The spin-wave spectrum of $s=1/2$ triangular lattice Heisenberg antiferromagnet

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The ground state and spin excitations of a Heisenberg antiferromagnet on a triangular lattice with nearest- and next-nearest-neighbor interactions are investigated. Ground state has long-range order and becomes unstable near $J_2/J_1 \cong 2/15$. The possibility of spin liquid state is discussed.

Two-dimensional spin systems have been studied extensively in connection with high-temperature superconductivity. A list of candidates for spin-liquid ground state is continuously reduced. Triangular lattice still remains one of them, because it has inherent frustration.

In the present letter we investigate spin excitations for $s=1/2$ triangular lattice Heisenberg antiferromagnet with nearest (NN) and next-nearest-neighbor (NNN) exchange J_1 and J_2. The Hamiltonian is

$$H=-\sum_{\langle ij\rangle} s_i s_j - \alpha \sum_{(ij)} s_i s_j; \quad \alpha = J_2/J_1; \quad J_1=1, \tag{1}$$

where the sum $\langle ij\rangle$ is over NN and (ij)-NNN pairs of sites. The essential feature of our approach is a block method, where the short-range order is taken into account in the zero approximation, without breaking the lattice symmetry. The blocks are triangles, regularly covering the plane (Fig. 1). For one block it is appropriate to choose eigenstates of chirality operator $\hat{K}=\mathbf{s}_1(\mathbf{s}_2\times\mathbf{s}_3)$[1] (1,2,3-block sites) as a basis. The complete set of such states consists of two doublets with energy $\epsilon_d=-3/4$ and block

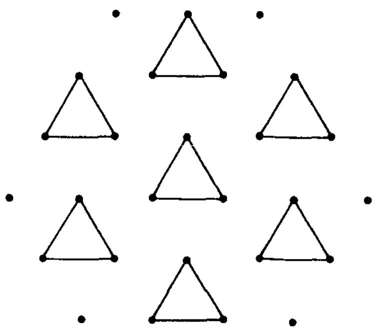

FIG. 1. Triangular lattice represented as a set of triangular blocks.

spin $S=1/2$ and a quartet with $\epsilon_q=3/4$ and $S=3/2$. Below we ignore energetically higher quartet states, so the problem is solved in the basis $\varphi^{\pm}$, $\chi^{\pm}$

$$|\varphi^+\rangle=\frac{1}{\sqrt{3}}\{|\downarrow\uparrow\uparrow\rangle+\omega^2|\uparrow\downarrow\uparrow\rangle+\omega|\uparrow\uparrow\downarrow\rangle\};$$

$$|\chi^+\rangle=\frac{1}{\sqrt{3}}\{|\downarrow\uparrow\uparrow\rangle+\omega|\uparrow\downarrow\uparrow\rangle+\omega^2|\uparrow\uparrow\downarrow\rangle\};\quad \omega=\exp(2\pi i/3) \tag{2}$$

$$\hat{K}|\varphi^{\pm}\rangle=-2\sqrt{3}|\varphi^{\pm}\rangle;\quad \hat{K}|\chi^{\pm}\rangle=2\sqrt{3}|\chi^{\pm}\rangle$$

($|\varphi^-\rangle$, $|\chi^-\rangle$ are obtained from $|\varphi^+\rangle$, $|\chi^+\rangle$ by arrowheads reversing). The dashed blocks, if considered as new sites, form a triangular lattice with the new states of the sites described by two doublets. Note that standard generalization of the usual $SU(2)$ Heisenberg Hamiltonian is a model with $SU(N)$ symmetry, which involves N slave bosons per site, so $1/N$ expansion is applicable.[2] Here another generalization naturally appears - a model with two $s=1/2$ spins of different color per "site" (i.e., block).

In the basis $\lambda^i=\{\varphi^{\pm}, \chi^{\pm}\}$, $i=1$–4 the Hamiltonian takes the form

$$H=H_0+T;\quad H_0=\epsilon_d\sum_n\sum_{i=1}^{4}Z_{\mathbf{n}}^{\lambda^i\lambda^i} \tag{3}$$

$$T=\sum_{\mathbf{n},\mathbf{g}}\sum_{i,j,k,l=1}^{4}t_{\mathbf{g}}(\lambda^i,\lambda^j;\lambda^k,\lambda^l)Z_{\mathbf{n}}^{\lambda^i\lambda^k}Z_{\mathbf{n}+\mathbf{g}}^{\lambda^j\lambda^l}.$$

Here $\mathbf{n}$ denotes the block, $\mathbf{g}$ is its nearest-neighbor blocks, $Z_{\mathbf{n}}^{\mu\nu}$ is the projection operator, H_0 is the Hamiltonian of the noninteracting blocks, and T is the interblock interaction. The coefficients $t_{\mathbf{g}}$ can be easily calculated; T is invariant under the operations of block's lattice symmetry group and rotations in spin space. Both NN and NNN intersite interactions in the site Hamiltonian (1) correspond to the nearest blocks in (3). Note that restriction by the set of states (2) is completely adequate for the case of triangular box lattice, where the exchange on the intrablock bonds is greater than the interblock interaction.

Let us first construct the Hartree ground state for Hamiltonian (2). It has the form $\Psi_{gr}=\Pi_{\mathbf{n}}\Phi_{\mathbf{n}}$, where $\Phi_{\mathbf{n}}$ are optimal linear combinations of the functions (2). One can show that for $\alpha < 1/3$ the simplest Φ can be assumed as any state from the orthonormal set $d^{\pm} = (\chi^{+} \pm \varphi^{-})/\sqrt{2}$, $p^{\pm} = (\varphi^{+} \pm \chi^{-})/\sqrt{2}$. The ground state Ψ_{gr} is degenerate under rotations in the space of block spins and, in particular, $d^{\pm}$ and $p^{\pm}$ are transformed, one into the another, by appropriate rotations. The state Ψ_{gr} has zero mean value of the block spin $\langle S_{\mathbf{n}} \rangle = 0$ and the energy per block $\epsilon_0 = -13/12 + \alpha$ (the energy per intersite bond $\epsilon_{00} = \epsilon_0/9 = -0.12 + \alpha*0.11$). Ψ_{gr} is not an eigenstate of the site spin operator; the vectors of the mean values of site spins form a three-sublattice 120° picture with $s \equiv \sqrt{\langle \mathbf{s}_i^2 \rangle} = 1/3$. Ψ_{gr} obviously has a long-range order.

If we construct Ψ_{gr} in the complete set (adding quartet), the mentioned properties of Ψ_{gr}: $\langle S_{\mathbf{n}} \rangle = 0$ will not be changed; Ψ_{gr} is degenerate and is obtained from the state

$$q = (1 + 2\nu^2)^{-1} [\nu(\delta^{+} + \delta^{-}) + d^{+}], \quad \delta^{+} = |\uparrow\uparrow\uparrow\rangle, \quad \delta^{-} = |\downarrow\downarrow\downarrow\rangle,$$

by rotations in the spin space of the block. For $\alpha = 0$ $\nu \cong 0.22$, $\epsilon_{00} = -0.14$, and $s = 0.48$. We recall that classical triangular AFM has 120° ground state with $\epsilon_{00} = -0.125$ (Ref. 3).

Now it is natural to consider spin excitations against the background of Ψ_{gr} with the choice, say, $\Phi_n = d_n^{+}$. The operators of spin excitations are then $b_{1,n}^{+} = Z_n^{d^{-}d^{+}}$, $b_{2,n}^{+} = Z_n^{p^{+}d^{+}}$, and $b_{3,n}^{+} = Z_n^{p^{-}d^{+}}$. We use the approach which is analogous to the linear spin wave theory. We consider $b_{\nu,n}^{+}$ as bosonic operators and keep only the quadratic terms $b_{\nu n}^{+} b_{\mu m}$, $b_{\nu n}^{+} b_{\mu m}^{+}$, $b_{\nu n} b_{\mu m}$ $\mu,\nu = 1,2,3$. The 6×6 Hamiltonian matrix is diagonalized by the generalized $u - v$ transformation.[4] One can see from the analytic form of the secular equation that there are three nondegenerate (in any direction) acoustic branches $\omega_\mu(\mathbf{k})$ of spin excitations. No branch changes under rotation of $\mathbf{k}$ by $\pi/3$.

The Brillouin zone (BZ) is a regular hexagon with the side $4\pi/3a = 4\pi/3\sqrt{3}a_0$, a and a_0 are the lattice constants of the block and site lattices, respectively. The spin-wave operators of the ω_μ branches are superimpositions of b_1^{+}, b_2^{+}, b_3^{+}. Hybridization disappears only at $\mathbf{k} = 0$ (the point Γ) and in the BZ corners K [$\mathbf{k} = (0, 4\pi/3a)$ and equivalent points].

The spectrum is softened with increasing α. When $\alpha \cong 2/15 \cong 0.133$, the instabilities at the three points appear almost simultaneously: At $\mathbf{k} = 0$ one of the sound velocities becomes zero ($\alpha \cong 0.126$), at point M (the midpoint of the BZ side) the frequency of one branch goes to zero ($\alpha \cong 0.132$), and at point K the frequencies of two branches go to zero ($\alpha = 2/15 \cong 0.133$).

Estimation of the Hartree energies near $\alpha = 2/15$ shows that the stripe phase (alternation of stripes of the blocks in the states, for example, d^{+} and d^{-}) is the most probable candidate for the ground state.

Investigation of the problem for a square lattice with frustration shows that a spin-liquid state can exist between the chess and the stripe phases.[5] The triangular lattice was mostly studied at $\alpha = 0$, where the question about the long-range order (LRO) is still open.[3,6] In particular, the resonating-valence-bond (RVB) state is a candidate for ground state at $\alpha = 0$.[7] Recently, the relationship between the variational RVB trial function and the fractional quantum Hall state was argued.[8] Nevertheless, numerical investigation of the variational wave function with LRO leads to the lowest energy[9] $\epsilon_{00}=-0.1789$. Our analysis shows that it is necessary to search for stable spin-liquid ground state near $\alpha=2/15$.

At $\alpha=0$, the zero-point motion lowers the energy to $\epsilon_{00}=-0.145$ (compare with $\epsilon_{00}\cong-0.18$, which was mentioned above). It is therefore necessary to consider spin waves in the complete block basis. Nevertheless, it should not change the transition picture qualitatively. In particular, such consideration retains three gapless branches, although the quartet states are separated from φ, χ by a finite gap. In the Hartree approximation, the transition point moves only slightly after taking the quartet states into account.

In summary, we constructed the long-range order ground state with the mean 120° structure, which loses stability at $\alpha\cong2/15$, where the search for the spin-liquid state should be carried out.

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