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THE DISAPPEARANCE OF TWO-DIMENSIONAL LONG RANGE ORDER IN THE HEISENBERG MODEL WITH COMPETING INTERACTIONS

A. F. BARABANOV, L. A. MAKSIMOV, O. A. STARYKH
Institute for High Pressure Physics, 142092, Troitsk, Moscow Region, USSR

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In the frustrated Heisenberg model with first (J_1) and second (J_2) nearest neighbours interactions on a square lattice the transition from the long range order state (LROS) to spin liquid state (SLS) is found at $\alpha = J_1/J_2 \cong 0.25$. SLS is characterized by the gap in spin excitation spectrum at $T = 0$ and, hence, by exponential decay of spin correlation function at large distance. As a result, correlation length is temperature independent in SLS in accordance with neutron experiments on doped La_2CuO_4.

1. Introduction

The behavior of the magnetic subsystem of undoped La_2CuO_4 is well described by the two-dimensional (2D) antiferromagnetic (AFM) $S = \frac{1}{2}$ Heisenberg model with interaction between nearest spins on the square lattice.[1,2] Experiments show that doping leads to so-called spin-liquid state (SLS).[1] As is known AFM Heisenberg model is equivalent to the Hubbard model in the strong coupling limit $U \gg t$ (U — on-site repulsion, t — kinetic energy) and at half-filled bands. On the other hand, hole doping causes frustration in spin subsystem, i.e. interaction with next-nearest-neighbours.[3] So one may expect the manifestation of spin-liquid features in the 2D AFM frustrated Heisenberg model, for example, the disappearance of long range order (LRO) at $T = 0$.

In this paper we consider 2D model with AFM interactions between first J_1 and second $J_2 = \alpha J_1$ neighbours (NN) on the square lattice ($J_1 - J_2$ model). This model differs from another one, where regularly located interacting Cu spins have additional interaction with randomly distributed localized oxygen hole spins.[4] That model describes the disappearance of the Neél order in the dielectric phase while $J_1 - J_2$ model with uniform frustration describes the influence of delocalized holes (i.e. metallic phase).

Let's note some possible states in the model at $T = 0$:

1) usual Neél-like state with two or more (depending on α) sublattices and with

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different nonzero $\langle S_i^z \rangle$ on each sublattice.[5] We mention that to stabilize this state at nonzero temperature it is necessary to take into account anisotropy of interactions or small exchange between planes.

2) long range order state (LROS): $\langle S_i^z \rangle = 0$, $m_0 \neq 0$[6,7]

3) spin-liquid state (SLS): $\langle S_i^z \rangle = 0$, $m_0 = 0$.

LROS is characterized by the nonzero value of the effective spin (or sublattice magnetization) m_0, where

$$m_0^2 = \lim_{r \to \infty} (-1)^r \sum_{\mu} K_r^{\mu\mu} , \qquad K_r^{\mu\nu} = \langle S_i^{\mu} S_{i+r}^{\nu} \rangle . \tag{1}$$

Moreover there are two possible LRO states: with spherical symmetry ($K_r^{\mu\mu}$ is independent of μ)[6] and anisotropic one ($K_r^{\mu\mu}$ depends on μ).[7] As is known from the Mermin-Wagner theorem LRO is possible only at $T = 0$.[8] At $T \neq 0$ there are macroscopic correlation length $\xi \sim \exp(\text{const} \cdot T^{-1})$ and exponentially small gap $\Delta \sim \xi^{-1}$ in the spin excitation spectrum.[6,7,9]

As to SLS it is expected that it is realized at $\alpha > \alpha_0$, where α_0 is some critical value. In Refs. 3,10 by using Jastrow variational wave function it was found that at $\alpha > 0.24$ SLS gains energy in comparison to LROS, but the transition from LROS to SLS is the first order one. Exact diagonalization study of 4×4 cluster indicate the nonstability of LROS at $\alpha \cong 0.6$.[11] Using modified spin-wave theory[7] to the case $\alpha \neq 0$ in Ref. 12 the coexistence of two different LRO phases with small values m_0 at $\alpha \cong 0.6$ was shown, this supports the possibility of SLS. It is worthwhile mentioning that on the triangular lattice SLS is close to the ground state and has nonzero gap in the spin excitation spectrum at $T = 0$.[13]

In this paper by means of a block method[14] we construct isotropic singlet ground state and found three degenerate spin wave branches which describe singlet-triplet block excitations. It will be shown that at small α the system possesses LROS and m_0 is in good agreement with numerical results at $\alpha = 0$. As α increases m_0 decreases and at $\alpha \cong 0.25$ there is a second order phase transition from LROS to SLS which results in the opening of the gap in spin excitation spectrum at $T = 0$. The transition to SLS allows us to explain the experimentally observed temperature independent spin correlation length in doped La_2CuO_4.

2. The Model and Equation of Motion

The Hamiltonian of the model under consideration is

$$H = J_1 \sum_{\langle i,j \rangle} S_i S_j + J_2 \sum_{(i,j)} S_i S_j \tag{2}$$

$\langle i,j \rangle$, (i,j) — denotes links with first and second NN on the square lattice (lattice spacing a), in the following $J_1 = 1$. To take into account short-range spin correlation in the zero approximation we based on the block method, developed

in Ref. 14. The procedure is as follows: let us divide the square lattice into four-spins square blocks (so that block lattice is also square, block lattice spacing is $g = 2a$; see Fig. 1) and find all block eigenstates. The complete set of eigenstates for the plaquette of four spins, interacting in accordance with (2), consists of 16 states — their full description is given in Appendix A. From this complete set we select four low-lying energy block states: singlet φ and triplet $\psi_m, m = \mp 1, 0$. Then we project the Hamiltonian (2) to the selected subspace $D = \langle \varphi, \psi_m \rangle$. The complete form of the projected Hamiltonian is derived in Appendix B. Omitting the "higher orders in ψ_m" terms, which describes the processes $|m_R\, m_{R'}\rangle \to |m'_R\, m''_{R'}\rangle$ and $|m_R\, \varphi_{R'}\rangle \to |m'_R\, m''_{R'}\rangle$ the resulting Hamiltonian takes the form ($|m\rangle \equiv |\psi_m\rangle$)

$$H = H_0 + T_g + T_b\,, \qquad H_0 = \varepsilon_\varphi N + \sum_R \sum_m e Z_R^{mm}$$

$$T_g = \frac{1}{2} V_g \sum_{R,\,g} \sum_m \{(-1)^m [Z_R^{m\varphi} Z_{R+g}^{\bar{m}\varphi} + \text{h.c.}] + 2 Z_R^{m\varphi} Z_{R+g}^{\varphi m}\} \tag{3}$$

$$V_g = -\frac{1}{3}(1 - \alpha)\,, \qquad V_b = \frac{1}{6}\alpha\,, \qquad e = \varepsilon_\psi - \varepsilon_\varphi$$

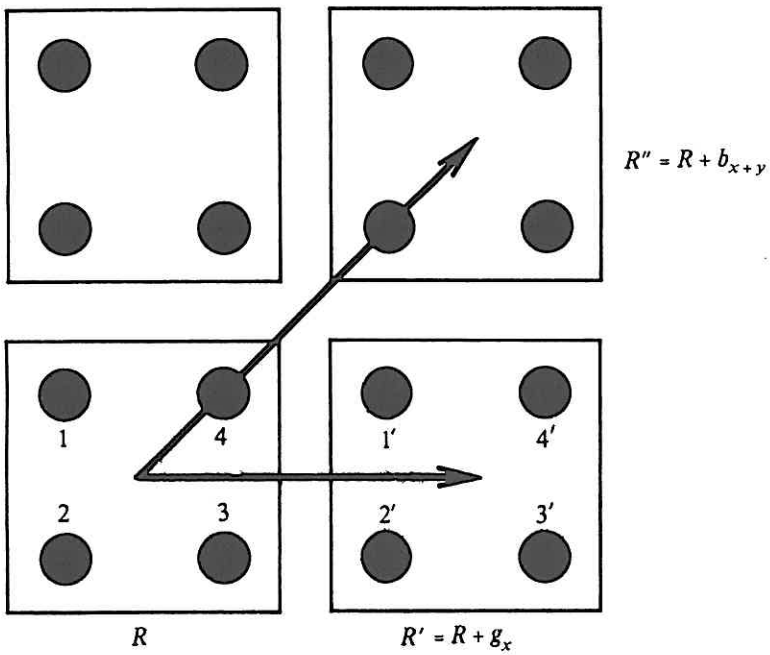


Fig. 1. Block covering of the lattice.

where **R**—block vector index, **g(b)** — vectors of the first (second) NN for the block lattice, $Z_R^{\lambda\mu} = |\lambda_R\rangle\langle\mu_R|$ — projection operator for block **R** states. One may obtain T_b from T_g by substituting vector **g** by **b**.

To clarify block approach let's consider for the moment the Hartree-type variational function, which one may construct from states φ and ψ_m, for simplicity $\alpha = 0$. The simplest variational function is the singlet's product over all block, $\Omega_s = \Pi_R \varphi_R$. As seen from (3) this state represent noninteracting singlets, nevertheless the energy per site $\varepsilon_s = -0.5$ is equal to the classical Neél energy. Note that $\langle\Omega_s|S_i^z|\Omega_s\rangle = 0$, $m_0 = 0$ and according to the classification in the Introduction Ω_s is SLS and by construction it is close to the short range RVB state.[15] At the next step it is natural to take into account block triplet states $\Omega_{st} = \Pi_R(A\varphi_R + \Sigma_m B_m \psi_{m,R})$, here $A, B_m (m = \mp 1, 0)$ are variational parameters with normalization condition $A^2 + \Sigma_m B_m^2 = 1$. Minimum energy is achieved when $B_{+1} = -B_{-1}$. This condition reflects the trial function symmetry with respect to the spin space rotations. As a result the variational procedure for Ω_{st} gives $\varepsilon_{st} = -0.565$ and $B_0^2 + 2B_{+1}^2 = \frac{5}{16}$.[16] This state is characterized by $\langle S_i^z\rangle = (-1)^i 0.38$ and corresponds to the Neél-type state 1) (note that here and elsewhere $i, j = 1,2,3,4$ runs over four block sites, **R** denotes block vector coordinate). The deviation of $|\langle S_i^z\rangle|$ from $\frac{1}{2}$ represents the quantum fluctuations in the variational function Ω_{st}. It is possible to construct block linear spin waves in this Neél state and to obtain $\varepsilon_{st} = -0.584$ which is close to the energy given in the mean-field approximation for the cluster approach.[17] Thus, the obtained energy ε_{st} is higher than the usual site spin waves value (which agrees with numerical results) $\varepsilon_{spinwave} = -0.66$. Moreover this variational function approach does not permit to generalize the theory for $T \neq 0$ (as well as the state 1), see Introduction.

In contrast to the Hartree state Ω_{st} we shall construct the state which contains coherent singlet pairs formed by the triplet states of the neighbouring blocks. In this sense our approach is close to the Schwinger boson one.[6]

One-particle excitations of the Hamiltonian (3) are described by the block projection operators $Z_k^{m\varphi}$, k — quasi-momentum. In order to find spin excitation spectrum ω_k and spin correlation we introduce the following averages and retarded Green functions G_k, $\tilde{G}_k$:

$$
\begin{aligned}
&P_\varphi = \langle Z_R^{\varphi\varphi}\rangle\,, \qquad P_\psi = \langle Z_R^{mm}\rangle\,, \qquad Q = P_\varphi - P_\psi \\
&B_k = (-1)^m \langle Z_k^{m\varphi} Z_{-k}^{-m\varphi}\rangle\,, \qquad C_k = \langle Z_k^{m\varphi} Z_k^{\varphi m}\rangle \\
&B_r = (-1)^m \langle Z_R^{m\varphi} Z_{R+r}^{-m\varphi}\rangle = N^{-1}\sum_k B_k \exp(i\mathbf{kr})\,, \qquad C_r = \langle Z_R^{m\varphi} Z_{R+r}^{\varphi m}\rangle \\
&G_k^m = \langle Z_k^{m\varphi} | Z_k^{\varphi m}\rangle\,, \qquad \tilde{G}_k^m = \langle Z_{-k}^{\varphi,-m} | Z_k^{\varphi m}\rangle\,.
\end{aligned}
\tag{4}
$$

We take B_r and C_r independent of m due to isotropy of the Hamiltonian, besides the anisotropic case is more difficult to calculate.

At the beginning let use construct the equation of motion for $G^{+1}_{R,R'} = \langle Z_R^{+1,\varphi} | Z_{R'}^{\varphi,+1} \rangle \equiv \langle Z_{\mathbf{R}}^{+1,\varphi} | \rangle$ with Hamiltonian $H_g = H_0 + T_g$

$$
\begin{aligned}
(\omega - e)\langle Z_R^{\varphi,1} | \rangle = {} & \delta_{R,R'} \langle Z_R^{\varphi\varphi} - Z_R^{11} \rangle - V_g \langle (Z_R^{\varphi\varphi} - Z_R^{11}) \sum_g (Z_{R+g}^{\bar{1}\varphi} - Z_{R+g}^{\varphi,1}) | \rangle \\
& + V_g \langle Z_R{}^{-1,1} \sum_g (Z_{R+g}^{1\varphi} - Z_{R+g}^{\varphi,-1}) | \rangle \\
& - V_g \langle Z_R^{0,1} \sum_g (Z_{R+g}^{0,\varphi} + Z_{R-g}^{\varphi,0}) | \rangle \ . \qquad (5)
\end{aligned}
$$

To get the close system for functions G^{+1}, $\tilde{G}^{+1}$ we exploit the following decoupling scheme using averages from (4)

$$
\begin{aligned}
\langle (Z_R^{\varphi\varphi} - Z_R^{11}) \sum_g (Z_{R+g}^{\bar{1},\varphi} - Z_{R+g}^{\varphi,1}) | \rangle &= Q \sum_g (\langle Z_{R+g}^{\bar{1},\varphi} | \rangle - \langle Z_{R+g}^{\varphi,1} | \rangle) \\
&= Q \sum_g (\tilde{G}^{+1}_{R+g,R'} - G^{+1}_{R+g,R'}) \\
\langle (Z_R^{\bar{1},1} \sum_g (Z_{R+g}^{1,\varphi} - Z_{R+g}^{\varphi,-1}) | \rangle &= \langle Z_R^{\bar{1},\varphi} Z_R^{\varphi,1} \sum_g (Z_{R+g}^{1,\varphi} - Z_{R+g}^{\varphi,-1}) | \rangle \\
&= \sum_g (\langle Z_R^{\bar{1},\varphi} Z_{R+g}^{1,\varphi} \rangle - \langle Z_R^{\bar{1},\varphi} Z_{R+g}^{\varphi,-1} \rangle) \langle Z_R^{\varphi,1} | \rangle \\
&= -4(B_g + C_g) G^{+1}_{R,R'} \\
\langle Z_R^{0,1} \sum_g (Z_{R+g}^{0,\varphi} + Z_{R+g}^{\varphi,0}) | \rangle &= \langle Z_R^{0,\varphi} Z_R^{\varphi,1} \sum_g (Z_{R+g}^{0,\varphi} + Z_{R+g}^{\varphi,0}) | \rangle \\
&= \sum_g (\langle Z_R^{0,\varphi} Z_{R+g}^{0,\varphi} \rangle + \langle Z_R^{0,\varphi} Z_{R+g}^{\varphi,0} \rangle) \langle Z_R^{\varphi,1} | \rangle \\
&= 4(B_g + C_g) G^{+1}_{R,R'} \ . \qquad (6)
\end{aligned}
$$

Then introducing $F_r = B_r + C_r$ we have for Green function $G^{+1}_{R,R'}$

$$
(\omega - e + 8V_g F_g) G^{+1}_{R,R'} = -V_g Q \sum_g (\tilde{G}^{+1}_{R,R'} - G^{+1}_{r+g,R'}) + Q\delta_{R,R'} \ . \qquad (7)
$$

The extension of (7) to the Hamiltonian $T_g + T_b$ is obvious.

As a result in the momentum representation we have

$$
\begin{aligned}
& (\omega - e + 8v_g F_g + 8v_b F_b - 4Qv_g\gamma_g - 4Qv_b\gamma_b) \\
& \quad \times G_k^{+1} = Q - 4Q(v_g\gamma_g + v_b\gamma_b)\tilde{G}_k^{+1} \\
& \gamma_g = \frac{1}{2}(\cos k_x g + \cos k_y g) \ , \qquad \gamma_b = \cos k_x g \cos k_y g \ . \qquad (8)
\end{aligned}
$$

The described procedure for $\tilde{G}^{+1}$ gives

$$(\omega + e - 8v_gF_g - 8v_bF_b + 4Qv_g\gamma_g + 4Qv_b\gamma_b)\tilde{G}_k^{+1} = 4Q(v_g\gamma_g + v_b\gamma_b)G_k^{+1} . \qquad (9)$$

It is easy to get the analogous equations for Green functions with $m = 0, -1$. After Eqs. (8) and (9) we have

$$G_k^m = Q(\omega + e_k)(\omega^2 - \omega_k^2)^{-1} , \quad \tilde{G}_k^m = (-1)^{m+1}Qw_k(\omega^2 - \omega_k^2)^{-1}$$

$$e_k = e - 8v_gF_g - 8v_bF_b + 4Q(v_g\gamma_g + v_b\gamma_b) , \quad w_k = 4Q(v_gF_g + v_bF_b) \qquad (10)$$

$$\omega_k^2 = (e_k - w_k)(e_k + w_k) .$$

Note that spin excitation spectrum ω_k is three-fold degenerate on m. It is obvious that accounting of twelve high-energy block states will result in high-energy spin modes separated from ω_k by the gap of order 1.

3. Self-consistent System and Correlation Function

Using the Green functions G_k, $\tilde{G}_k$ we can construct the self-consistent equations for averages (4), for example

$$\begin{aligned} P_\psi &= \langle Z_R^{11} \rangle \\ &= -\frac{1}{\Pi}\sum_k \int d\omega v(\omega)\mathrm{Im}G_k(\omega + i0) \\ &= -\frac{1}{2}Q + N^{-1}\sum_k Qe_k\omega_k^{-1}\left(v_k + \frac{1}{2}\right) \end{aligned}$$

$$v_k = v(\omega_k) = (\exp(\beta\omega_k) - 1)^{-1} , \qquad \beta \equiv T^{-1} .$$

The complete system for P_φ, P_ψ, F_g, F_b (we should remind ourselves that ω_k, Q and F_r are expressed over these quantities) has the form

$$P_\psi = -\frac{1}{2}Q + N^{-1}\sum_k Qe_k\omega_k^{-1}\left(v_k + \frac{1}{2}\right)$$

$$F_g = Q(e - 8v_gF_g - 8v_bF_b)N^{-1}\sum_k \gamma_g\omega_k^{-1}\left(v_k + \frac{1}{2}\right) \qquad (11)$$

$$F_b = Q(e - 8v_gF_g - 8v_bF_b)N^{-1}\sum_k \gamma_b\omega_k^{-1}\left(v_k + \frac{1}{2}\right)$$

$$P_\varphi + 3P_\psi = 1 .$$

Here Σ_k means the sum over the first Brillouin zone for block lattice. The last equation in (11) results from the completeness of the basis states in the chosen subspace D.

System (11) is solved for $T \to 0$. Depending on the α value there are two possible physically different solutions. For $\alpha < \alpha_0 = 0.253$ the spectrum ω_k has a gap Δ which is exponentially small on temperature $\Delta \sim T \exp\left(\frac{-\text{const.}}{T}\right)$. The presence of such a gap is necessary for fulfilling the constraint condition (the last equation in (11)) at $\alpha < \alpha_0$.[6] In this case one must take into account a macroscopic part in the summations with Bose-function ν_k at $k = 0$, analogous to the case of Bose-Einstein condensation.[18] As it was shown in Refs. 6, 18 the presence of such a contribution corresponds to the long range order in the system. It will be shown that frustration (interaction J_2) leads to decrease of the "condensate" contribution at $k = 0$ (see also Ref. 12). In contrast, for $\alpha > \alpha_0$ the solution gives the temperature independent gap for the spectrum and, hence, SLS is realized.

To make our description clear let us analyse spin correlation function in detail. First of all it is necessary to express site spin operators by the block projection operators

$$S^z_{R,i} = (-1)^{i+1} 6^{-1/2} (Z^{\varphi,0}_R + Z^{0,\varphi}_R) + \frac{1}{4} S^z_R$$

$$S^+_{R,i} = (-1)^{i+1} 3^{-1/2} (Z^{\varphi,-1}_R - Z^{1,\varphi}_R) + \frac{1}{4} S^+_R \ , \quad S^-_{R,i} = (S^+_{R,i})^+ \tag{12}$$

$$S^z_R = Z^{11}_R - Z^{-1,-1}_R \ , \quad S^+_R = 2^{1/2} (Z^{1,0}_R + Z^{0,-1}_R) \ , \quad S^-_R = 2^{1/2} (Z^{0,1}_R + Z^{-1,0}_R)$$

here $S^\mu_{R,i}$ μ-component of the site i spin operator ($i = 1,2,3,4$) in block **R**, as usual $S^\pm_{R,i} = S^x_{R,i} \pm i S^y_{R,i}$; S_R — block **R** spin operator, which, as seen, is fully determined by the block states ψ_m. Straightforward calculations gives

$$K^{zz}_{r,ij} \equiv \langle S^z_{R,i} S^z_{R+r,j} \rangle = (-1)^{i+j} \frac{1}{3} (C_r + B_r) + \frac{1}{8} (C_r^2 - B_r^2) \ . \tag{13}$$

The second term in (13) originates from the spin interaction between triplet block states. We caution the reader that formula (13) is correct for spins belonging to the different blocks, correlators for spins in one block must be calculated by diagonal block projection operators. The isotropy of correlation function $K^{xx}_{r,ij} = K^{yy}_{r,ij} = K^{zz}_{r,ij}$ may be checked by direct test.

In LROS $K_{r,ij} = \Sigma_\mu K^{\mu\mu}_{r,ij}$ has the asymptotic ($T \ll 1$)

$$K_{r,ij} = (-1)^{i+j} \begin{cases} m_0^2(\alpha) + \dfrac{3}{8\pi(1-2\alpha)r} \ , & g \ll r \ll \xi \\ \dfrac{3T}{2^{3/2}\pi(1-2\alpha)} (\xi/r)^{1/2} \exp(-r/\xi) \end{cases} \tag{14}$$

where correlation length ξ is

$$\xi = \frac{c}{T}\exp(2\pi\vartheta(\alpha)T^{-1}), \qquad \vartheta(\alpha) = \frac{2}{3}(1 - 2\alpha)m_0^2(\alpha) \tag{15}$$

$$c^2 = \frac{2}{3}(1 - 2\alpha)Q\left(e + \frac{8}{3}(1 - 2\alpha)F_g - \frac{4}{3}\alpha F_b\right)$$

c — spin wave velocity: $\omega_k = ck$, $k \to 0$ ($T = 0$). From (14) at $T = 0$ $\lim_{r\to\infty} K_{r,ij} = (-1)^{i+j}m_0^2(\alpha)$, so effective spin $m_0(\alpha)$ is the order parameter of the problem under consideration. The m_0 and ϑ dependence on α is presented in Fig. 2 and it may be approximated by the following expressions

$$m_0(\alpha) = m_0(0)(1 - 2\alpha_0^{-1}\alpha)^{1/2}(1 - 2\alpha)^{-1/2}, \qquad m_0(0) = 0.356 \tag{16}$$

$$\vartheta(\alpha) = \frac{1}{6}(0.1693 - 0.67\alpha)$$

so $m_0(\alpha)$ has a critical index $\frac{1}{2}$. The value $m_0(0)$ is in good agreement with numerical calculations: 0.34,[19] 0.33.[20] The linear ϑ dependence on α is also known from usual spin-wave approach.[21] The exponential decay of $K_{r,ij}$ at nonzero temperature confirms the fulfilling of the Mermin-Wagner theorem.

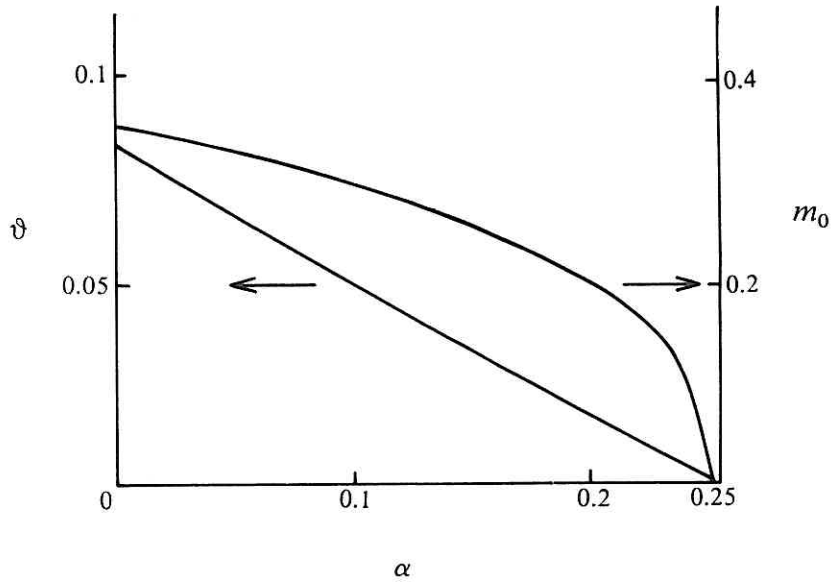


Fig. 2. Effective spin m_0 and ϑ dependence on $\alpha = J_1/J_2$ in LROS.

SLS ($\alpha > \alpha_0$) is characterized by the following properties at $T = 0$

$$\omega_{k\to 0} = (\Delta^2 + c^2k^2)^{1/2}, \qquad \Delta = c\eta,$$

$$K_{r,ij} = (-1)^{i+j} \frac{3c}{8\pi(1-2\alpha)} r^{-1} \exp(-r/\zeta) \tag{17}$$

$$+ \frac{3}{8}\{\frac{1}{4\pi} Q\eta r^{-1} \exp(-r/\zeta)\}^2, \quad r \gg \zeta = \eta^{-1}.$$

As mentioned in the Introduction we have for SLS $\lim_{r\to\infty} K_{r,ij} = 0$ and $\omega(k = 0) = \Delta$ in accordance with the results of Ref. 13. Moreover, as seen from Fig. 3, ζ decreases with α increase and at $\alpha \geq 0.4$ ζ is about several lattice spacing as well in Ref.13. Figure 3 demonstrates the linear dependence Δ on α: $\Delta \simeq 1.47(\alpha - \alpha_0)$. It is difficult to obtain K_r in analytical form for $r < \zeta$, but it is obvious that at this region the exponential decay must be changed to power one. The important moment is the temperature independence of ζ, this independence was demonstrated in the neutron experiments.[1] Unusual behavior of $K_{r,ij}$ is seen from (17): there is a rapidly decaying ferromagnetic correlations (second term) together with usual AFM correlations (first term). This FM correlation, as mentioned above, arise from the interaction of two blocks both in triplet states. We want to emphasize that $\langle S_{R,i}\rangle = 0$, as seen from (11), for any α.

4. Discussion and Conclusion

Divergency of the correlation length at $T \to 0$ for $\alpha < \alpha_0$ and its finite value for $\alpha > \alpha_0$ may be interpreted as LROS–SLS transition. Either m_0 or Δ (critical index

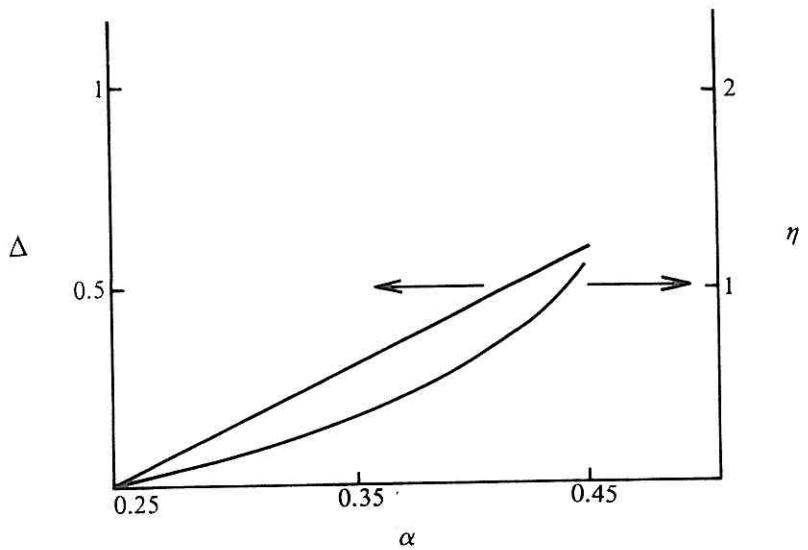


Fig. 3. Inverse correlation length η (in units $g^{-1} = (2a)^{-1}$) and gap Δ dependence on α in SLS.

1) serve as order parameter, hence it is second order phase transition. Note that any choice gives nonlocal order parameter.

To clarify the nature of constructed state one may compare it with "singlet" Ω_s state. Despite the small energy difference $\Delta\varepsilon\cong 0.01$ of SLS and Ω_s at $\alpha \to \frac{1}{2}$ (see Fig. 4) these states are essentially distinct. For SLS (and moreover for LROS) the spin wave dispersion is determined by the condition $P_\psi \neq 0$, consequently all obtained results are due to the presence of triplet fluctuations in the considered system. Spin excitations are submitted by three degenerate waves with different m-projections analogous to the one-dimensional AFM model.

Based on the connection between J_2 and hole concentration[3] δ the reasonable choice of parameters $U/t = 5$ gives that LROS–SLS transition takes place at $\delta_0 \cong 0.07$. Of course, the interaction with third next-neighbours may decrease δ_0 up to experimentally observed 2–3% in La_2CuO_4.

In conclusion, we have presented the theory of spin excitations in the frustrated Heisenberg model on the square lattice. The theory describes the

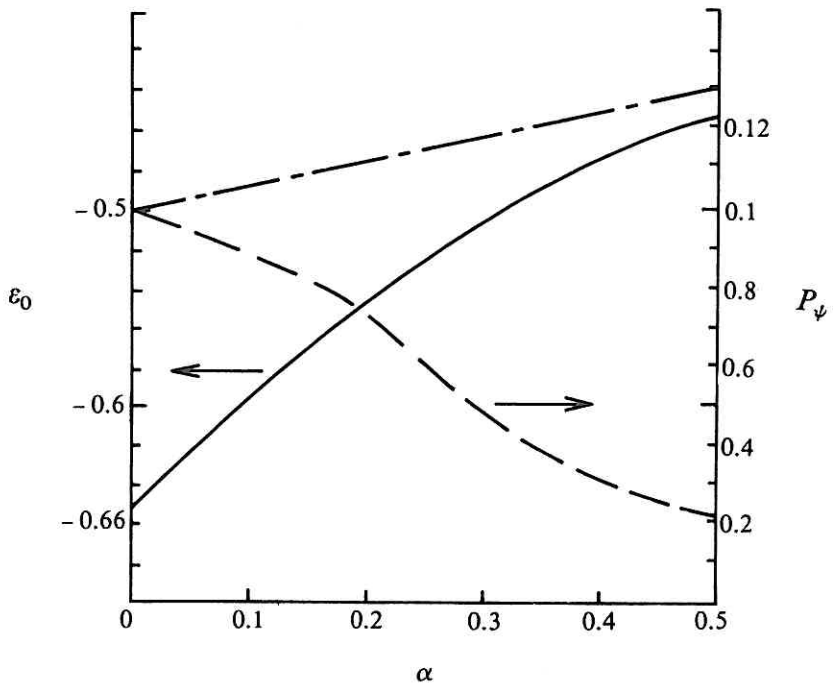


Fig. 4. Ground state energy ε_0 (solid line) and number of triplet states P_ψ (dashed line) dependence on α. By the dashed-dotted line $\varepsilon_\varphi(\alpha)$–$\Omega_s$ state energy.

second order phase transition from the "spin crystal state" (LROS) to the "spin liquid state" (SLS). The transition is accompanied by the lack of the long range order and by appearance of the gap in the spin excitation spectrum of SLS. This is in agreement with arguments of Ref. 13. The energy per site $\varepsilon_0 = -0.655$ and effective spin $m_0(0) = 0.356$ at $\alpha = 0$ are close to the numerical results.[19,20] For $\alpha < \alpha_0$ the T and α dependence of the correlation length agree with recent theories[2,6,7] and experiment.[1] The temperature independence of the correlation length at $\alpha < \alpha_0$[1] is naturally explained in our approach.

Appendix A

The space $\{X_s\}$ of sixteen square four spin block eigenstates is convenient to classify according to irreducible symmetry group representations of the square and by eigenvalues of operator S and its projection S^z. Let's introduce, as shown in (A1), next operators: $\hat{C}$ — rotation by $\pi/2$, $\hat{\sigma}_x(\hat{\sigma}_y)$ — reflection by OX (OY) axis, $\hat{\vartheta}$ — reflection by block diagonal, $\hat{T}$ — spin inversion.

$$\hat{C}\begin{vmatrix}\sigma_1 & \sigma_4\\ \sigma_2 & \sigma_3\end{vmatrix} = \begin{vmatrix}\sigma_4 & \sigma_3\\ \sigma_1 & \sigma_2\end{vmatrix}, \quad \hat{\sigma}_x\begin{vmatrix}\sigma_1 & \sigma_4\\ \sigma_2 & \sigma_3\end{vmatrix} = \begin{vmatrix}\sigma_2 & \sigma_3\\ \sigma_1 & \sigma_4\end{vmatrix},$$

$$\hat{\sigma}_y\begin{vmatrix}\sigma_1 & \sigma_4\\ \sigma_2 & \sigma_3\end{vmatrix} = \begin{vmatrix}\sigma_4 & \sigma_1\\ \sigma_3 & \sigma_2\end{vmatrix}, \quad \hat{\vartheta}_y\begin{vmatrix}\sigma_1 & \sigma_4\\ \sigma_2 & \sigma_3\end{vmatrix} = \begin{vmatrix}\sigma_1 & \sigma_2\\ \sigma_4 & \sigma_3\end{vmatrix}, \tag{A1}$$

$$\hat{T}\begin{vmatrix}\sigma_1 & \sigma_4\\ \sigma_2 & \sigma_3\end{vmatrix} = \begin{vmatrix}\tilde{\sigma}_1 & \tilde{\sigma}_4\\ \tilde{\sigma}_2 & \tilde{\sigma}_3\end{vmatrix}$$

$\begin{vmatrix}\sigma_1 & \sigma_4\\ \sigma_2 & \sigma_3\end{vmatrix}$ denotes block states with site spin projection $\frac{1}{2}\sigma_i$, $\sigma_i \equiv \sigma_i = \pm 1$, $\tilde{\sigma}_i = -\sigma_i$, $i = 1,2,3,4$ — numerate the block sites.

The space $\{X_s\}$ consists of two one-dimensional singlets φ and $\varphi^{(1)}$, one one-dimensional triplet $\psi_m(m = 0, \pm 1)$, two two-dimensional triplets $Y_m^{(1)}$, $Y_m^{(2)}$ and one-dimensional quintet $M_l(l = 0, \pm 1, \pm 2)$. These states are transformed according to the Table (we also give energy and eigenvalues for one-dimensional representations).

Table

	$\hat{C}$	$\hat{\vartheta}'$	$\hat{\sigma}_x$	$\hat{T}$	S	S^z	ε
φ	+1	+1	+1	+1	0	0	$-2+0.5\alpha$
$\varphi^{(1)}$	−1	−1	+1	+1	0	0	-1.5α
ψ_m	−1	+1	−1	$-\psi_{-m}$	1	m	$-1+0.5\alpha$
$Y_m^{(1)}$	$Y_m^{(2)}$	$Y_m^{(1)}$	$Y_m^{(2)}$	$-Y_{-m}^{(1)}$	1	m	-0.5α
$Y_m^{(2)}$	$-Y_m^{(1)}$	$-Y_m^{(2)}$	$Y_m^{(1)}$	$-Y_m^{(2)}$	1	m	-0.5α
M_1	+1	+1	+1	M_{-1}	2	1	$1+0.5\alpha$

The explicit form of these states is

$$\varphi = 12^{-1/2}\left(\left|\begin{matrix}+&+\\-&-\end{matrix}\right| + \left|\begin{matrix}+&-\\+&-\end{matrix}\right| + \left|\begin{matrix}-&-\\+&+\end{matrix}\right| + \left|\begin{matrix}-&+\\-&+\end{matrix}\right| - 2\left\{ \left|\begin{matrix}+&-\\-&+\end{matrix}\right| + \left|\begin{matrix}-&+\\+&-\end{matrix}\right| \right\} \right) \tag{A2}$$

$$\psi_0 = 2^{-1/2}\left(\left|\begin{matrix}+&-\\-&+\end{matrix}\right| - \left|\begin{matrix}-&+\\+&-\end{matrix}\right| \right),$$

$$\psi_{+1} = -\frac{1}{2}\left(\left|\begin{matrix}+&+\\-&-\end{matrix}\right| - \left|\begin{matrix}+&-\\+&-\end{matrix}\right| + \left|\begin{matrix}-&-\\+&+\end{matrix}\right| - \left|\begin{matrix}-&+\\-&+\end{matrix}\right| \right), \quad \psi_{-1} = -\hat{T}\psi_{+1}$$

$$\varphi^{(1)} = \frac{1}{2}\left(\left|\begin{matrix}+&+\\-&-\end{matrix}\right| - \left|\begin{matrix}+&-\\+&-\end{matrix}\right| + \left|\begin{matrix}-&-\\+&+\end{matrix}\right| - \left|\begin{matrix}-&+\\-&+\end{matrix}\right| \right)$$

$$Y_0^{(1)} = \frac{1}{2}\left(\left|\begin{matrix}+&+\\-&-\end{matrix}\right| + \left|\begin{matrix}+&-\\+&-\end{matrix}\right| - \left|\begin{matrix}-&-\\+&+\end{matrix}\right| - \left|\begin{matrix}-&+\\-&+\end{matrix}\right| \right) \tag{A3}$$

$$Y_0^{(2)} = -\frac{1}{2}\left(\left|\begin{matrix}+&+\\-&-\end{matrix}\right| - \left|\begin{matrix}+&-\\+&-\end{matrix}\right| - \left|\begin{matrix}-&-\\+&+\end{matrix}\right| + \left|\begin{matrix}-&+\\-&+\end{matrix}\right| \right)$$

$$M_0 = 6^{-1/2}\left(\left|\begin{matrix}+&+\\-&-\end{matrix}\right| + \left|\begin{matrix}+&-\\+&-\end{matrix}\right| + \left|\begin{matrix}-&-\\+&+\end{matrix}\right| + \left|\begin{matrix}-&+\\-&+\end{matrix}\right| + \left|\begin{matrix}+&-\\-&+\end{matrix}\right| + \left|\begin{matrix}-&+\\+&-\end{matrix}\right| \right).$$

Functions $Y_m^{(1,2)}$, $M_1(m, l\neq 0)$ are constructed by raising (lowering) block spin operators $\Sigma_i\sigma_i^+$ ($\Sigma_i\sigma_i^-$) on the corresponding functions with $m, l = 0$.

Energy comparison in the Table shows that restriction of the $\{X_s\}$ by the subspace $D = \{\varphi, \psi_m\}$ is possible for $\alpha < \frac{1}{2}$. As to the state $\varphi^{(1)}$ (its energy became close to ε_φ, ε_ψ with α increase) we argue that the full Hamiltonian connect $\varphi^{(1)}$ with φ, ψ_m only through the higher lying block states, not belonging to D.

Appendix B

Here we describe how to project the Hamiltonian (2) on the subspace $D = \{\varphi, \psi_m\}$. Taking block covering of the plane H (2) is a sum of an intrablock H_{intra} and an interblock part H_{inter}. It is clear that term H_0 in (3) coincides with H_{intra} in the subspace D. In this subspace H_{inter} takes the form

$$\begin{aligned} H_{\text{inter}} &= \sum_{R,f} \sum_{\{\lambda,\mu\}\in D} |\lambda_R \mu_{R+f}\rangle\langle\lambda_R \mu_{R+f}| H_{\text{inter}} |\lambda'_R \mu'_{R+f}\rangle\langle\lambda'_R \mu'_{R+f}| \\ &= \sum_{R,f} \sum_{\{\lambda,\mu\}\in D} \langle\lambda_R \mu_{R+f} H_{\text{inter}} |\lambda'_R \mu'_{R+f}\rangle Z_R^{\lambda\lambda'} Z_{R+f}^{\mu\mu'} \end{aligned} \tag{B1}$$

$\mathbf{f} = \mathbf{g}(\mathbf{b})$ — vectors for the first (second) NN. So, it is necessary to know the matrix elements of H between pairs of different states on neighbouring blocks.

These matrix elements are calculated directly by using the explicit form for φ, ψ_m and their symmetry (Appendix A). As an example, we shall explain the calculation proportional to J_1 matrix elements of H_{inter}. These matrix elements link only first NN blocks $\mathbf{R}$ and $\mathbf{R}' = \mathbf{R} + \mathbf{g}$ and H_{inter} for them has the form $h = \mathbf{S}_4\mathbf{S}_{1'} + \mathbf{S}_3\mathbf{S}_{2'}$ ($4,3 \in \mathbf{R}; 1',2' \in \mathbf{R}$ — see Fig. 1.). By straightforward calculations one may check the following equalities

$$h\varphi_R\varphi_{R'} = \frac{1}{3}(\psi_{1,R}\psi_{-1,R'} - \psi_{0,R}\psi_{0,R'} + \psi_{-1,R}\psi_{1,R'})$$

$$h\varphi_R\psi_{m,R'} = -\frac{1}{3}\psi_{m,R}\psi_{R'}$$

$$h\psi_{1,R}\psi_{-1,R'} = \frac{1}{3}\varphi_R\varphi_{R'} + \frac{1}{8}(\psi_{0,R}\psi_{0,R'} - \psi_{1,R}\psi_{-1,R'})$$

$$h\psi_{\pm 1,R}\psi_{\pm 1,R'} = \frac{1}{8}\psi_{\pm 1,R}\psi_{\pm 1,R'}$$

$$h\psi_{\pm 1,R}\varphi_{0,R'} = \frac{1}{8}\psi_{0,R}\psi_{\pm 1,R'}$$

$$h\psi_{0,R}\psi_{0,R'} = -\frac{1}{3}\varphi_R\varphi_{R'} + \frac{1}{8}(\psi_{1,R}\psi_{-1,R'} + \psi_{-1,R}\psi_{1,R'}) \tag{B2}$$

which permit to find matrix elements for $\mathbf{f} = \mathbf{g}$ in (B1). Analogous procedure gives matrix elements for $\mathbf{f} = \mathbf{b}$.

As a result the projected Hamiltonian has the form

$$H = H_0 + T_g + T_b + W_g + W_b + U_b$$

$$H = H_0 + T_g + T_b\,, \qquad H_0 = \varepsilon_\varphi N + \sum_R \sum_m e Z_R^{mm}$$

$$T_g = \frac{1}{2} V_g \sum_{R,g} \sum_m \{(-1)^m [Z_R^{m\varphi} Z_{R+g}^{\bar{}\,m\varphi} + \text{h.c.}] + 2 Z_R^{m\varphi} Z_{R+g}^{\varphi m}\}$$

$$V_g = -\frac{1}{3}(1 - \alpha)\,, \qquad V_b = \frac{1}{6}\alpha\,, \qquad e = \varepsilon_\psi - \varepsilon_\varphi \tag{B3}$$

$$W_g = \frac{1}{8}(1 + \alpha)\frac{1}{2}\sum_{R,g} S_R S_{R+g}$$
$$= \frac{1}{8}(1 + \alpha)\frac{1}{2}\sum_{R,g} S^z_R S^z_{R+g} + \frac{1}{2}(S^+_R S^-_{R+g} + S^-_R S^+_{R+g})$$

$$W_b = \frac{1}{16}\frac{1}{2}\sum_{R,b} S_R S_{R+b}$$

$$U_b = -\frac{\alpha}{2\sqrt{6}}\frac{1}{2}\sum_R\sum_b d(\mathbf{b})\{Z^{\varphi,0}_R(Z^{-1,-1}_{R+b} - Z^{1,1}_{R+b}) + Z^{\varphi,1}_R(Z^{1,0}_{R+b} + Z^{0,-1}_{R+b}) - Z^{\varphi,-1}_R(Z^{-1,0}_{R+b} + Z^{0,1}_{R+b}) + \text{h.c.}\}\ .$$

Here $d(\mathbf{b}) = +1$ for $\mathbf{b} = \mathbf{g}_x + \mathbf{g}_y$; $-\mathbf{g}_x - \mathbf{g}_y$ and $d(\mathbf{b}) = -1$ for $\mathbf{b} = \mathbf{g}_x - \mathbf{g}_y$; $-\mathbf{g}_x + \mathbf{g}_y$, the operator S_R is the **R** block spin (see (12)).

In our consideration of the problem we omitted the terms W_g, W_b, U_b in Hamiltonian (B3) (see (3)). These terms describe the processes with three or four triplet states. Such processes lead to quadratic or the triplet number $P_\psi = \langle Z^{mm}_R \rangle$ corrections in the equations of motion for the Green functions. As P_ψ is small (Fig. 4) these corrections cannot change our results.

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Note added: After completion of this work we learned of the work[22] where "double spiral state" is found. The spin excitation spectrum of this state is characterized by the gap at $T = 0$, which is determined by the hole concentration. This confirms our results.

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