\left(\frac{E_i(k)U_i(k) + A_i(k)}{E_i(k)[\omega' - E_i(k)]} + \frac{E_i(k)U_i(k) - A_i(k)}{E_i(k)[\omega' + E_i(k)]}\right), \tag{10a}$$

$$G^{BA}(k, \omega) = -4\sum_{i=1}^{3}\left(\frac{E_i(k)U_i'(k) + A_i'(k)}{E_i(k)[\omega' - E_i(k)]} + \frac{E_i(k)U_i'(k) - A_i'(k)}{E_i(k)[\omega' + E_i(k)]}\right), \tag{10b}$$

$$G^{CA}(k, \omega) = (G^{BA}(k, \omega))^+, \tag{10c}$$

where $\omega' = 4\omega/M$, $A_i(k) = \Delta_i(k)/\Delta(k)$, $U_i(k) = \Delta_i'(k)/\Delta(k)$, $A_i'(k) = \Phi_i(k)/\Delta(k)$, $U_i'(k) = \Phi_i'(k)/\Delta(k)$, and

$$\begin{aligned}
\Delta(k) &= [E_1^2(k) - E_2^2(k)]E_3^2(k)E_2^2(k) + [E_3^2(k) - E_1^2(k)]E_3^2(k)E_1^2(k) \\
&\quad + [E_2^2(k) - E_3^2(k)]E_2^2(k)E_3^2(k), \\
\Delta_1(k) &= [E_2^2(k) - E_3^2(k)][-12E_1^4(k) + \sigma_2(k)E_1^2(k) + \sigma_1(k)], \\
\Delta_2(k) &= [E_3^2(k) - E_1^2(k)][-12E_2^4(k) + \sigma_2(k)E_2^2(k) + \sigma_1(k)], \\
\Delta_3(k) &= [E_1^2(k) - E_2^2(k)][-12E_3^4(k) + \sigma_2(k)E_3^2(k) + \sigma_1(k)], \\
\Delta_1'(k) &= [E_2^2(k) - E_3^2(k)][-E_1^4(k) + \sigma_2'(k)E_1^2(k) + \sigma_1'(k)], \\
\Delta_2'(k) &= [E_3^2(k) - E_1^2(k)][-E_2^4(k) + \sigma_2'(k)E_2^2(k) + \sigma_1'(k)], \\
\Delta_3'(k) &= [E_1^2(k) - E_2^2(k)][-E_3^4(k) + \sigma_2'(k)E_3^2(k) + \sigma_1'(k)], \\
\Phi_1(k) &= [-\gamma_k^*E_1^4 + (6E_0\gamma_k^2 - 24\gamma_k\gamma_k^{*2})E_1^2(k) + \sigma_3](E_2^2(k) - E_3^2(k)), \\
\Phi_2(k) &= [-\gamma_k^*E_2^4 + (6E_0\gamma_k^2 - 24\gamma_k\gamma_k^{*2})E_2^2(k) + \sigma_3](E_3^2(k) - E_1^2(k)), \\
\Phi_3(k) &= [-\gamma_k^*E_3^4 + (6E_0\gamma_k^2 - 24\gamma_k\gamma_k^{*2})E_3^2(k) + \sigma_3](E_1^2(k) - E_2^2(k)), \\
\Phi_1'(k) &= [(8\gamma_k^2 - 2E_0\gamma_k^*)E_1^2(k) + \sigma_3'](E_2^2(k) - E_3^2(k)), \\
\Phi_2'(k) &= [(8\gamma_k^2 - 2E_0\gamma_k^*)E_2^2(k) + \sigma_3'](E_3^2(k) - E_1^2(k)), \\
\Phi_3'(k) &= [(8\gamma_k^2 - 2E_0\gamma_k^*)E_3^2(k) + \sigma_3'](E_1^2(k) - E_2^2(k)), \\
\sigma_1(k) &= 64(\gamma_k^*\gamma_k^4 + \gamma_k^{*4}\gamma_k) - 28E_0^2(\gamma_k^3 + \gamma_k^{*3})
\end{aligned}$$

$$
\begin{aligned}
&- 192E_0\gamma_k^{*2}\gamma_k^2 + 40E_0^3\gamma_k\gamma_k^* - E_0^5,\\
\sigma_2(k) &= 8(\gamma_k^3 + \gamma_k^{*3}) - 36E_0\gamma_k^*\gamma_k + 2E_0^3,\\
\sigma_3(k) &= -64\gamma_k^5 + 112E_0\gamma_k^*\gamma_k^3 - 10E_0^3\gamma_k^2 - 64\gamma_k^{*2}\gamma_k^2\\
&\quad + 24E_0^2\gamma_k^{*2}\gamma_k + E_0^4\gamma_k^* - 80E_0\gamma_k^{*4},\\
\sigma_1'(k) &= -16E_0(\gamma_k^3 + \gamma_k^{*3}) - 192\gamma_k^{*2}\gamma_k^2 + 36E_0^2\gamma_k\gamma_k^* - E_0^4,\\
\sigma_2'(k) &= -32\gamma_k\gamma_k^* + 2E_0^2,\\
\sigma_3'(k) &= 128\gamma_k^*\gamma_k^3 - 12E_0^2\gamma_k^2 + 2E_0^3\gamma_k^* - 60\gamma_k^{*4}.
\end{aligned}
$$

With the above Green's functions and spectral representation (6), we can obtain the sublattice magnetization

$$
\begin{aligned}
M &= \frac{1}{2} - < S_i^{A-} S_i^{A+} >\\
&= \frac{1}{2} - \frac{\mathrm{i}}{N}\sum_{k(\mathrm{red})}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\frac{[G^{AA}(\boldsymbol{k},\omega + \mathrm{i}0^-) - G^{AA}(\boldsymbol{k},\omega - \mathrm{i}0^+)]}{\mathrm{e}^{\beta\omega} - 1},
\end{aligned}
\tag{11}
$$

and the correlation function

$$
< S_i^{A-} S_{i+\eta}^{B+} > = \frac{\mathrm{i}}{N}\sum_{k(\mathrm{red})}\gamma_k\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\frac{[G^{BA}(\boldsymbol{k},\omega + \mathrm{i}0^+) - G^{BA}(\boldsymbol{k},\omega - \mathrm{i}0^+)]}{\mathrm{e}^{\beta\omega} - 1}, \tag{12}
$$

where $\beta = 1/k_B T$, (red) means that the summation is carried only over the reduced Brillouin zone, k_B is the Boltzmann constant, T is the temperature.

We are now ready to discuss the ground-state properties of the system. At zero temperature, we have performed the numerical calculation for the sublattice magnetization

Table 1. A comparison of the ground-state energy per bond for the antiferromagnetic Heisenberg model on a 2D triangular lattice.

Authors	Ground-state energy per bond	Method
Kalmeyer and Laughlin[12]	-0.157	variational Monte Carlo
Huse and Elser[8]	-0.170	variational Monte Carlo
Nishimori and Nakanishi[13]	-0.183	finite lattice
Lee and Feng[14]	-0.161	variational Monte Carlo
The present work	-0.166	Green's function method

(11) and correlation function (nearest-neighbor spin bond-order amplitude) (12), and the sublattice magnetization and correlation function are evaluated to be $M = 0.241$ and $< S_i^{A-} S_{i+\eta}^{B+} > = -0.105$. Then according to Eq. (1), we obtain the ground-state energy per bond $E_g/NZJ = -0.166$ (Z is the number of nearest-neighbor sites). For comparison with other results obtained by the numerical simulations, our present theoretical result is also shown in Table 1. Our result of the sublattice magnetization is equal to about 48% of the classical value, and the ground-state energy is in very good agreement with

variational Monte Carlo results obtained by Huse and Elser[8] and Lee and Feng[14], but higher than the exact diagonalization result obtained by Nishimori and Nakanishi.[13] This is due to the finite lattice effects in the exact diagonalization calculation. Moreover, Huse and Elser[8] have estimated that the ground-state energy per bond of the AF Heisenberg model is $E_g/NZJ \leqslant -0.179$, then our result is only 7% higher than this estimates. The present theoretical study seems to confirm that there is AFLRO in the ground-state of the AF Heisenberg model on a triangular lattice.[8,13,15]

Finally we also note the result obtained by Bernu *et al*.[16] Based on the finite lattice analysis, they obtained a ground-state energy per bond E_g/NZJ of -0.187, which is consistent with that obtained by Nishimori and Nakanshi.[13] Recently using the coupled-cluster method, Zeng *et al*.[17] have a result consistent with the present study.

In summary, we have studied the ground-state property of the 2D AF Heisenberg model on a triangular lattice within the Tyablikov's decoupling scheme. It is shown that the sublattice magnetization is $M=0.241$, and the ground-state energy per bond is $E_g/NZJ = -0.166$, which are consistent with the numerical simulations.

ACKNOWLEDGMENTS

The authors would like to thank Dr. Huang Zhong-bing and Dr. Song Yun for helpful discussions.

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