Unconventional state
with two coexisting long-range orders
for frustrated Heisenberg model
at quantum phase transition

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Abstract

For the frustrated two-dimensional $S = 1/2$ antiferromagnetic Heisenberg model close to quantum phase transition we consider the singlet ground states retaining both translational and SU(2) symmetry. Besides usually discussed checkerboard, spin-liquid and stripe states an unconventional state with two coexisting long-range orders appears to be possible at sufficiently large damping of spin excitations. The problem is treated in the frames of self-consistent spherically symmetric approach.

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1. The general quantum phase transition problem [1-3] is commonly considered in the frames of 2D Heisenberg quantum antiferromagnet. The main interest in this context is concentrated around the maximally frustrated point $J_2/J_1 \sim 0.5$ (frustration parameter $p = J_2/(J_1 + J_2) \sim 0.3$). In this region several energetically competitive states with different symmetry appear to be possible ground state $\Psi_0$ at $T = 0$. That is why the recent theoretical efforts are aimed at quantum phase transition near $p \sim 0.3$ with several possible scenarios.

There is firstly a class of states which brake either translational $\hat{T}_l$ (l - lattice vector) symmetry or spin SU(2) symmetry of the Hamiltonian. These are semiclassical Neel checkerboard state ($p < 0.3$) and semiclassical stripe phase ($p > 0.3$), where both $\hat{T}_l$ and SU(2) symmetries are broken. Another states of the class are singlet $\langle S_z^r \rangle = 0$ valence bond crystal (VBC) states ($p \approx 0.3$, $\hat{T}_l$ symmetry is broken, SU(2) symmetry is restored). Spins in VBC are coupled in pairs forming singlet valence bonds, the
latter being arranged in a periodic pattern. Usually only the simplest — columnar and plaquette — VBC are considered. The aforementioned states are sketched in Fig. 1.

Let us note, that an accurate comparison of competitive states is of course permissible only within one and the same method.

Hereinafter we will consider only another class of pretender states — singlet states which differ from semiclassical ones and do not brake neither $T_l$ nor SU(2) symmetry. The simplest state of this class can be constructed in the frames of the mentioned nearest neighbour valence bond approach. The wavefunction of this state is a sum of terms represented in Fig. 2a. Each term is given by disorderly placed valence bonds, but the whole spin liquid (SL) state picture is periodical.

One can generalize the nearest neighbour valence bond concept and consider also arbitrary range valence bonds (see Fig. 2b). In the latter picture spin-spin correlation functions $\langle S^z_{r}|S^z_{0}\rangle_{r \to \infty}$ for infinitely distant sites can become non-zero under certain circumstances, thus opening the way to consider the transition between spin liquid singlet state without long-range order (LRO) to singlet state with LRO.

In the present work we investigate singlet states with and without LRO in the frames of Kondo–Yamaji–Shimahara–Takada self-consistent spherically symmetric theory (SST) [4, 5], adapted for frustrated Heisenberg model [6, 7]. SST does not brake neither translational nor SU(2) symmetry. The method describes the singlet ground state in terms of spin-spin correlation functions and allows to find the triplet excitations spectrum. Note, that the arising description of Neel and stripe states differs from common semiclassical ones, presented in Fig.1, namely, a mean site spin in SST is equal to zero $\langle S^z_r \rangle = 0$ in any phase, sublattices are absent and the long-range order (or its absence) is controlled by spin-spin correlators $\langle S^z_{r}|S^z_{0}\rangle_{r \to \infty}$ for infinitely distant sites, or equivalently by the presence or absence of the gap in the spin spectrum at the symmetrical points $(\pm \pi, \pm \pi), (0, \pm \pi), (\pm \pi, 0)$.

In more detail, at zero temperature the structure factor $c_q = \langle S^z_q S^z_{-q}\rangle$ in SST is a superposition of smooth part $c_0q$ and, for long-range order cases, $\delta$-terms $c_0q\delta(q - q_0^\nu)$ at symmetric points $q_0^\nu$ of the Brilloine zone. This means that in the coordinate space the spin-spin correlation function acquires the form

$$c_r = \langle S^z_{n+r}|S^z_n\rangle = \frac{1}{N} \sum_q c_0 q e^{iqr} + \sum_\nu c_0 q \delta(q - q_0^\nu)$$

(1)

The first term in the right-hand side of (1) defines local correlations and it vanishes at infinite distance $r \to \infty$, the second (condensation) part controls LRO. The existence of non-zero condensation part is equivalent to zero spin gaps at the appropriate points $q_0^\nu$ of the Brillouin zone.

In particular for spherically symmetric Neel-type state (SST-Neel) $q_0^\nu = Q = (\pi, \pi)$ and the long-range order has a checkerboard pattern

$$\langle S^z_{\nu} | S^z_{0} \rangle_{r \to \infty} = c_0^\text{Neel} (-1)^{n_x + n_y}$$

(2)

where $r = n_x g_x + n_y g_y$, and $g_x = (1, 0)$, $g_y = (0, 1)$ are lattice vectors. The effective magnetization $m^\text{Neel} = \sqrt{c_0^\text{Neel}}$ depends on frustration. SST-Neel state is realized at low frustration. $m^\text{Neel}$ decreases from its maximal value at $p = 0$ to zero at point $p^*_N$, which is
where LRO disappears ($p_N^* \sim 0.2$, [8, 9]). Let us remind, that in SST $\langle S^z \rangle = 0$ in any phase.

Spherical symmetric stripe state (SST-Stripe) differs from the presented in Fig.1 semiclassical picture also in the following sense – it is the coherent superposition of stripe pictures with horizontal (as in Fig.1) and vertical stripes. For this state $q_0^{\nu=2,3} = \mathbf{X} = (0, \pi), (\pi, 0)$ and the long-range order pattern is

$$\langle S^z(r) | S^z(0) \rangle_{r \to \infty} = \frac{c_0^{\text{Stripe}}}{2} \sum_{n_y} (-1)^{n_x} (-1)^{n_y}$$

(3)

SST-Stripe state is realized for higher frustrations. The effective magnetization $m^{\text{Stripe}} = \sqrt{c_0^{\text{Stripe}}}$ increases from zero at $p^*_S \sim 0.5$ [7] to the maximal value at $p = 1$.

The solution with $c_0^{\text{Neel}} = c_0^{\text{Stripe}} = 0$, i.e. without long-range order, corresponds to SL. In this case spin gaps in the symmetrical points of the Brillouine zone are opened, their value depending on frustration. The correlation length is defined by the lowest spin gap and also depends on frustration. In this sense the solution involved is the arbitrary range spin liquid (compare Fig.2b). Self-consistent SL solution is realized in the intermediate frustration region $p \sim 0.3$ [7, 8, 9].

Note, that besides three aforenamed types of solutions the approach allows to consider the exotic state with two mutually penetrating long-range orders – checkerboard and stripe. The spin gaps in this state must be closed both at $Q$ and at $X$. The main result of this work is that at sufficiently large damping of spin excitations the solution of this type does exist and at the point of quantum phase transition is degenerate with another (two) solutions.

The paper is organized as follows. In part 2 we briefly remind the SST calculation procedure in the mean field realization. In part 3 the damping of spin excitations is introduced in the simplest semiphenomenological way. As it is shown in part 4, at sufficiently large but still realistic damping there appears a new type of self-consistent solution – with two long-range orders. In passing it is demonstrated that the width of spin liquid solution region strongly depends on damping. This part is also devoted to brief discussion.

2. The Hamiltonian of the frustrated Heisenberg model for $S = 1/2$ spins on a square lattice is

$$\hat{H} = \frac{1}{2} J_1 \sum_{i,g} \mathbf{S}_i \mathbf{S}_{i+g} + \frac{1}{2} J_2 \sum_{i,d} \mathbf{S}_i \mathbf{S}_{i+d}$$

(4)

here the first term in the right-hand side stands for the nearest-neighbour interaction ($J_1$ – antiferromagnetic exchange constant, $\mathbf{g}$ – nearest-neighbour vector), and the second – for the next-nearest-neighbour one (with corresponding quantities $J_2$ and $\mathbf{d}$). Standard parameter $p$ is a measure of frustration $p = J_2/J$, $J_1 = (1-p)J$, $J_2 = pJ$, $J = J_1 + J_2$. All the energetic parameters are expressed in the units of $J$, hereafter we put $J = 1$.

In the frames of SST the calculations come to the chain of equations of motion for spin retarded Green’s function $G^z_{nm} = \langle S^z_n | S^z_m \rangle_{\omega+is} = -i \int_0^\infty dt e^{i\omega t} \langle [S^z_i(t), S^z_j] \rangle$. The
chain is closed at the second step by the approximation of the following type

\[ S_{n+1}^i + g_1 S_{n+2}^i S_n^\gamma \approx \alpha g_1 (\delta j_1 (S_{n+1}^i + g_2 S_{n}^\gamma) + \alpha g_1 + g_2 \delta j_2 S_n^\gamma) + \alpha g_1 + g_2 \delta j_1 S_n^\gamma + \alpha g_1 \delta j_2 S_n^\gamma \]

(5)

where \( \alpha \) – so called vertex corrections \([5]\). In the mean-field approximation Green's function \( G_z (q, \omega) = (S_z^q \mid S_{-q})_\omega \) has the form

\[ G_z (q, \omega) = \frac{F_q}{\omega^2 - \omega_q^2}, \quad S_z^q = \frac{1}{\sqrt{N}} \sum_q e^{-iqr} S_z^q \]

(6)

where the numerator \( F_q \) and the spin excitations spectrum \( \omega_q \) are functions of lattice sums, involving spin–spin pair correlation functions \( c_r = (S_z^{n+r} \mid S_z^n) \) for first five coordination spheres (see \([8, 10]\) for details).

\( G_z (q, \omega) \) defines the structure factor, i.e. Fourier-transform of a correlation function

\[ c_q = (S_z^q \mid S_{-q}^z) = -\frac{1}{\pi} \int d\omega m(\omega) \text{Im} G_z (q, \omega) = \frac{F_q}{2\omega_q} (2m(\omega_q) + 1) ; \]

(7)

which, in turn, leads to five self-consistent equations:

\[ c_r = \frac{1}{N} \sum_q c_q e^{irq} ; \quad (r = g, d, 2g, 2d, g + d) \]

(8)

The system of equations (8) is then solved numerically.

At \( T = 0 \) the structure factor \( c_q \) (7) is a superposition of smooth part and, possibly, \( \delta \)-terms \( \delta(q - q_0^\nu) \) at symmetric points \( q_0^\nu \) of the Brillouin zone. The latter solution corresponds to the presence of long-range order, the condensation part appears in Eq.(8), and \( \delta(q - q_0^\nu) \) transforms into

\[ c_r = \frac{1}{N} \sum_q c_q e^{irq} + \sum_{\nu} c_0^\nu e^{iq_0^\nu r} \]

(9)

where \( c_0^\nu = \frac{F_{q_0^\nu}}{2\omega_{q_0^\nu}} \) defines local correlations, and \( c_0^\nu \) controls the long-range order. Non-zero condensation part leads to additional condition in the self-consistent system of equations (8) — the zero spin gap at the appropriate point of the Brillouin zone (\( q_0^\nu = Q = (\pi, \pi) \) for SST-Neel and \( q_0^\nu = 2.3 = X = (0, \pi), (\pi, 0) \) for SST-Stripe phase). Solution with all \( c_0^\nu = 0 \), i.e. without long-range order corresponds to spin liquid. As it is seen from (9), in particular, the scheme allows to search for the states with several mutually penetrating long-range orders, defined by the points \( q_0^\nu \).

3. The described starting approach leads to spin excitations without damping, being the mean-field realization of SST. Nevertheless, at this stage it is possible to trace the evolution of the ground state with the frustration increase from SST-Neel phase to spin liquid and further to SST-Stripe phase \([7, 10]\).
But, as it was shown in [8, 10], the damping of spin excitations is qualitatively important, even if it is introduced in the semiphenomenological way. The scheme, based on formally exact expression for the Green’s function [11], in the simplest case is reduced to the following Green’s function form (instead of (6)):

$$G^z(q, \omega) = \frac{F_q}{\omega^2 - \omega^2 q + i\omega\gamma}$$  \hspace{1cm} (10)$$

here only the imaginary part of the polarization operator is taken into account and it is written down as the trivial odd function of \(\omega\). Damping constant \(\gamma\) must be considered as an external parameter, defined by whatever additional arguments.

The rest of the self-consistent calculations procedure remains the same (of course, it must be recalculated at any fixed \(\gamma\)).

4. As it was mentioned above, in principle one can seek four types of self-consistent solutions. The first is the spin-liquid solution without long-range order \(c|_{r \to \infty} \to 0\). There are also two types of the "sole" long-range order solutions: with checkerboard \(c|_{r \to \infty} \sim e^{iQr} \sim (-1)^{n_x + n_y}\) and quantum stripe \(c|_{r \to \infty} \sim e^{iXr} \sim \frac{1}{2}([-1]^{n_x} + (-1)^{n_y}]\) correlators pattern. The fourth possible type of solution corresponds to two mutually penetrating long-range orders, when the spin-spin correlator at infinitely distant sites is the linear combination on checkerboard and stripe laws.

In the mean-field approximation with zero damping only three self-consistent solutions are realized in SST – SST-Neel for small frustration \(p\), spin-liquid for intermediate \(p\) and SST-Stripe for large frustration [7].

Fig.3 represents the energy for all types of self-consistent solutions (found in the present work) in the whole range of frustration parameter \(p\) for different values of damping parameter \(\gamma\). It is seen, that at small \(\gamma\) (\(\gamma \lesssim 0.3\)) the picture remains qualitatively unchanged: for different values of \(\gamma\) only three types of solutions are realizes.

With growing damping \(\gamma\) the points of transitions \(p^*_N\) (Neel$$\leftarrow$$Liquid) and \(p^*_S\) (Liquid$$\leftarrow$$Stripe) are shifted towards each other. It was shown in our previous work [8], that \(p\)-region of SL solution shrinks from the left side with the increase of \(\gamma\), i.e. the value \(p^*_N\) increases. Current results show, that the same is true for the right side of SL region, corresponding to SL$$\leftarrow$$Stripe transition.

But at \(\gamma \gtrsim 0.3\) for intermediate frustrations \(p \approx 0.3\) there appears another self-consistent solution – with two coexisting long-range orders. For \(0.3 \lesssim \gamma \lesssim 0.6\) this solution is metastable in the whole region of its existence and is disconnected by energy with the other solutions.

At \(\gamma \gtrsim 0.6\) this biordered solution is energetically connected with the SL one for \(p \lesssim 0.3\) and with stripe state for \(p \gtrsim 0.3\), in the intermediate interval it remains metastable. This is clearly seen from Fig.4, where for \(\gamma = 0.65\) the energies of all four solutions – SST-Neel, SST-Stripe, SL and biordered are depicted. The corresponding condensates for long-range ordered solutions are also shown.

Note that the value \(\gamma \sim 0.6\) can be considered as absolutely realistic [12, 13].

As it is seen from Figs.3–4, three states of different types (SST-Neel, SL and biordered) at \(\gamma \gtrsim 0.5\) are degenerate at the quantum transition point \(p^{OPT} \approx 0.28\).
Thus we come to a conclusion, that in the maximally frustrated region quantum fluctuations in addition to usually discussed states (checkerboard, SL and other mentioned above states) can select the exotic state with two long-range orders.

Let us mention, that in the biordered state at $p \gtrsim p_{\text{OPT}}$ with decrease of $p$ the checkerboard condensate increases and the stripe condensate rapidly decreases.

The typical spin excitations spectrum $\omega_q$ for this state is presented in Fig.5. The spectrum is gapless at points $\mathbf{X}$ and $\mathbf{Q}$.

As it was noted above for intermediate damping $0.3 \lesssim \gamma \lesssim 0.6$ the biordered solution is disconnected by energy with other ones (see Fig.3, curves for $\gamma = 0.35$ and $\gamma = 0.45$). To reveal the states which could be energetically connected with the biordered state, one must examine other candidates, for example the helicoidal solution with $\mathbf{q}^\nu_0 = (q, \pi), (\pi, q)$. Its semiclassical prototype is the helicoidal state, which is realized in $J_1 - J_2 - J_3$ Heisenberg model $[14]$. Nevertheless this speculation is a matter of further study.

In conclusion, we have found that in the frames of self-consistent spherically symmetric approach for the 2D frustrated Heisenberg model at $T = 0$ the unconventional state with two coexisting long-range orders can appear near the point of quantum phase transition $p_{\text{OPT}} \approx 0.28$ at sufficiently large damping of spin excitations.

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Figure 1: Commonly considered states for 2D Heisenberg model. Upper left – semiclassical Neel checkerboard state, upper right – semiclassical stripe state, thick arrow implies the transition with the frustration increase. Lower left – columnar VBC, lower right – plaquette VBC.

Figure 2: a) Nearest neighbour valence bond spin-liquid state. b) Arbitrary range valence bond spin-liquid state. The oriented bond between two sites $i$ and $j$ stands for singlet valence bond $(1/\sqrt{2})(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)$. 
Figure 3: The energy for all found types of self-consistent solutions for $0 \leq p \leq 1$ and different values of damping $\gamma$. Solid lines on the left correspond to SST-Neel solutions, solid lines on the right – SST-Stripe, intermediate dotted lines are SL solutions, small solid curves above SL at $p \sim 0.3$ correspond to biordered solution. The ordinate axis scale fits the curves with $\gamma = 0.001$, other lines are downshifted by $0.2\gamma$. 
Figure 4: The energy of SST-Neel, SL, biordered and SST-Stripe states in the vicinity of quantum phase transition for damping $\gamma = 0.65$.

The upper graphs show the condensates for the LRO solutions. For checkerboard LRO $c_{|r|\rightarrow\infty} \sim C^N_0(-1)^{n_x+n_y}$, for stripe LRO $c_{|r|\rightarrow\infty} \sim C^S_0(1/2)[(-1)^{n_x} + (-1)^{n_y}]$. Solid lines are for the SST-Neel (left) and SST-Stripe (right) states. The dashed and dashed-dotted curves are checkerboard and stripe condensates for the biordered state.
Figure 5: Spin excitations spectrum $\omega_q$ for the state with two coexisting long-range orders. Frustration and damping parameters are $p = 0.285$ and $\gamma = 0.65$. The spectrum is gapless at points $X$ and $Q$. 