Spin-Liquid State for Two-Dimensional Heisenberg Antiferromagnets on a Triangular Lattice

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The spin liquid state of the antiferromagnetic Heisenberg model on a triangular lattice is studied within the self-consistent Green’s function method. It is shown that the spin excitation spectra is gapless, and ground-state energy per site is $E_g/NJ = -0.966$, which is in very good agreement with the results obtained within the variational Monte Carlo method based on the resonating-valence-bond state. Some thermodynamic properties are also discussed.

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In the last decades, a large amount of work has been devoted to the understanding of the property of the two-dimensional (2D) quantum Heisenberg antiferromagnets. This is motivated partly by the search for quantum disordered ground-state and their possible relationship to the high temperature superconductivity \[1\]. The numerical simulations strongly support the existence of the antiferromagnetic (AF) long-range-order (AFLRO) for the Heisenberg antiferromagnet on a square lattice with the reduced magnetic moment of about 60% of its classical value \[9\]. It has been shown that this magnetic moment is reduced further by considering the spin frustration arising from the next-nearest-neighbors coupling \[9\]. In contrast with the Heisenberg antiferromagnet on the square lattice, the Heisenberg antiferromagnet on a triangular lattice is the three-sublattice spin system with geometric frustration. Anderson \[4\] argued that the strong spin frustration on the triangular lattice may generate a novel resonating-valence-bond (RVB) spin liquid ground-state without AFLRO. Since then some different types of quantum ground-state have been proposed, in particular, Kalmeyer and Laughlin \[5\] argued that RVB state for the triangular lattice is similar to the fractional quantum Hall state for bosons. Moreover, various numerical techniques and analytical approaches have been used to study this system \[6,7\]. The variational energy reported by Lee and Feng \[8\] was essentially identical to the results obtained within the variational Monte Carlo method based on the RVB state. Huse and Elser \[9\] subsequently constructed wave functions exhibiting AFLRO which reportedly had a lower variational energy than Anderson’s \[4\]. Therefore the nature of the ground-state, especially the existence of AFLRO for the AF Heisenberg antiferromagnet on the triangular lattice, is still controversial.

Apart from the numerical techniques, a popular method to study the quantum spin problem is the spin-wave theory, where the quantum spin is mapped onto the boson representation in terms of the Holstein-Primakoff transformation. However, the native spin-wave theory, an expansion and linear approximation in Holstein-Primakoff bosons, leads to violation of the commutation rule of the quantum spin, this is because that the quantum spins obey the Pauli algebra, i.e., the spin one-half raising and lowering operators behave as fermions on the same site and as bosons on different sites. In this paper, we study the spin liquid state of the AF Heisenberg antiferromagnet on the triangular lattice within the Green’s function theory under the Kondo-Yamaji \[10\] decoupling scheme. With the help of the spectral representations of the correlations, the self-consistent equations are obtained to determine the order parameters. The spin excitation spectral is gapless and spin liquid ground-state energy per site is $E_g/NJ = -0.966$. Some thermodynamic properties are also discussed.

The standard AF Heisenberg model on the triangular lattice is written as,

$$H = J \sum_{i\eta} S_i \cdot S_{i+\eta},$$  \hspace{1cm} (1)

where the sum is over all sites $i$ and, for each $i$, over nearest-neighbors $\eta$. Since the quantum spin operators obey the Pauli spin algebra, then it can be discussed in terms of the Tyablikov’s two-time Green’s function method \[11\]. We define the spin two-time Green’s function $G$ as

$$G(i-j, t-t’) = -i\theta(t-t’) \langle [S_i^+(t), S_j^-(t’)] \rangle = \langle \langle S_i^+(t) S_j^-(t’) \rangle \rangle,$$  \hspace{1cm} (2)

with $\theta(t)$ is the step function, $S_i^+$ and $S_i^-$ are the raising and lowering operators of $S_i^z$, respectively, and $\langle \cdot \cdot \cdot \rangle$ is an average over the ensemble. The time-Fourier transform of the two-time Green’s function satisfies the equation,

$$\omega \langle \langle A; B \rangle \rangle = \frac{1}{2\pi} \left[ \langle [A, B] \rangle + \langle \langle A, H \rangle; B \rangle \right],$$  \hspace{1cm} (3)

\hspace{1cm}
and the correlation functions can be obtained by the spectral representations as,
\[
< B(t')A(t) > = i \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{<< A; B >>_{\omega+i0^+} - << A; B >>_{\omega-i0^+}}{e^{\beta\omega} - 1} e^{-i\omega(t-t')}.
\]

With the help of the Eq. (3), the equation of motion of the spin Green’s function (3) is evaluated as,
\[
\omega G(i-j, \omega) = \delta_{ij} < S_i^z > + 2J \sum_{\eta} << S_{i+\eta}^- S_i^z - S_i^z S_{i+\eta}^- S_j^- >> \omega.
\]

Since the three-sublattice ordering for the triangular lattice is still controversial, and the spin liquid hypothesis is not convincingly discarded, then in the following discussions, we only study the system in the case \(< S_i^z > = 0\), i.e., the spin liquid state without AFLRO. In this case, the basic equation for the spin Green’s function in the one-dimension equations to determine the order parameters \(G(k, \omega)\) has been discussed in detail by Kondo and Yamaji \([10]\), and 2D by many authors \([12]\). Following their discussions, we can obtain the spin Green’s function (5) as,
\[
G(k, \omega) = \frac{ZJC_1}{\pi} \left( \frac{\gamma_k - 1}{\omega^2 - \omega^2(k)} \right),
\]
where \(Z\) is the number of the nearest neighbor sites, \(\gamma_k = (1/Z) \sum_\eta e^{i\eta k}\), and spin excitation spectra,
\[
\omega^2(k) = ZJ^2 \left[ \frac{1}{2} + \alpha C_2 - \alpha C_1 (1 + Z \gamma_k) (1 - \gamma_k) \right],
\]
with the order parameters \(C_1 = << S_i^z S_{i+\eta}^+ >, C_2 = \sum_{\eta' (\eta' \neq \eta)} << S_{i+\eta}^- S_{i+\eta'}^+ >>\). In order not to violate the sum rule of the correlation function \(< S_i^z S_j^- >= 1/2\) in the case \(< S_i^z > = 0\), the important decoupling parameter \(\alpha\) has been introduced as these discussed by Kondo and Yamaji \([10]\), which is regarded as the vertex corrections. With the help of the Green’s function (6) and the spectra representation of the correlation functions (4), we obtain the self-consistent equations to determine the order parameters \(C_1, C_2,\) and \(\alpha\) as,
\[
C_1 = -\frac{ZJC_1}{N} \sum_k \frac{\gamma_k - \gamma_k}{\omega(k)} \coth \left[ \frac{1}{2} \beta \omega(k) \right],
\]
\[
C_2 = -\frac{ZJC_1}{N} \sum_k (Z \gamma_k^2 - 1) \frac{1 - \gamma_k}{\omega(k)} \coth \left[ \frac{1}{2} \beta \omega(k) \right],
\]
\[
\frac{1}{2} = -\frac{ZJC_1}{N} \sum_k \frac{1 - \gamma_k}{\omega(k)} \coth \left[ \frac{1}{2} \beta \omega(k) \right].
\]

We have performed the numerical calculation for the above self-consistent equations. The ground-state energy per site is \(E_g/NJ = -0.966\). For comparison with the other results obtained by the numerical simulations, the present theoretical result is also shown in Table I. It is obvious that our result of the ground-state energy is in very good agreement with those obtained by Lee and Feng \([8]\) based on the variational d-wave RVB state without AFLRO, but higher than the results of Huse and Elser \([9]\) for a AFLRO state and Nishimori and Nakanishi’s \([6]\) finite lattice exact diagonalization. Huse and Elser \([9]\) have estimated that the ground-state energy per site is \(E_g/NJ \leq -1.074\), then our ground-state energy is more than 10% higher this estimates. But the present low energy of the spin liquid state and the short range of its spin correlations indicate that longer-range spin interactions, e.g., second-near-neighbor coupling, can push the system further into the liquid phase. More interestingly, the excitation spectra of the RVB state for the triangular lattice obtained by Kalmeyer and Laughlin \([11,12]\) or Lee and Feng \([8]\) has a large gap, but in the present result, the excitation spectra of the spin liquid state is gapless, which is shown in Fig. 1, and the minimum-energy excitation is the spinon at \(k_c = (0,0)\). Our spin liquid state has spin-\(1/2\) bosonic spinons, and this structure clearly disagree with the Kalmeyer and Laughlin \([11,13]\) state on the triangular lattice, which was argued to possess semionic spinons. We have also computed the spin structure factor \(S(k) = (1/N) \sum_\langle ij \rangle < S_i^z S_j^z > e^{ik \cdot (R_i - R_j)}\) in the zero temperature, and the result is plotted in Fig. 2, the maxima of \(S(k)\) occur at six wave vectors, which is consistent with the result obtained within the large-N expansion \([14]\).

Some interesting properties associated the present spin liquid state, such as, the specific heat and susceptibility \(\chi = (g^2 \mu_B^2/k_B T) \sum_{ij} < S_i^z S_j^z >\) with \(g\) is the Landau factor and \(\mu_B\) is the Bohr magneton, have been discussed, and the results are shown in Fig. 3(a) and Fig. 3(b), respectively. The specific heat display a broad peak near \(k_B T \sim 0.5J\), which is in qualitative agreement with results of the AF Heisenberg model on the square lattice \([5]\).
The susceptibility is very weakly dependent on $T$, and the similar behavior has been obtained on the square lattice [15]. Therefore, our present results seem to indicate that the global behavior of the AF Heisenberg model on the triangular lattice, which is the system with geometric frustration, is qualitative consistent with the frustrated AF Heisenberg model on the square lattice.

In summary, we have studied the spin liquid state of the AF Heisenberg model on the triangular lattice within the Kondo-Yamaji’s decoupling scheme. It is shown that the spin excitation spectra is gapless, and the ground-state energy per site is $E_g/NJ = -0.966$. The energy of this spin liquid is very good consistent with the RVB state, but higher than the result for the AFLRO state. The behaviors of the specific heat and susceptibility are similar to these obtained on the square lattice.

A natural question is what is the reason why this self-consistent mean-field Green’s function theory is so useful to treat the quantum spin systems without AFLRO? To our present understanding, there are at least two reasons: (1) the commutation rule (Pauli algebra) of the quantum spin is exactly satisfied in the actual calculations. (2) The sum rule of the spin Green’s function is always satisfied, and the rotational symmetry is not unphysically broken in this self-consistent mean-field Green’s function theory. For the spin systems without AFLRO, the low lying excitations described are essentially spin waves propagating in a short-range-order with a correlation length. Kondo and Yamaji [10], and Shimahara and Takada [12] have employed this self-consistent mean-field Green’s function theory to study the one-dimensional Heisenberg spin system and 2D AF Heisenberg spin system on the square lattice, respectively, they obtained the results which have satisfactory temperature dependence over whole temperature region from qualitative view point.

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FIG. 1. Momentum dependence of the spin excitation spectra $\omega(k)$ of the spin liquid state. The minimum-energy excitation is the spinon at $k_c = (0,0)$

FIG. 2. Zero temperature structure factor $S(k)$ of the spin liquid state. The global maxima are at six wave vectors.
FIG. 3. (a) The specific heat and (b) susceptibility as a function of temperature.

TABLE I. A comparison of the ground-state energy per site for the antiferromagnetic Heisenberg model on the two-dimensional triangular lattice

| Author(s)                   | $E_g/NJ$    | Method               |
|-----------------------------|-------------|----------------------|
| Kalmeyer and Laughlin       | $-0.94(2)$  | Variational RVB      |
| Huse and Elser              | $-1.02(2)$  | Variational AF       |
| Nishimori and Nakanishi     | $-1.10(2)$  | Finite lattice       |
| Lee and Feng                | $-0.908(4)$ | Variational RVB      |
| The present work            | $-0.966$    | Green’s function method |