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ON THE SPIN-WAVE SPECTRUM OF $s = 1/2$ TRIANGULAR LATTICE HEISENBERG ANTIFERROMAGNET

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

Two-dimensional spin systems are intensively studied 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.

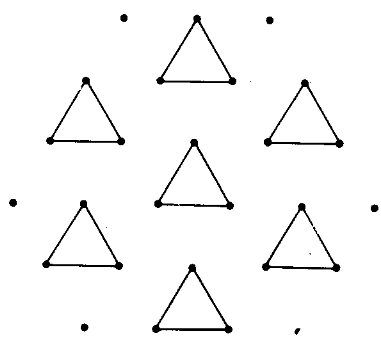

Figure capture. Triangular lattice as a set of triangular blocks

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

$$H = -\sum_{<ij>} \mathbf{s}_i\mathbf{s}_j - \alpha\sum_{(ij)} \mathbf{s}_i\mathbf{s}_j; \quad \alpha = J_2/J_1; \quad J_1 = 1 \qquad (1)$$

where the sum $< ij >$ 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.). For one block it is appropriate to choose eigenstates of chirality operator $\hat{K} = \mathrm{s}_1(\mathrm{s}_2 \times \mathrm{s}_3)$ [1] (1,2,3-block sites) as a basis. Complete set of such states consists of two doublets with energy $\epsilon_d = -3/4$ and block spin $S = 1/2$ and a quartet with $\epsilon_q = 3/4$ and $S = 3/2$. Hereinafter we neglect energetically higher quartet states, so the problem is solved in the basis $\varphi^{\pm}$, $\chi^{\pm}$

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

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

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

($|\varphi^->, |\chi^->$ are obtained from $|\varphi^+>, |\chi^+>$ by arrowheads reversing) Dashed blocks, if considered as new sites, form triangular lattice with the new sites' states 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 $\lambda^i = \{\varphi^{\pm}, \chi^{\pm}\}$, $i = 1 \div 4$ 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 block, $\mathbf{g}$ – its nearest-neighbor blocks, $Z_{\mathbf{n}}^{\mu\nu}$ – projection operator, H_0 – Hamiltonian of non-interacting blocks, T – inter-block interaction. Coefficients $t_{\mathbf{g}}$ are 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 site Hamiltonian (1) correspond to nearest blocks in (3). Note, that restriction by the set of states (2) is completely adequate for the case of triangular box-lattice, where exchange on intra-block bonds is greater than inter-block interaction.

Let's at first construct Hartree ground state for Hamiltonian (2). It has the form $\Psi_{gr} = \prod_{\mathbf{n}} \Phi_{\mathbf{n}}$, where $\Phi_{\mathbf{n}}$ are optimal linear combinations of functions (2). One can show, that for $\alpha < 1/3$ the simplest Φ can be taken as any state from ortonormal set $d^{\pm} = (\chi^+ \pm \varphi^-)/\sqrt{2}$, $p^{\pm} = (\varphi^+ \pm \chi^-)/\sqrt{2}$. 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 to another by appropriate rotations. State Ψ_{gr} has zero mean value of block spin $< S_{\mathbf{n}} >= 0$ and energy per block $\epsilon_0 = -13/12 + \alpha$ (energy per intersite bond $\epsilon_{00} = \epsilon_0/9 = -0,12 + \alpha * 0,11$). Ψ_{gr} is not an eigenstate of site spin operator, the vectors of mean values of site spins forming three-sublattice 120^0 picture with $s \equiv \sqrt{< \mathrm{s}_i^2 >} = 1/3$. Ψ_{gr} obviously has long-range order.

If we construct Ψ_{gr} in the complete set (adding quartet,) it does not change the mentioned properties of Ψ_{gr}: $< S_{\mathbf{n}} >= 0$; Ψ_{gr} is degenerate and is obtained from the state

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

by rotations in block's spin spase. For $\alpha=0$ $\nu \cong 0,22$, $\epsilon_{00}=-0,14$, $s=0,48$. Let's remind that classical triangular AFM has 120^0 ground state with $\epsilon_{00}=-0,125$ [3].

Now it is natural to consider spin excitations on the background of Ψ_{gr} with the choice, say, $\Phi_n = d_n^+$. Operators of spin excitations are then $b_{1,n}^+ = Z_n^{d^- d^+}$, $b_{2,n}^+ = Z_n^{p^+ d^+}$, $b_{3,n}^+ = Z_n^{p^- d^+}$. We use the approach, analogous to linear spin waves theory, considering $b_{\nu,n}^+$ as bosonic operators and keeping 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 analytical form of secular equation, that there are three non-degenerate (in any direction) acoustic branches $\omega_\mu(\mathbf{k})$ of spin excitations. Any branch is not changed under rotation of $\mathbf{k}$ by $\pi/3$.

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 lattice constants of block and site lattices respectively. The spin-waves operators of ω_μ branches are superpositions of b_1^+, b_2^+, b_3^+. Hybridization disappears only for $\mathbf{k}=0$ (point Γ) and in BZ corners K ($\mathbf{k}=(0,4\pi/3a)$ and equivalent points).

Spectrum is softened with increasing α. When $\alpha \cong 2/15 \cong 0,133$, instabilities at three points appear almost simultaneously: at $\mathbf{k}=0$ one of the sound velocities becomes zero ($\alpha \cong 0,126$), at point M (middle of BZ side) frequency of one branch goes to zero ($\alpha \cong 0,132$), at point K - frequencies of two branches ($\alpha=2/15 \cong 0.133$).

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

Investigation of the problem for square lattice with frustration shows, that spin-liquid state can exist between chess and stripe phases [5]. Triangular lattice mostly studied at $\alpha=0$, where the guestion about the long-range order (LRO) is still open [3,6]. In particular, resonating-valence-bond (RVB) state is a candidate for ground state at $\alpha=0$ [7]. Recently the relationship between variational RVB trial function and the fractional quantum Hall state was argued [8]. Nevertheless, numerical investigation of variational wave function with LRO leads to the lowest energy $\epsilon_{00}=-0,1789$ [9]. Our consideration shows that it is necessary to search for stable spin-liquid ground state near $\alpha=2/15$.

At $\alpha=0$ zero-point motion lowers the energy to $\epsilon_{00}=-0,145$. (compare with $\epsilon_{00} \cong -0,18$, mentioned above). So it is necessary to consider spin waves in complete block basis. Nevertheless, it shouldn't change the transition picture qualitatively. In particular, such consideration retains three gapless branches, though quartet states are separated from φ,χ by finite gap. In Hartree approximation transition point only slightly moves after taking quartet states into account.

To summarize, we constructed long-range order ground state with mean 120^0 structure, which looses stability at $\alpha \cong 2/15$, where spin-liquid state is to be searched for.

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