Magnetic properties of the two-dimensional Heisenberg model on a triangular lattice

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Abstract

The spin Green's function of the antiferromagnetic Heisenberg model on a triangular lattice is calculated using Mori's projection operator technique. At $T = 0$ the spin excitation spectrum is shown to have gaps at the wave vectors of the classical Néel ordering. This points to the absence of the antiferromagnetic long-range order in the ground state. The calculated spin correlation on the neighboring sites of the same sublattice is in good agreement with the value derived from exact diagonalization. The temperature dependencies of the spin correlations and the gaps are calculated.

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\textit{Key words:} Heisenberg antiferromagnet, triangular lattice

Strong electron correlations are expected to play an essential role in the recently discovered electron doped cobaltate $\text{Na}_x\text{CoO}_2*\text{yH}_2\text{O}$ \cite{1,2,3,4}. This system has layered structure which consists of two-dimensional $\text{CoO}_2$ planes separated by $\text{Na}^+$ and $\text{H}_2\text{O}$ layers and resembles the structure of cuprate high-$T_c$ superconductors. However, in contrast to square $\text{CuO}_2$ planes the Co ions form a triangular lattice. It is supposed that for moderate Na concentrations $x$ the low-energy physics of $\text{CoO}_2$ planes can be described by the $t$-$J$ model \cite{5}. For small $x$ the major part of Co ions are in the Co$^{4+}$ state with the spin $S = 1/2$ and the $t$-$J$ model is reduced to the two-dimensional $S = 1/2$ Heisenberg model. The knowledge of the spin excitation spectrum of this model is necessary for further investigation of spectral and magnetic properties of the $\text{CoO}_2$ planes. Various numerical and analytical methods were used for elucidating the ground state properties of the Heisenberg model on a triangular lattice \cite{6}. In Refs. \cite{6,7} it is argued that the ground state of this system has the long-range antiferromagnetic order. The opposite conclusion was made in Refs. \cite{8,9} analyzing the data of the exact diagonalization of small clusters.

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In this work we use the method [10] based on Mori’s projection operator technique [11] in which the spin Green’s function is represented by a continued fraction. The elements of the fraction are calculated in the recursive procedure which is similar to Lanczos’ orthogonalization. The decoupling is used in calculating the terms of the fraction. By analogy with Ref. [12] the decoupling is corrected by introducing vertex parameters the values of which are determined from the constraint of zero site magnetization following from the rotational symmetry of the Hamiltonian and the nearest-neighbor spin correlation derived from exact diagonalization. The used approach retains the rotation symmetry of spin components and does not contain any preset magnetic ordering. With this procedure the energies of magnetic excitations and spin-spin correlations are calculated. The calculated spin correlation on neighboring sites of the same sublattice is in good agreement with the value available from exact diagonalization [8,9]. The spectrum of magnetic excitations is found to have finite gaps at wave vectors of the classical Néel ordering \( \mathbf{Q} = \left( \frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}} \right), \left( \frac{4\pi}{3}, 0 \right) \) for zero temperature. This indicates that the ground state of the Heisenberg model on a triangular lattice has no long-range magnetic ordering.

The Hamiltonian of this model reads

\[
H = \frac{1}{2} \sum_{nm} J_{nm} \left( s^z_n s^z_m + s^z_{n+1} s^z_{m-1} \right),
\]

where \( s^z_n \) and \( s^z_m \) are the components of the spin-\( \frac{1}{2} \) operators, \( n \) and \( m \) label sites of the triangular lattice, \( \sigma = \pm 1 \). We take into account nearest neighbor interactions only, \( J_{nm} = J \sum_a \delta_{n,m+a} \) where \( J \) is the exchange constant and the six vectors \( \mathbf{a} \) connect nearest neighbor sites.

Magnetic properties of the model are inferred from the spin retarded Green’s function

\[
D(\mathbf{k} t) = -i \theta(t) \langle [s^z_{\mathbf{k}}(t), s^z_{-\mathbf{k}}] \rangle,
\]

where \( s^z_{\mathbf{k}} = N^{-1/2} \sum_n \exp(-i \mathbf{k} \mathbf{n}) s^z_n \), \( N \) is the number of sites, \( s^z_{\mathbf{k}}(t) = \exp(i H t) s^z_{\mathbf{k}} \exp(-i H t) \) and \( \langle \ldots \rangle = \text{Sp}[\exp(-H/T) \ldots]/\text{Sp}[\exp(-H/T)] \) with the temperature \( T \). As mentioned, we apply Mori’s projection operator technique [10,11]. To obtain the spin Green’s function we use the continued fraction representation for Kubo’s relaxation function \( \langle s^z_{\mathbf{k}}|s^z_{-\mathbf{k}} \rangle_\omega = \int_{-\infty}^{\infty} dt \exp(i \omega t) \langle (s^z_{\mathbf{k}}|s^z_{-\mathbf{k}})_t \rangle_{t} = \theta(t) \int_{0}^{\infty} dt' \langle [s^z_{\mathbf{k}}(t), s^z_{-\mathbf{k}}] \rangle \),

\[
\langle s^z_{\mathbf{k}}|s^z_{-\mathbf{k}} \rangle_\omega = \frac{\langle s^z_{\mathbf{k}}, s^z_{-\mathbf{k}} \rangle}{\omega - E_0 - \frac{V_0}{\omega - E_1 - \frac{V_1}{\ldots}}},
\]

and the relation

\[
D(\omega t) = \omega \langle s^z_{\mathbf{k}}|s^z_{-\mathbf{k}} \rangle_\omega - \langle s^z_{\mathbf{k}}, s^z_{-\mathbf{k}} \rangle,
\]
where \((A, B) = i \int_0^\infty dt \langle [A(t), B] \rangle\).

The elements of the fraction \(E_i\) and \(V_i\) are determined from the recursive procedure

\[
[A_n, H] = E_n A_n + A_{n+1} + V_{n-1} A_{n-1}, \quad E_n = ([A_n, H], A_n) (A_n, A_n^\dagger)^{-1},
\]

\[
V_{n-1} = (A_n, A_n^\dagger) (A_{n-1}, A_{n-1}^\dagger)^{-1}, \quad V_{-1} = 0, \quad A_0 = s_z^k, \quad n = 0, 1, 2, \ldots
\]

The operators \(A_i\) constructed in this procedure form an orthogonal set, \((A_i, A_j^\dagger) \propto \delta_{ij}\).

Using procedure (5) we get

\[
E_0 = (i s_z^k, s_z^\dagger_{-k})(s_z^k, s_z^\dagger_{-k})^{-1} = \langle [s_z^k, s_z^\dagger_{-k}] \rangle = 0, \quad A_1 = i s_z^k,
\]

\[
F_0 = 6J|C_1|(1 - \gamma_k')(s_z^k, s_z^\dagger_{-k})^{-1}, \quad E_1 = (i^2 s_z^k, -i s_z^\dagger_{-k})(i s_z^k, -i s_z^\dagger_{-k})^{-1} = 0,
\]

where \(\gamma_k' = \frac{1}{2} \cos(k_x) + \frac{2}{3} \cos(k_y) \cos(\frac{k_z \sqrt{7}}{2})\) in the orthogonal system of coordinates, \(C_1 = \langle s_{n-z}^{\dagger} s_{n+a}^{-1} \rangle\) is the spin correlation on neighboring sites. At this point we interrupt the continued fraction and calculate \((s_z^k, s_z^\dagger_{-k})\). In the accepted approximation \(V_1 \propto (A_2, A_2^\dagger) = 0\). From this equation we find [10]

\[
\langle i^2 s_z^k, -i s_z^\dagger_{-k} \rangle = 36 J^2 C_1^2 (1 - \gamma_k'^2)(s_z^k, s_z^\dagger_{-k})^{-1}.
\]

The quantity \(i^2 s_z^k\) in the left-hand side of this equation contains terms of the type \(s_z^n s_{n-1}^{\dagger}\) which, following Refs. [12,13], are approximated by \((\alpha_1 P_{nm} + \alpha_2 (1 - P_{nm})) \langle s_{n-1}^{\dagger} s_{m}^{-1} \rangle (1 - \delta_{nm}) + \frac{1}{2} \delta_{nm} s_z^n\). Here \(\alpha_{1,2}\) are the vertex corrections, \(P_{nm} = 1\) if the sites \(n\) and \(m\) belong to the same magnetic sublattice and zero in the opposite case. In the decoupling the constraint of zero site magnetization

\[
\langle s_z^n \rangle = \frac{1}{2} = \langle s_{n-1}^{\dagger} s_n^{-1} \rangle = 0
\]

was taken into account. This constraint is fulfilled both in the paramagnetic and in the ordered states; in the latter case due to the averaging over all possible directions of the magnetization. Using this approximation for \(i^2 s_z^k\) from Eq. (6) we find \((s_z^k, s_z^\dagger_{-k})\) and from Eqs. (3) and (4) we get

\[
D(\mathbf{k}, \omega) = \frac{6(1 - \gamma_k') J |C_1|}{\omega^2 - \omega_k'^2},
\]

where

\[
\omega_k^2 = 36 J^2 \alpha_2 |C_1|(1 - \gamma_k') \left( \Delta + \frac{1}{2} + \gamma_k' \right), \quad \Delta = \frac{\alpha_1 C_2' + \alpha_2 C_2''}{\alpha_2 |C_1|} - \frac{1}{3} + \frac{(1 - \alpha_1)}{12 \alpha_2 |C_1|},
\]
where \( C' \) with the vector \( \mathbf{a}' \) connecting nearest neighbor sites of a magnetic sublattice and \( C'' = 2C_1 + \langle s_n^+s_{n+2a}^- \rangle \). The quantity \( \omega_k \) is the frequency of spin excitations and the parameter \( \Delta \) describes the spin gap at the wave vectors \( \mathbf{Q} \) of the classical Néel ordering. As seen from Eq. (9), the frequency of spin excitations tends to zero when \( k \to 0 \) (the Goldstone mode) and has local minima at \( k = Q \).

To finish the calculations we have to find the parameters \( \alpha_1, \alpha_2, C_1, C'_2 \) and \( C''_2 \) in Eq. (8) and (9). For this purpose we use Eq. (7) and the relations connecting the spin correlations with Green’s function (8)

\[
\langle s_n^+s_m^- \rangle = \frac{6J|C_1|}{N} \sum_k \cos (k(n-m)) \frac{1 - \gamma_k'}{\omega_k} \coth \left( \frac{\omega_k}{2T} \right).
\]

However, these relations – the three equations (10) for \( C_1, C'_2, C''_2 \) and the constraint (7) – give only four equations for the above five parameters. At zero temperature this deficiency can be made up by using results of exact diagonalization. More specifically, we use the value \( C_1 = -0.1215 \) derived for an infinite crystal from results of exact diagonalization [8]. If the assumption is made that for \( T = 0 \) the system has the long-range antiferromagnetic order then the frequencies of spin excitations at \( \mathbf{Q} \) have to vanish. In this case one more unknown parameter – the condensation part \( C \) – appears in the calculations [13]. This part is the contribution of points \( \mathbf{Q} \) to the spin correlations (10),

\[
\langle s_n^+s_m^- \rangle = C \cos (\mathbf{Q}(n-m)) + \frac{6J|C_1|}{N} \sum_{k \neq \mathbf{Q}} \cos (k(n-m)) \frac{1 - \gamma_k'}{\omega_k}.
\]

Also the above set of equations is supplemented by the equation \( \Delta = 0 \) with \( \Delta \) given by Eq. (9). The sublattice magnetization \( m \) is directly connected with the condensation part:

\[ m = \sqrt{3C}/2. \]

Solving the mentioned set of equations for an infinite crystal we found that \( C = -0.05 \). This result contradicts to the assumption of the long-range order for which \( C \) has to be positive. We arrived at the conclusion that either there is no long-range order in the ground state of the 2D Heisenberg model on the triangular lattice or the ordering parameter is too small to be determined by the present approximate method. Notice also that the value of \( \langle s_n^+s_{n+a}^- \rangle = 0.077 \) obtained in our calculations is in good agreement with the value 0.0803 \( \pm \) 0.004 derived from exact diagonalization [8] (to our knowledge \( C_1 \) and \( \langle s_n^+s_{n+a}^- \rangle \) are the only correlations with the values well-defined from exact diagonalization for the triangular lattice). One of the manifestations of the short-range order is a finite frequency \( \omega_\mathbf{Q} \) of spin excitations at the wave vectors \( \mathbf{Q} \).

To consider the temperature variation of the spin correlations and spectrum we decreased the number of parameters, setting \( \alpha_1 = \alpha_2 = \alpha \). In this approximation we have four equations for four parameters. The range of temperatures \( 0 \leq T \leq 1.3J \) and a 1000 \( \times \) 1000 lattice with periodic boundary conditions were used in these calculations. The approximation \( \alpha_1 = \alpha_2 \) is cruder than the previous one where \( \alpha_1 \) and \( \alpha_2 \) could differ. Therefore the gap \( \omega_\mathbf{Q} \) in the spectrum of spin excitations at the wave vectors \( \mathbf{Q} \), the existence of which is an indication
of the short-range order, is somewhat larger in the former approximation than in the latter. The temperature dependencies of this gap, the spin correlation $C_1$ and the dispersion of the spin excitations in the approximation $\alpha_1 = \alpha_2$ are shown in Fig. 1 – 3. The gap $\omega_\mathbf{Q}$ grows with temperature which corresponds to the decrease of the correlation length.

In summary, Mori’s projection operator technique was used for investigating the excitation spectrum of the two-dimensional Heisenberg model on a triangular lattice. The zero-temperature spin-excitation spectrum has gaps at the wave vectors $\left(\frac{2\pi}{3}, \frac{2\pi}{\sqrt{3}}\right)$, $\left(\frac{4\pi}{3}, 0\right)$ of the classical Néel ordering which is an indication of the lack of the long-range antiferromagnetic ordering in the ground state of the system. Temperature dependencies of the spin correlations and the gaps were calculated.

Acknowledgements

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Figure captions

Fig. 1. The dependence of the spin correlation $C_1 = \langle s_{n+1}^+ s_{n+a}^- \rangle$ on temperature.

Fig. 2. The dependence of the energy of the spin excitations at the wave vector of the classical Néel ordering $Q$ on temperature.

Fig. 3. The dispersion of the spin excitations at zero temperature.
\[ \omega(k)/J \]