

Quantum Spin Liquid in the FCC Lattice

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Abstract—The properties of the spin system in the FCC lattice described by the Heisenberg model ($s = 1/2$) with antiferromagnetic interactions between the nearest neighbors were studied. It was shown within the framework of spin-wave theory that long-range antiferromagnetic order was absent because of frustration of exchange coupling and transverse quantum spin fluctuations. The system was in the quantum spin liquid state. A method for describing it within linear second-order theory with self-consistently calculated parameters was suggested. It was proved that the ground spin liquid state was singlet. The thermodynamic properties of the spin liquid in the whole temperature range and the character of spatial spin correlations, which had alternating signs and a finite correlation length, were determined. The theory was constructed based on the method of two-time Green temperature functions. © 2003 MAIK “Nauka/Interperiodica”.

1. INTRODUCTION: A CRITERION OF ANTIFERROMAGNETISM IN THE FCC LATTICE

A system of localized spins is described by the Heisenberg model with the Hamiltonian

$$H = -\frac{1}{2} \sum_{\mathbf{f}, \mathbf{R}} J(\mathbf{R}) \mathbf{s}_{\mathbf{f}} \cdot \mathbf{s}_{\mathbf{f}+\mathbf{R}}, \quad (1)$$

$$J(\mathbf{R}) = J(-\mathbf{R}), \quad J(0) = 0,$$

defined on an ideal lattice with periodic boundary conditions. Here, \mathbf{f} are the coordinates of lattice sites, $J(\mathbf{R})$ are the exchange integrals at intersite distance \mathbf{R} , and \mathbf{R} , $\mathbf{s}_{\mathbf{f}} = (s_{\mathbf{f}}^+, s_{\mathbf{f}}^-, s_{\mathbf{f}}^z)$ is the spin operator on site \mathbf{f} . For three-dimensional systems, Hamiltonian (1) is largely used to describe long-range magnetic order. The exact first-order equation of motion ($\hbar = 1$) is linearized (the Tyablikov splitting) as

$$i\dot{s}_{\mathbf{f}} \approx \sum_{\mathbf{R}} J(\mathbf{R}) (\langle s_{\mathbf{f}+\mathbf{R}}^z \rangle s_{\mathbf{f}}^+ - \langle s_{\mathbf{f}}^z \rangle s_{\mathbf{f}+\mathbf{R}}^+) \quad (2)$$

on the assumption that $\langle s_{\mathbf{f}}^z \rangle \neq 0$. Equation (2) is the base equation of spin-wave theory at various regular exchange $J(\mathbf{R})$ distributions and mean $\langle s_{\mathbf{f}}^z \rangle$ values. To describe collinear antiferromagnetic states, subsystems A ($N/2$ sites α with spins “upward,” N is the number of sites) and B ($N/2$ sites β with spins “downward”) are introduced. We then have $\langle s_{\alpha}^z \rangle = \bar{s}$, $s_{\beta}^z = -\bar{s}$, where $\bar{s} = \bar{s}(T)$ and T is the temperature in energy units.

Of special interest is the FCC lattice with exchange antiferromagnetic interactions between the nearest neighbors: $J(\Delta) = -J, J > 0$, where Δ are the vectors con-

necting $z_1 = z = 12$ nearest neighbors. There are four types of ordering in the FCC lattice [1]. For any of them, frustrated (energetically unfavorable) exchange J -couplings always arise. For instance, for antiferromagnetic order of the first type characterized by alternating ferromagnetic xy planes with spins upward and downward, that is, antiferromagnetically coupled planes, all four J -couplings in these planes are frustrated. The remaining eight (interplanar) antiferromagnetic couplings are, however, normal, and the effective molecular field is $\pm 4J\bar{s}$ (“plus” sign for spins upward and “minus” for spins downward). Stabilizing such an antiferromagnetic structure requires taking into account at least ferromagnetic exchange between next-nearest neighbors, $J(\mathbf{a}) = K, K > 0$, where \mathbf{a} are the vectors connecting $z_2 = 6$ next-nearest neighbors ($|\mathbf{a}| = a$ is the FCC lattice parameter, and $|\Delta| = a/\sqrt{2}$).

Lines [2, 3] showed that antiferromagnetic order could only exist at $K \neq 0$ in a quantum spin system with Hamiltonian (1) in the FCC lattice. This conclusion is valid for the first ($K > 0$) and third ($K < 0$) types of ordering. In any event, the $\bar{s} = \bar{s}(\lambda)$ order parameter and the $T_N(\lambda)$ Néel temperature are functions of the $\lambda = |K|/J$ ratio and vanish at $\lambda = 0$ ($K = 0$). Apart from frustrations, this phenomenon is related to the substantial role played by transverse quantum spin fluctuations, which, at $\lambda = 0$, destroy long-range antiferromagnetic order. Note that the antiferromagnetic state “survives” in the system of classical spins [4, 5].

The conclusion on the absence of antiferromagnetic order at $K = 0$ also follows from work [6]. The authors considered a primitive cubic cell with antiferromagnetic interactions J_1 and J_2 for the nearest and next-nearest neighbors, respectively ($s = 1/2$), and intro-

duced the $p = J_2/(J_1 + J_2)$ parameter. At $J_1 = 0$, we nearly have the FCC spin lattice, and antiferromagnetic order is absent in this limit ($p = 1$).

To summarize, it follows from [2, 3, 6] that long-range antiferromagnetic order is absent in the FCC lattice for quantum spins with antiferromagnetic exchange J only between the nearest neighbors. What is the state of such a system? Below, we suggest the concept of a spin liquid.

2. QUANTUM SPIN LIQUID

We continue our consideration of a system with Hamiltonian (1) and total spin operator \mathbf{S} taking into account antiferromagnetic exchange interactions J only between the nearest neighbors,

$$h = \frac{H}{zJ} = \frac{1}{2z} \sum_{\mathbf{f}, \Delta} \mathbf{s}_{\mathbf{f}} \cdot \mathbf{s}_{\mathbf{f}+\Delta}, \quad \mathbf{S} = \sum_{\mathbf{f}} \mathbf{s}_{\mathbf{f}}, \quad s = \frac{1}{2}. \quad (3)$$

In the absence of stabilizing factors, there is no antiferromagnetic FCC lattice state. Let us therefore analyze the spin system with dimensionless Hamiltonian (3) as a quantum spin liquid.

We define the spin liquid as a system without symmetry loss and without long-range magnetic order in which

(1) spin correlation functions are isotropic,

$$\begin{aligned} \frac{1}{N} \sum_{\mathbf{f}} \langle s_{\mathbf{f}}^x s_{\mathbf{f}+\mathbf{r}}^x \rangle &= \frac{1}{N} \sum_{\mathbf{f}} \langle s_{\mathbf{f}}^y s_{\mathbf{f}+\mathbf{r}}^y \rangle \\ &= \frac{1}{N} \sum_{\mathbf{f}} \langle s_{\mathbf{f}}^z s_{\mathbf{f}+\mathbf{r}}^z \rangle \equiv \frac{1}{4} K_r, \end{aligned} \quad (4)$$

and only depend on the modulus of distance $r = |\mathbf{r}|$; in addition, $K_0 = 1$ (the sum rule);

(2) the mean values for an arbitrary spin component on lattice sites and for an arbitrary total spin operator component are zero,

$$\langle s_{\mathbf{f}}^{\alpha} \rangle = 0, \quad \langle S^{\alpha} \rangle = 0, \quad (5)$$

where $\alpha = x, y, z$ or $+, -, z$;

(3) the mean values of the products of spin operators on an odd number of different sites are zero,

$$\langle s_{\mathbf{f}}^{\alpha} s_{\mathbf{m}}^{\beta} s_{\mathbf{n}}^{\gamma} \rangle = 0, \quad \mathbf{f} \neq \mathbf{m} \neq \mathbf{n}. \quad (6)$$

Here and throughout, the symbol $\langle \dots \rangle$ denotes thermodynamic averaging at temperature $\tau = T/zJ$ and over the ground state wave function at $\tau = 0$.

The whole collection of the properties of the spin liquid, namely, its ground state, the excitation spectrum, and the thermodynamic properties, should be described based on Hamiltonian (3) and postulates (4)–(6). Note that postulate (6) was introduced for the first time by this author in [7]; the corollaries to it will be considered

below. It will be shown that the ground state is singlet and has a total spin of $S = 0$, which is equivalent to the equality

$$\langle \mathbf{S}^2 \rangle_{\tau=0} = 0. \quad (7)$$

The properties of the spin liquid state are largely determined by the spatial and temperature dependences of the $K_r(\tau)$ spin correlation functions. The spin liquid state energy per bond in J units is

$$\varepsilon = \frac{\langle H \rangle}{(1/2)zNJ} = -\frac{3}{4} K_1, \quad (8)$$

where $K_{|\Delta|} = -K_1$ ($K_1 > 0$) is the correlator between the nearest neighbors.

To describe the state of the spin liquid, we use the Fourier transforms of the spin operators

$$s^{\alpha}(\mathbf{q}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{f}} e^{i\mathbf{q} \cdot \mathbf{f}} s_{\mathbf{f}}^{\alpha}$$

(similarly for all the other operators), where vectors \mathbf{q} belong to the first Brillouin zone of the FCC lattice, and we introduce the Fourier transform of the correlation function

$$\begin{aligned} K(\mathbf{q}) &= \sum_{\mathbf{r}} e^{-i\mathbf{q} \cdot \mathbf{r}} K_r \\ &= 4 \langle s^z(\mathbf{q}) s^z(-\mathbf{q}) \rangle = 2 \langle s^+(\mathbf{q}) s^(-\mathbf{q}) \rangle, \quad (9) \\ K_r &= \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}} K(\mathbf{q}) \end{aligned}$$

with the obvious property $K(\mathbf{q}) = K(-\mathbf{q})$. Calculations of $K(\mathbf{q})$ are performed by the method of two-time Green temperature functions [8]. Because the correlators are isotropic, it suffices to calculate the retarded commutator Green function

$$\langle \langle s^z(\mathbf{q}) | s^z(-\mathbf{q}) \rangle \rangle_{\omega} \equiv G(\mathbf{q}, \omega), \quad (10)$$

where ω is the dimensionless spectral variable used to determine $K(\mathbf{q})$ by the spectral theorem,

$$\frac{1}{4} K(\mathbf{q}) = \langle s^z(\mathbf{q}) s^z(-\mathbf{q}) \rangle = \int_{-\infty}^{\infty} J(\mathbf{q}, \omega; \tau) d\omega,$$

$$J(\mathbf{q}, \omega; \tau) = \frac{e^{\omega/\tau}}{e^{\omega/\tau} - 1} \left(-\frac{1}{\pi} \right) \quad (11)$$

$$\times \text{Im} \langle \langle s^z(\mathbf{q}) | s^z(-\mathbf{q}) \rangle \rangle_{\omega+i0},$$

where $J(\mathbf{q}, \omega; \tau)$ is the spectral intensity.

3. EQUATIONS OF MOTION AND THE GREEN FUNCTION OF LINEAR SECOND-ORDER THEORY

The theory of spin liquids is based on equations of an order not lower than second because $\langle s_f^\alpha \rangle = 0$, and, in contrast to spin-wave theory, first-order equations can not be linearized. The exact equations of motion have the form ($\hbar = 1$)

$$i\dot{s}_f^+ = \frac{1}{z} \sum_{\Delta} (s_f^z s_{f+\Delta}^+ - s_{f+\Delta}^z s_f^+), \quad (12)$$

$$i\dot{s}_f^z = \frac{1}{2z} \sum_{\Delta} (s_f^+ s_{f+\Delta}^- - s_{f+\Delta}^+ s_f^-) \equiv M_f,$$

$$i\dot{M}_f = -\frac{\partial^2 s_f^z}{\partial t^2} = \frac{1}{2z^2} \sum_{\Delta} (s_f^z - s_{f+\Delta}^z) + R_f, \quad (13)$$

where

$$R_f = \frac{1}{z} \sum_{\substack{\Delta \\ \Delta \neq \Delta'}} [s_f^z s_{f+\Delta}^+ s_{f+\Delta'}^- + (s_{f+\Delta}^z s_{f+\Delta'}^- - s_{f+\Delta'}^z s_f^-) s_f^+ s_{f+\Delta}^- - s_{f+\Delta}^z s_f^+ s_{f+\Delta'}^-]. \quad (14)$$

The second-order equation takes into account the kinematic properties of the spin operators on one node.

Let us truncate the chain of linked equations at the second step by linearizing the R_f operator, which contains the products of the spin operators on three different nodes. We suggest the following linearization scheme:

$$\begin{aligned} s_f^z s_n^+ s_m^- &\approx s_f^z \alpha_{|n-m|} \langle s_n^+ s_m^- \rangle \\ &= \frac{1}{2} \alpha_{|n-m|} K_{|n-m|} s_f^z, \quad \mathbf{f} \neq \mathbf{n} \neq \mathbf{m}, \end{aligned} \quad (15)$$

where $\alpha_{|n-m|}$ are the parameters that introduce corrections into the splitting (linearization). This scheme is a simple generalization of the linearization procedure applied in [6, 7, 9–11]. Using (15), we obtain

$$\begin{aligned} (R_f)_{\text{lin}} &= \frac{1}{2z^2} \sum_{\substack{\Delta, \Delta' \\ (\Delta \neq \Delta')}} [\alpha_{|\Delta-\Delta'|} K_{|\Delta-\Delta'|} (s_f^z - s_{f+\Delta}^z) \\ &+ \alpha_1 K_1 (s_{f+\Delta'}^z - s_{f+\Delta-\Delta'}^z)], \quad K_{|\Delta|} = -K_1. \end{aligned} \quad (16)$$

The sum over Δ' in the first term is

$$\begin{aligned} \tilde{K} &\equiv \frac{1}{z} \sum_{\substack{\Delta' \\ (\Delta' \neq \Delta)}} \alpha_{|\Delta-\Delta'|} K_{|\Delta-\Delta'|} \\ &= \frac{1}{12} (-4\alpha_1 K_1 + 2\alpha_2 K_2 + 4\alpha_3 K_3 + \alpha_4 K_4), \end{aligned} \quad (17)$$

where indices 1, 2, 3, and 4 denote the coordination zones with the corresponding $|\Delta - \Delta'|$ distances. The linearized R_f operator can now be written as

$$\begin{aligned} (R_f)_{\text{lin}} &= \frac{1}{2} \left[\left(\tilde{K} + \frac{\alpha_1 K_1}{z} \right) \frac{1}{z} \sum_{\Delta} (s_f^z - s_{f+\Delta}^z) \right. \\ &\left. + \frac{\alpha_1 K_1}{z^2} \sum_{\Delta, \Delta'} (s_{f+\Delta}^z - s_{f+\Delta+\Delta'}^z) \right], \end{aligned} \quad (18)$$

where the $\Delta' \neq \Delta$ restriction is removed in the second term.

The above transformations allow us to replace the exact equation (13) by the linearized one,

$$(i\dot{M}_f)_{\text{lin}} = \left(-\frac{\partial^2 s_f^z}{\partial t^2} \right)_{\text{lin}} \quad (19)$$

$$= \frac{1}{2z^2} \sum_{\Delta} (s_f^z - s_{f+\Delta}^z) + (R_f)_{\text{lin}},$$

which, after the Fourier transform, takes the form

$$(i\dot{M}(\mathbf{q}))_{\text{lin}} = \left(-\frac{\partial^2 s^z(\mathbf{q})}{\partial t^2} \right)_{\text{lin}} = \frac{1}{2} (1 - \Gamma_{\mathbf{q}}) \quad (20)$$

$$\times \left[\left(\tilde{K} + \frac{1 + \alpha_1 K_1}{z} \right) + \alpha_1 K_1 \Gamma_{\mathbf{q}} \right] s^z(\mathbf{q}) \equiv \Omega_{\mathbf{q}}^2 s^z(\mathbf{q}).$$

Here,

$$\begin{aligned} \Gamma_{\mathbf{q}} &= \frac{1}{z} \sum_{\Delta} e^{i\mathbf{q} \cdot \Delta} = \frac{1}{3} (c_x c_y + c_x c_z + c_y c_z), \\ c_j &\equiv \cos \frac{q_j}{2}. \end{aligned} \quad (21)$$

Using the notation

$$\frac{\alpha_1 K_1}{2} \equiv \lambda^2, \quad \frac{\tilde{K} + (1 + \alpha_1 K_1)/z}{\alpha_1 K_1} \equiv D, \quad (22)$$

we can write

$$\Omega_{\mathbf{q}}^2 = \lambda^2 (1 - \Gamma_{\mathbf{q}}) (D + \Gamma_{\mathbf{q}}) \equiv \lambda^2 E_{\mathbf{q}}^2. \quad (23)$$

Applying the Fourier transform to equations of motion (12) and (13) yields the following equations for the Green functions:

$$\omega G(\mathbf{q}, \omega) = \langle \langle M(\mathbf{q}) | s^z(-\mathbf{q}) \rangle \rangle_{\omega},$$

$$\omega \langle \langle M(\mathbf{q}) | s^z(-\mathbf{q}) \rangle \rangle_{\omega} = A_{\mathbf{q}} + \langle \langle i\dot{M}(\mathbf{q}) | s^z(-\mathbf{q}) \rangle \rangle_{\omega},$$

where

$$A_{\mathbf{q}} = \langle [M(\mathbf{q}), s^z(-\mathbf{q})] \rangle = \frac{K_1}{2}(1 - \Gamma_{\mathbf{q}}). \quad (24)$$

Using the $i\dot{M}(\mathbf{q}) \approx (i\dot{M}(\mathbf{q}))_{\text{lin}}$ approximation [see (20)], we obtain the Green function of linear second-order theory in the form

$$G(\mathbf{q}, \omega) = \frac{A_{\mathbf{q}}}{\omega^2 - \Omega_{\mathbf{q}}^2}. \quad (25)$$

Its spectral intensity (11) is

$$J(\mathbf{q}, \omega; \tau) = \frac{e^{\omega/\tau} A_{\mathbf{q}}}{e^{\omega/\tau} - 1} \frac{1}{2\Omega_{\mathbf{q}}} \times [\delta(\omega - \Omega_{\mathbf{q}}) - \delta(\omega + \Omega_{\mathbf{q}})], \quad \Omega_{\mathbf{q}} \geq 0. \quad (26)$$

By the spectral theorem, the one-time average is

$$\begin{aligned} \langle s^z(\mathbf{q})s^z(-\mathbf{q}) \rangle &\equiv \frac{1}{4}K(\mathbf{q}) \\ &= \int_{-\infty}^{\infty} J(\mathbf{q}, \omega; \tau) d\omega = \frac{A_{\mathbf{q}}}{2\Omega_{\mathbf{q}}} \coth \frac{\Omega_{\mathbf{q}}}{2\tau} \end{aligned}$$

or

$$K(\mathbf{q}) = \frac{K_1}{\lambda} \frac{1 - \Gamma_{\mathbf{q}}}{E_{\mathbf{q}}(D)} \coth \frac{\lambda E_{\mathbf{q}}(D)}{2\tau}. \quad (27)$$

Equation (27) shows that the suggested version of spin liquid theory contains three unknown parameters, which are functions of temperature, namely, the modulus of the correlator between the nearest neighbors $K_1(\tau)$, the ‘‘stiffness’’ parameter of the excitation spectrum $\lambda(\tau)$, and the pseudogap in the spectrum $D(\tau)$. All these parameters should be calculated self-consistently from three equations (see below). Note in advance that, because $-1/3 \leq \Gamma_{\mathbf{q}} \leq 1$ in the Brillouin zone of the FCC lattice, we can conveniently separate the limiting spectrum point ($-1/3$) and write the D parameter as

$$D = 1/3 + \delta, \quad \delta = \delta(\tau) \geq 0, \quad (28)$$

which is necessary for satisfying the $\Omega_{\mathbf{q}} \geq 0$ or $E_{\mathbf{q}}(\delta) \geq 0$ condition.

4. THE SELF-CONSISTENCY EQUATION

Using the definition of spatial correlators K_r [Eq. (9)], we obtain the system of equations

$$\begin{aligned} K_0 = 1 &= \frac{1}{N} \sum_{\mathbf{q}} K(\mathbf{q}) = \frac{K_1}{\lambda} I_0(\delta, \tau), \\ K_1 &= \frac{1}{N} \sum_{\mathbf{q}} (-\Gamma_{\mathbf{q}}) K(\mathbf{q}) = \frac{K_1}{\lambda} I_1(\delta, \tau), \end{aligned} \quad (29)$$

$$K_{\text{tot}} = \frac{1}{N} \sum_{\mathbf{q}} (\Gamma_{\mathbf{q}})^2 K(\mathbf{q}) = \frac{K_1}{\lambda} I_2(\delta, \tau),$$

where

$$I_n(\delta, \tau) = \frac{1}{N} \sum_{\mathbf{q}} (-\Gamma_{\mathbf{q}})^n \frac{1 - \Gamma_{\mathbf{q}}}{E_{\mathbf{q}}(\delta)} \coth \frac{\lambda E_{\mathbf{q}}(\delta)}{2\tau},$$

$$E_{\mathbf{q}}(\delta) = \sqrt{(1 - \Gamma_{\mathbf{q}}) \left(\frac{1}{3} + \Gamma_{\mathbf{q}} + \delta \right)}, \quad (30)$$

$$\begin{aligned} K_{\text{tot}} &= \frac{1}{z^2} \sum_{\Delta, \Delta'} K_{|\Delta + \Delta'|} \\ &= \frac{1 - 4K_1 + 2K_2 + 4K_3 + K_4}{z}, \quad z = 12. \end{aligned}$$

Equations (29) have the formal solution (the arguments of the functions are omitted)

$$\lambda = I_1, \quad K_1 = I_1/I_0, \quad (31)$$

$$K_{\text{tot}} = I_2/I_0, \quad \alpha_1 = 2I_0I_1.$$

Note that the $D = 1/3 + \delta$ parameter [see Eq. (28)] is written as a complex combination of unknown correlators and splitting parameters. Calculating them separately is meaningless. For this reason, we further calculate the δ value as one of the most important characteristics of the system, which describes correlations in an ‘‘extended’’ cluster. We cannot, however, determine δ from (31) and will therefore use the method of moments [7] to calculate it self-consistently.

Let us define and exactly calculate the first three moments,

$$\begin{aligned} M_0 &\equiv \langle s_{\mathbf{f}}^z(t) s_{\mathbf{f}}^z(0) \rangle_{t=0} = \langle s_{\mathbf{f}}^z s_{\mathbf{f}}^z \rangle = \frac{1}{4}, \\ M_1 &\equiv \left\langle i \frac{\partial s_{\mathbf{f}}^z(t)}{\partial t} s_{\mathbf{f}}^z(0) \right\rangle_{t=0} \\ &= \left\langle \frac{1}{2z} \sum_{\Delta} (s_{\mathbf{f}}^+ s_{\mathbf{f}+\Delta}^- - s_{\mathbf{f}+\Delta}^+ s_{\mathbf{f}}^-) s_{\mathbf{f}}^z \right\rangle = \frac{K_1}{4}, \\ M_2 &\equiv \left\langle \left(-\frac{\partial^2 s_{\mathbf{f}}^z(t)}{\partial t^2} \right) s_{\mathbf{f}}^z(0) \right\rangle_{t=0} \\ &= \left\langle \left(\frac{1}{2z^2} \sum_{\Delta} (s_{\mathbf{f}}^z - s_{\mathbf{f}+\Delta}^z) + R_{\mathbf{f}} \right) s_{\mathbf{f}}^z \right\rangle \\ &= \frac{1}{8} \left(\frac{K_1}{z} + K_{\text{tot}} \right). \end{aligned} \quad (32)$$

These calculations are performed using the rules of the multiplication of operators on one node and the definitions of $K_1 = -K_{|\Delta|}$ and K_{tot} [see Eq. (30)]; importantly,

by virtue of condition (6), only the first term of the R_f operator [Eq. (14)] contributes to the $\langle R_f s_f^z \rangle$ mean.

Based on the spectral theorem, the one-node mean can be represented as

$$\langle s_f^z(t) s_f^z(0) \rangle = \int_{-\infty}^{\infty} e^{-i\omega t} J_0(\omega) d\omega, \quad (33)$$

$$J_0(\omega) = \frac{1}{N} \sum_{\mathbf{q}} J(\mathbf{q}, \omega; \tau),$$

where the $J(\mathbf{q}, \omega; \tau)$ spectral intensity generally corresponds to the exact Green function $G(\mathbf{q}, \omega)$. It follows from (33) that

$$\begin{aligned} M_0 &= \int_{-\infty}^{\infty} J_0(\omega) d\omega, & M_1 &= \int_{-\infty}^{\infty} \omega J_0(\omega) d\omega, \\ M_2 &= \int_{-\infty}^{\infty} \omega^2 J_0(\omega) d\omega. \end{aligned} \quad (34)$$

Above, we calculated approximate Green function (25). The corresponding $J(\mathbf{q}, \omega; \tau)$ spectral intensity is given by (26). It follows that

$$\begin{aligned} J_0(\omega) &= \frac{K_1}{4\lambda N} \sum_{\mathbf{q}} \frac{e^{\omega/\tau}}{e^{\omega/\tau} - 1} \frac{1 - \Gamma_{\mathbf{q}}}{E_{\mathbf{q}}} \\ &\times [\delta(\omega - \Omega_{\mathbf{q}}) - \delta(\omega + \Omega_{\mathbf{q}})], \quad \Omega_{\mathbf{q}} = \lambda E_{\mathbf{q}}. \end{aligned} \quad (35)$$

Let us impose the requirement that exact equations (34) should be satisfied in the linear second-order theory under consideration. The M_0 zero moment is given by the equation that precisely reproduces the sum rule $K_0 = 1$. It is easy to see that substituting (35) into (34) to obtain M_1 leads to an identity. Substituting (35) into (34) to determine M_2 , however, yields

$$M_2 = \frac{\lambda K_1}{4} P(\delta), \quad (36)$$

$$P(\delta) \equiv \frac{1}{N} \sum_{\mathbf{q}} (1 - \Gamma_{\mathbf{q}}) E_{\mathbf{q}} \coth \frac{\Omega_{\mathbf{q}}}{2\tau}.$$

Using the exact expression for M_2 [Eq. (32)] and solutions (31), we obtain the equation for self-consistently calculating gap parameter δ ,

$$P(\delta) = \frac{I_2(\delta) + I_1(\delta)/12}{2I_1^2(\delta)}, \quad \delta = \delta(\tau). \quad (37)$$

It follows that consistent linear second-order theory is based on the observance of the sum rule $K_0 = 1$, the definitions of the K_1 and K_{tot} correlators [Eqs. (29)], and the requirement of the exact second moment value, which leads to (37). Equation (37) plays an important

role. Indeed, it makes the theory of spin liquids internally closed, and there appears a possibility of self-consistently calculating all system parameters.

The sums over the Brillouin zone in the equations for I_n and P will be written in terms of integrals with the density of states $D(\varepsilon)$. The $D(\varepsilon)$ density of states that corresponds to the isoenergy surfaces $\Gamma_{\mathbf{q}} = \varepsilon$ in the FCC lattice should satisfy the exact relations

$$\begin{aligned} D_0 &= \int_{-1/3}^1 D(\varepsilon) d\varepsilon = 1, \\ D_1 &= \int_{-1/3}^1 \varepsilon D(\varepsilon) d\varepsilon = 0, \\ D_2 &= \int_{-1/3}^1 \varepsilon^2 D(\varepsilon) d\varepsilon = \frac{1}{2}. \end{aligned} \quad (38)$$

The $D(x)$ density of states was approximated as

$$D(x) = \begin{cases} A(x), & -1/3 \leq x \leq 0 \\ B(x), & 0 \leq x \leq 1, \end{cases} \quad (39)$$

where

$$A(x) = -0.366664 \ln \left[0.0671182 \left(x + \frac{1}{3} \right) \right] - 0.456693x,$$

$$B(x) = 0.226573 \sqrt{1-x} + \frac{0.202745}{x + 0.151142} - 0.174703.$$

In selecting this approximation, we were first and foremost guided by the logarithmic divergence of $D(\varepsilon)$ at $\varepsilon = -1/3$ and the fulfillment of integral equations (38), because self-consistency equations (31) and (37) are also integral.

Combining (31) and (37) yields the system of three equations for self-consistently calculating the spin liquid parameters,

$$\lambda = I_1, \quad (40a)$$

$$K_1 = I_1/I_0, \quad (40b)$$

$$P = \frac{I_2 + I_1/12}{2I_1^2}. \quad (40c)$$

Here,

$$I_n(\delta, t) = \int_{-1/3}^1 d\varepsilon D(\varepsilon) (-\varepsilon)^n \frac{1 - \varepsilon}{E(\varepsilon, \delta)} \coth \frac{E(\varepsilon, \delta)}{2t},$$

$$P(\delta, t) = \int_{-1/3}^1 d\varepsilon D(\varepsilon) (1 - \varepsilon) E(\varepsilon, \delta) \coth \frac{E(\varepsilon, \delta)}{2t}, \quad (41)$$

$$E(\varepsilon, \delta) = \sqrt{(1-\varepsilon)\left(\frac{1}{3} + \varepsilon + \delta\right)}, \quad t = \frac{\tau}{\lambda}.$$

5. THE GROUND STATE

Consider the properties of the spin liquid at $\tau \equiv 0$ (the hyperbolic cotangent equals one). The I_n and P integrals only depend on $\delta(0)$, and $K_1 = I_1/I_0$ monotonically decreases as $\delta(0)$ increases and has a maximum at $\delta(0) = 0$. Equation (40c) at $\tau \equiv 0$ is an equation with respect to $\delta(0)$ and has the solution $\delta(0) = 1.04 \times 10^{-3} \neq 0$. We therefore have the following characteristics of the ground state of the system:

$$\begin{aligned} \delta(0) &= 1.04 \times 10^{-3}, & \lambda(0) &= 0.538, \\ K_1(0) &= 0.178, & \varepsilon_0 &= -0.133. \end{aligned} \quad (42)$$

In addition, $I_0 = 3.026$, $I_2 = 0.212$, $\alpha_1 = 3.256$, and $P = 0.442$.

Solution (42) being available, it is pertinent to make some comments on the method for linearizing (15). It is known that, in first-order theory, the linearization (Tyablikov splitting) is performed without any correcting factor (the correcting factor is taken to be one). With α_i set equal to one in the second-order theory under consideration, equations (29) have no solutions of any kind. If all $\alpha_i = \alpha$ are equal, we can, without invoking the method of moments, obtain the gap parameter in the form

$$\delta = \frac{I_2(\delta)}{I_1(\delta)} - \frac{1}{4} - \frac{1}{12} \frac{2I_0(\delta)I_1(\delta) - 1}{2I_1^2(\delta)}.$$

This equation has the solution $\delta^*(0) = 0.0435$ at $\tau = 0$, and we obtain

$$\begin{aligned} \lambda^*(0) &= 0.319, & K_1^*(0) &= 0.143, \\ \varepsilon_0^* &= -0.107, & \alpha &= 1.418. \end{aligned}$$

Clearly, this variant gives a substantial loss in the ground state energy compared with (42). Note also that the singlet state energy obtained by applying the method of moments [7] to the spin liquid in a square lattice is $\varepsilon_0 = -0.352$, which is lower than the energy of the antiferromagnetic state at $\tau = 0$.

Let us show that the ground state is singlet (total spin $S = 0$). We will introduce the function (the mean of the square of the total spin of the system referred to one spin)

$$\begin{aligned} S^2(\tau) &\equiv \frac{1}{N} \langle \mathbf{S}^2 \rangle = \frac{1}{N} \sum_{\mathbf{f}\mathbf{m}} \langle \mathbf{s}_{\mathbf{r}} \cdot \mathbf{s}_{\mathbf{m}} \rangle \\ &= \sum_{\mathbf{r}} \frac{1}{N} \sum_{\mathbf{f}} \langle \mathbf{s}_{\mathbf{r}} \cdot \mathbf{s}_{\mathbf{f}+\mathbf{r}} \rangle = \frac{3}{4} \sum_{\mathbf{r}} K_{\mathbf{r}} = \frac{3}{4} K(0), \end{aligned} \quad (43)$$

which can be expressed via the Fourier transform of correlation function (27) at $\mathbf{q} = 0$. At $\tau \equiv 0$, it follows from (27) that $K(0) = 0$ and $S^2(0) = 0$, which proves the singlet character of the ground state in conformity with (7). On the other hand, (43) can be treated as the limit

$$\begin{aligned} K(0) &= \lim_{\mathbf{q} \rightarrow 0} K(\mathbf{q}) = \frac{K_1}{\lambda} \lim_{\mathbf{q} \rightarrow 0} \frac{1 - \Gamma_{\mathbf{q}}}{E_{\mathbf{q}}(\delta)} \coth \frac{\lambda E_{\mathbf{q}}(\delta)}{2\tau} \\ &= \frac{4\tau}{\alpha_1 \left(\frac{1}{3} + \Gamma_0 + \delta \right)}. \end{aligned} \quad (44)$$

From this equation, we again obtain $K(0)$ as $\tau \rightarrow 0$ (a singlet). At $\tau \neq 0$, triplet excitations, however, arise in the system, which results in $S^2(\tau) \neq 0$. Equation (44) will be used to analyze the temperature properties of the spin liquid.

6. CALCULATIONS OF THE THERMODYNAMIC PROPERTIES OF THE SPIN LIQUID

System (40) was solved numerically. A t value was set, and δ was found by (40c). At these t and $\delta(t)$, the I_0 , $I_1 = \lambda$, $K_1 = I_1/I_0$, and $\alpha_1 = 2I_0I_1$ integrals and temperature $\tau = \lambda t$ were calculated. As a result, all the parameters found numerically were functions of temperature $\tau = T/zJ$ ($z = 12$).

The calculated temperature dependence of the $\delta(\tau)$ gap parameter is shown in Fig. 1. In the low-temperature region, $\delta(\tau)$ grows almost as a power function of τ , $\delta(\tau) \propto \tau^2$ according to our data. However, already at $\tau \geq 0.5$, the $\delta(\tau)$ parameter virtually coincides with its asymptotic value 4τ .

The temperature dependence of the $\lambda(\tau)$ stiffness parameter of the excitation spectrum with the asymptotic behavior $\lambda(\tau) \propto 1/\sqrt{\tau}$ is shown in Fig. 2.

It is known that the thermodynamic properties of a system are determined by its excitation spectrum. The temperature evolution of the spectrum

$$\Omega_{\mathbf{q}}(\tau) = \sqrt{1 - \Gamma_{\mathbf{q}}} \lambda(\tau) \sqrt{1/3 + \Gamma_{\mathbf{q}} + \delta(\tau)}$$

is shown in Fig. 3; it was obtained by self-consistently calculating the $\lambda(\tau)$ and $\delta(\tau)$ parameters. The spectrum is gapless and acoustic; that is, $\Omega_{\mathbf{q}} \propto q$ as $q \rightarrow 0$ (as with phonons or antiferromagnetic magnons). The mean excitation energy (recall that all the energy parameters of the system are reduced to the dimensionless form through dividing by zJ) is

$$\begin{aligned} \bar{\Omega}(\tau) &= \lambda(\tau) \sum_{-1/3}^1 D(\varepsilon) E(\varepsilon, \delta(\tau)) d\varepsilon \\ &\approx \lambda(\tau) \sqrt{\delta(\tau)}. \end{aligned} \quad (45)$$

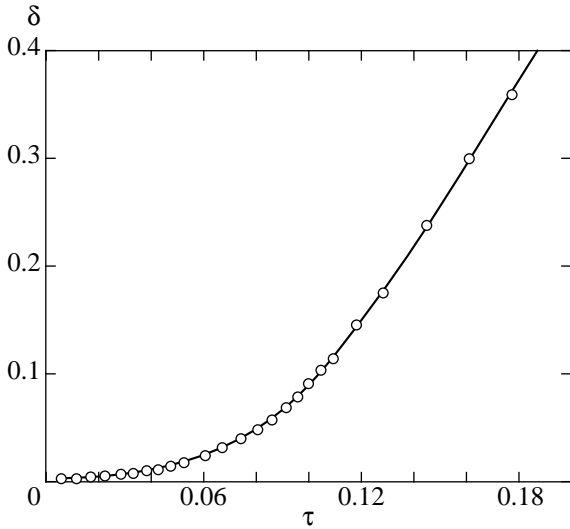


Fig. 1. Dependence of gap parameter δ on dimensionless temperature $\tau = T/zJ$ at low temperatures.

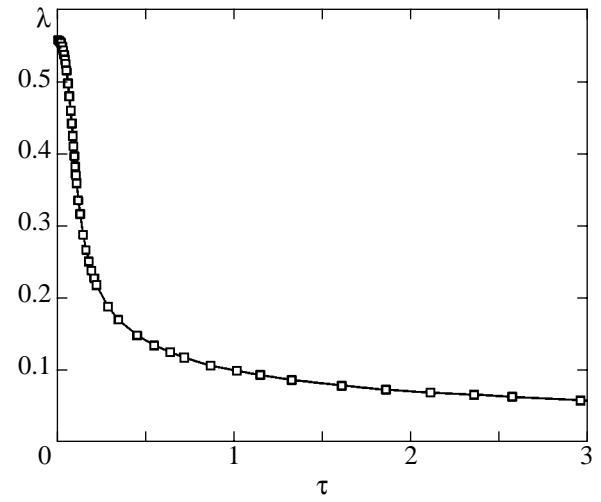


Fig. 2. Temperature dependence of spectrum stiffness parameter $\lambda(\tau)$.

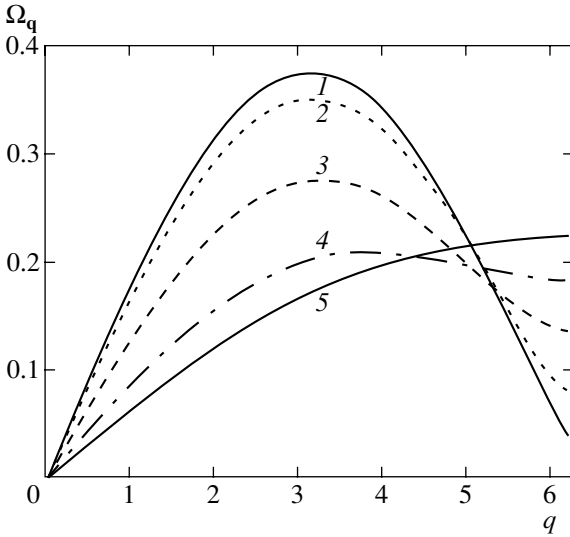


Fig. 3. Temperature evolution of excitation spectrum $\Omega_q(\tau)$ in the [001] direction at self-consistently calculated $\delta(\tau)$ and $\lambda(\tau)$ parameters: (1) $\tau = 0$, $\lambda = 0.56$, and $\delta = 0.0032$; (2) $\tau = 0.05$, $\lambda = 0.518$, and $\delta = 0.0172$; (3) $\tau = 0.1$, $\lambda = 0.385$, and $\delta = 0.091$; (4) $\tau = 0.2$, $\lambda = 0.23$, and $\delta = 0.47$; and (5) $\tau = 1.0$, $\lambda = 0.1$, and $\delta = 3.68$.

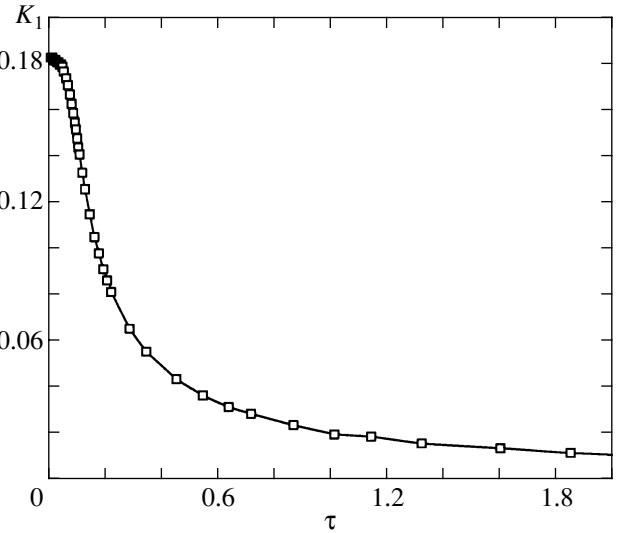


Fig. 4. Temperature dependence of the correlator modulus between nearest neighbors $K_1(\tau)$; system energy $\varepsilon(\tau) = -(3/4)K_1(\tau)$.

This is an increasing function of temperature, which reaches “saturation” at $\tau > 2$; that is, $\bar{\Omega} \rightarrow 0.2$.

The temperature behavior of the $K_1(\tau)$ modulus of the correlator between the nearest neighbors is shown in Fig. 4. At $\tau \geq 0.5$, its temperature dependence is close to asymptotic, $K_1(\tau) \propto 1/\tau$. According to the calculations, the dimensionless heat capacity

$$c(\tau) = \frac{\partial \varepsilon(\tau)}{\partial \tau} = -\frac{3}{4} \frac{\partial K_1(\tau)}{\partial \tau} \quad (46)$$

has a form similar to that of the heat capacity of a two-level system (Schottky anomaly), namely, it has a maximum at $\tau \approx 0.1 \approx \bar{\Omega}/2$ and the $c(\tau) \propto 1/\tau^2$ asymptotic behavior. In the low-temperature region, it, however, exhibits the behavior of a power function, $c(\tau) \propto \tau^3$.

Magnetic susceptibility. The dynamic susceptibility of a spin system in dimensionless units is determined by the equation [8]

$$\chi^{\alpha\beta}(\mathbf{q}, \omega) = -\langle \langle s^\alpha(\mathbf{q}) | s^\beta(-\mathbf{q}) \rangle \rangle_\omega.$$

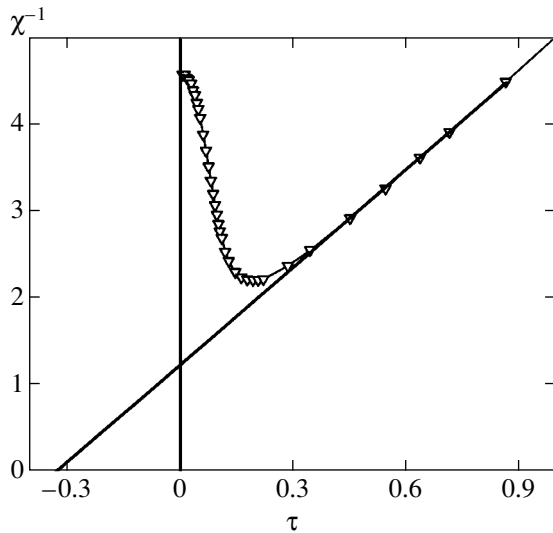


Fig. 5. Temperature dependence of reciprocal susceptibility χ^{-1} ; at $\tau > 0.5$, the $\chi^{-1}(\tau)$ function virtually reaches its asymptotic value with the Curie paramagnetic point $\Theta = 1/3$.

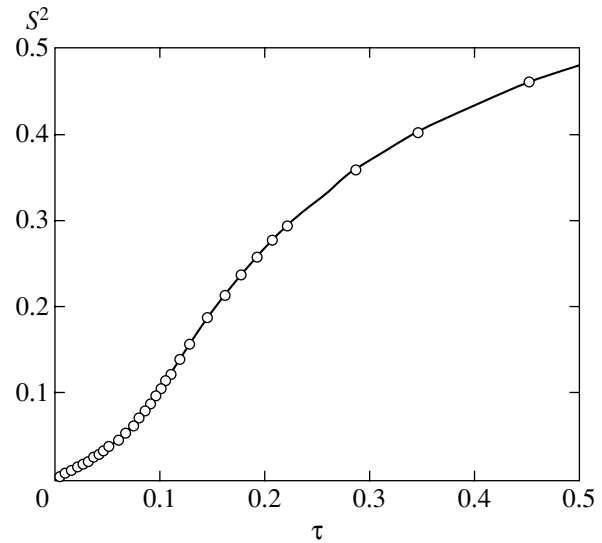


Fig. 6. Low-temperature behavior of the $S^2(\tau) \equiv N^{-1}\langle \mathbf{S}^2 \rangle$ function, where \mathbf{S} is the total spin operator of the system; asymptotically, $S^2(\tau) \rightarrow 3/4$.

In the spin liquid state under consideration, we have

$$\chi^{+-}(\mathbf{q}, \omega) = 2\chi^{zz}(\mathbf{q}, \omega) = -2G(\mathbf{q}, \omega)$$

because of the isotropic character of the correlation functions. According to (24) and (25), the expression for the static susceptibility ($\omega = 0$) has the form

$$\begin{aligned} \chi^{zz}(\mathbf{q}, 0) &= \frac{K_1}{2} \frac{1 - \Gamma_{\mathbf{q}}}{\Omega_{\mathbf{q}}^2} = \frac{K_1}{2\lambda^2} \frac{1}{1/3 + \Gamma_{\mathbf{q}} + \delta} \\ &= \frac{1}{\alpha_1} \frac{1}{1/3 + \Gamma_{\mathbf{q}} + \delta}. \end{aligned} \quad (47)$$

It follows from (47) that

$$\chi^{zz}(0, 0) \equiv \chi(\tau) = \frac{1}{\alpha_1(\tau)[4/3 + \delta(\tau)]}, \quad (48)$$

$$\chi^{zz}(0, 0)|_{\tau=0} \equiv \chi(0) = 0.23,$$

$$\chi^{zz}(\mathbf{Q}_{1,2}, 0) = \frac{1}{\alpha_1(\tau)\delta(\tau)}, \quad (49)$$

$$\chi^{zz}(\mathbf{Q}_{1,2}, 0)|_{r=0} = 295.31,$$

where $\mathbf{Q}_1 \equiv X = (0, 0, 2\pi)$ and $\mathbf{Q} \equiv W = (\pi, 0, 2\pi)$ are the special points of the FCC lattice Brillouin zone at which $\Gamma_{\mathbf{Q}_1} = \Gamma_{\mathbf{Q}_2} = -1/3$. Because $\delta(0) \neq 0$ in the spin liquid, (49) does not diverge as $\tau \rightarrow 0$, which is evidence of spin liquid stability with respect to short-wave perturbations corresponding to the $\mathbf{Q}_{1,2}$ wave vectors and of correlation length finiteness.

Compare susceptibility (48) with the longitudinal thermodynamic susceptibility. By definition [8], it is given by

$$\tilde{\chi}^{zz}(\tau) = \frac{1}{\tau} [\langle (s^z(0))^2 \rangle - \langle s^z(0) \rangle^2] \equiv \frac{1}{\tau} \chi_0(\tau), \quad (50)$$

where $s^z(0)$ is the operator Fourier transform at $\mathbf{q} = 0$. As $\langle s^z(0) \rangle = 0$ in the spin liquid state, it follows from the isotropic character of the spin correlators that

$$\begin{aligned} \chi_0(\tau) &= \frac{1}{N} \langle (S^z)^2 \rangle = \frac{1}{3} S^2(\tau) \\ &= \frac{1}{4} K(\mathbf{q} = 0) = \frac{\tau}{\alpha_1(3/4 + \delta)}, \end{aligned} \quad (51)$$

where the $S^2(\tau)$ function is given by (43). A comparison of expressions (50) and (51) with (48) shows that the longitudinal thermodynamic susceptibility coincides with the dynamic susceptibility at $\omega = 0$ and $\mathbf{q} = 0$; that is, $\tilde{\chi}^{zz}(\tau) = \chi(\tau)$. In addition,

$$3\tau\chi(\tau) = S^2(\tau). \quad (52)$$

The $\chi^{-1}(\tau)$ reciprocal susceptibility calculated numerically is shown in Fig. 5. This function has a minimum at $\tau \approx 0.2$ and becomes close to the $\chi^{-1}(\tau) \approx \tau + \Theta$ function already at $\tau \geq 0.5$; here, $\Theta = 1/3$ is an analog of the paramagnetic Curie point for antiferromagnets. The $S^2(\tau)$ function calculated by (52) is shown in Fig. 6. The $\alpha_1(\tau)$ parameter rapidly reaches its asymptotic value (one) at $\tau \geq 0.5$.

7. INTERPRETATION OF THE RESULTS

In the region of maximally low temperatures, the $\coth(x/2) = 1 + 2n(x)$ representation, where $n(x)$ is the Bose distribution function, can conveniently be used. The spectrum in this region is acoustic (proportional to q), and the parameters in this region therefore behave as power functions,

$$\lambda(\tau) = \lambda(0) - B\tau^4, \quad K_1(\tau) = K_1(0) - A\tau^4. \quad (53)$$

As the energy of the system is $\varepsilon = -(3/4)K_1$, the heat capacity of the spin liquid in this region,

$$c(\tau) = \partial\varepsilon/\partial\tau = 4A\tau^3, \quad (54)$$

is similar to the heat capacity of Debye phonons (or antiferromagnetic magnons).

At temperatures $\tau \geq \tau_0$, where $\tau_0 = \lambda(0)(2/\sqrt{3})\sqrt{\delta(0)}$ is the excitation energy at the boundary ($\varepsilon = -1/3$ or $\mathbf{q} = \mathbf{Q}_{1,2}$), the thermodynamic properties of the system become more complex, because this region also contributes to the temperature dependence of the parameters. Initially, the quadratic dependence of δ predominates, but, at $\tau > 1$, the dependence becomes linear.

Asymptotic behavior ($\tau \rightarrow \infty$). The coefficients of the asymptotic behaviors of all the functions when correlations disappear can be determined analytically using the following obvious physical conditions:

(1) $S^2(\tau) \rightarrow 3/4$; $3/4$ is the value of the square of the spin on a lattice site.

(2) $\alpha_1(\tau) \rightarrow 1$; that is, the uncoupling parameter for noncorrelated spins becomes equal to one.

The first condition leads to the Curie law for susceptibility (52),

$$\chi(\tau) = \frac{S^2(\tau)}{3\tau} \rightarrow \frac{1}{4\tau}.$$

On the other hand, the other (equivalent) definition of susceptibility [Eq. (48)] gives

$$\chi(\tau) \rightarrow \frac{1}{4/3 + \delta(\tau)}$$

when both conditions are satisfied. For the Curie law to be obeyed, it is necessary that

$$\delta(\tau) \rightarrow 4\tau. \quad (55)$$

Asymptotically, the integrals take the form

$$I_n(\tau) \rightarrow \frac{1}{2\lambda(\tau)} \int_{-1/3}^1 D(\varepsilon)(-\varepsilon)^n \left(1 - \frac{\varepsilon}{4\tau}\right) d\varepsilon.$$

This result and properties (38) of the density of states give

$$\begin{aligned} I_0(\tau) &\rightarrow \frac{1}{2\lambda(\tau)}, & I_1(\tau) &\rightarrow \frac{1}{z} \frac{1}{2\lambda(\tau)} \frac{1}{4\tau}, \\ I_2(\tau) &\rightarrow \frac{1}{z} \frac{1}{2\lambda(\tau)}, & z &= 12. \end{aligned} \quad (56)$$

As $I_1 = \lambda$ [according to self-consistency equation (40a)], it follows from (56) that $\lambda^2 = 1/8z\tau$; that is,

$$\lambda \rightarrow \frac{1}{\sqrt{2z}2\sqrt{\tau}}, \quad \bar{\Omega} = \lambda\sqrt{\delta} = \frac{1}{\sqrt{2z}}. \quad (57)$$

To summarize, the behavior of the thermodynamic characteristics of the system (spin liquid) as $\tau \rightarrow \infty$ is as follows:

$$\begin{aligned} \chi(\tau) &\rightarrow \frac{1}{4\tau}, & \delta(\tau) &\rightarrow 4\tau, \\ \lambda(\tau) &\rightarrow \frac{\bar{\Omega}}{2} \frac{1}{\sqrt{\tau}} = \frac{0.102}{\sqrt{\tau}}, \\ K_1(\tau) &\rightarrow \frac{\bar{\Omega}^2}{2} \frac{1}{\tau} = \frac{0.021}{\tau}. \end{aligned} \quad (58)$$

8. SPATIAL CORRELATIONS IN THE SPIN LIQUID

By definition,

$$K_r = 4 \frac{1}{N} \sum_{\mathbf{f}} \langle s_{\mathbf{f}}^z s_{\mathbf{f}+\mathbf{r}}^z \rangle = \frac{4}{3N} \sum_{\mathbf{f}} \langle \mathbf{s}_{\mathbf{f}} \mathbf{s}_{\mathbf{f}+\mathbf{r}} \rangle.$$

The general equation for the spatial correlation functions [see (14) and (34)] has the form

$$\begin{aligned} K_r &= \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}} K(\mathbf{q}), \\ K(\mathbf{q}) &= \frac{K_1}{\lambda} \frac{1 - \Gamma_{\mathbf{q}}}{E_{\mathbf{q}}(\delta)} \coth \frac{\lambda E_{\mathbf{q}}(\delta)}{2\tau}, \end{aligned}$$

where the $g \equiv K_1/\lambda$ and δ parameters are functions of temperature.

Consider the character of spatial correlations in the ground (singlet) spin liquid state. At $\tau \equiv 0$, we have

$$K(\mathbf{q}) = g(0)R(\mathbf{q}), \quad R(\mathbf{q}) \equiv \sqrt{\frac{1 - \Gamma_{\mathbf{q}}}{1/3 + \Gamma_{\mathbf{q}} + \delta(0)}}. \quad (59)$$

The determination of K_r at arbitrary r is a technically complex computational problem because the summation (integration) is over the first Brillouin zone, which has a fairly complex form in the FCC lattice [12].

First, note that Eq. (43),

$$\sum_r K_r = 0,$$

is evidence that spatial correlation functions are alternating in the ground singlet spin liquid state and cancel each other when the summation is performed.

It follows from (59) that the largest contribution to the formation of spatial correlations is made by those Brillouin zone regions in which $\Gamma_{\mathbf{q}} \rightarrow -1/3$; that is, by the neighborhoods of points $\mathbf{Q}_1 = (0, 0, 2\pi)$ and $\mathbf{Q}_2 = (\pi, 0, 2\pi)$ and other points with similar symmetry properties.

The neighborhood of point \mathbf{Q}_1 . Set $\mathbf{q} = \mathbf{Q}_1 + \mathbf{p}$, where $|\mathbf{p}| = p \ll 1$. In this region,

$$\begin{aligned} \Gamma_{\mathbf{Q}_1 + \mathbf{p}} &\approx -\frac{1}{3} + \frac{1}{12}p_z^2, \\ R(\mathbf{Q}_1 + \mathbf{p}) &\approx \frac{4}{\sqrt{p_z^2 + \kappa^2}}, \quad \kappa^2 \equiv z\delta(0) \end{aligned} \quad (60)$$

and the Fourier transform of the correlation function is anisotropic and has a singular direction (z). Then,

$$\begin{aligned} K_r &\approx 4g e^{i\mathbf{Q}_1 \cdot \mathbf{r}} C_{an}(r), \\ C_{an}(r) &= \frac{1}{(2\pi)^3} \int_{(p_0)} d\mathbf{p} \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{\sqrt{p_z^2 + \kappa^2}}. \end{aligned} \quad (61)$$

The integration is performed in the spherical coordinates over a sphere of small radius p_0 (the \mathbf{r} vector is directed along z axis),

$$\begin{aligned} C_{an}(r) &= \frac{1}{2\pi^2} \int_0^{p_0} p^2 dp \int_0^1 \frac{dx \cos(prx)}{\sqrt{p^2 x^2 + \kappa^2}} \\ &= \frac{1}{2\pi^2} \int_0^{p_0} p^2 dp \frac{1}{p} \int_0^{pr} \frac{dz \cos z}{\sqrt{z^2 + A^2}}, \end{aligned}$$

where $A^2 = r^2 \kappa^2$. At large r values, the integral is [13]

$$\int_0^\infty \frac{dz \cos z}{\sqrt{z^2 + A^2}} \approx \frac{\pi}{2A} e^{-A}, \quad A \gg 1.$$

As a result, we obtain the following asymptotic behavior:

$$C_{an}(r) \propto \frac{\exp(-r/\xi)}{\sqrt{r/\xi}}, \quad \xi = \frac{1}{\kappa} = \frac{1}{\sqrt{z\delta(0)}}, \quad (62)$$

where ξ is the correlation length. As $\delta(0) \approx 10^{-3}$ and $z = 12$, we have $\xi \approx 8.95$; that is, approximately nine lattice parameters or 12–13 distances between the nearest neighbors. It follows from these estimates that short-range order is fairly well established in the spin liquid.

The $\coth x \approx 1/x$ approximation can be used at high temperatures to obtain

$$K(\mathbf{q}) \approx \frac{4\tau}{\alpha_1(\tau)} \frac{1}{1/3 + \Gamma_{\mathbf{q}} + \delta(\tau)} \quad (63)$$

[recall that, asymptotically, $\alpha_1(\tau) \rightarrow 1$ and $\delta(\tau) \rightarrow 4\tau$]. We then have

$$\begin{aligned} K_r &= \frac{4\tau}{\alpha_1(\tau)} \frac{1}{v_B} \int_{(v_B)} d\mathbf{q} \frac{e^{i\mathbf{q} \cdot \mathbf{r}}}{1/3 + \Gamma_{\mathbf{q}} + \delta(\tau)}, \\ v_B &= 4(2\pi)^3, \end{aligned}$$

where v_B is the volume of the Brillouin zone. As previously, the neighborhoods of the points at which $\Gamma = -1/3$ are assumed to make the major contribution to the integral. In the neighborhood of point \mathbf{Q}_1 , we have

$$\begin{aligned} K_r &\approx \frac{z\tau}{\alpha_1(\tau)} C_{an}^*(r), \\ C_{an}^*(r) &= \frac{1}{(2\pi)^3} \int_{(p_0)} d\mathbf{p} \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{p_z^2 + \kappa^2}. \end{aligned} \quad (64)$$

As opposed to $C_{an}(r)$, the $C_{an}^*(r)$ function contains a linear term rather than a root in the denominator. The integration by the method specified above gives

$$\begin{aligned} C_{an}^*(r) &\approx \frac{p_0^2}{(2\pi)^2} r \int_0^\infty \frac{dz \cos z}{z^2 + \kappa^2 r^2} \\ &= \frac{p_0^2}{(2\pi)^2} r \frac{\pi}{2\kappa r} e^{-\kappa r} \propto e^{-\kappa r}. \end{aligned} \quad (65)$$

The $\xi = 1/\kappa$ correlation length becomes small under high-temperature conditions ($\xi \propto 1/\sqrt{\tau}$). As a result, virtually the only remaining correlations are those between the nearest neighbors.

It follows that spatial correlations in the main directions oscillate with a $\mathbf{Q}_1 \cdot \mathbf{r} = 2\pi r$ period and decay following the behavior of the $C_{an}(r)$ function.

9. CONCLUSION

Let us summarize the results obtained in this work.

In systems with frustrated exchange interactions between the nearest neighbors (as in the FCC lattice), quantum fluctuations of transverse spin components become substantial and can destroy the Ising antiferromagnetic state in the absence of additional stabilizing factors (exchange between the next-nearest neighbors or anisotropy).

In the absence of a long-range order in the FCC lattice, the system is in the spin liquid state. This state is characterized by an isotropic spin correlation function (Hamiltonian symmetry is not destroyed), and the

ground state of the spin liquid is singlet (the total spin of the system is $S = 0$), in conformity with the quantum-mechanical classification of states according to the total spin value.

We described the spin liquid within second-order theory by the method of Green functions. A method for self-consistently calculating spin liquid parameters, namely, the parameter of excitation spectrum stiffness λ , the modulus of the spin correlator between the nearest neighbors K_1 , and the gap parameter δ , as functions of the temperature was suggested. The spin liquid energy (in units of exchange parameter per bond) is $\varepsilon = -(3/4)K_1$, and the ground state energy is $\varepsilon_0 = -0.133$. The $\delta \neq 0$ parameter plays an important role. It preserves the translational invariance of the principal lattice in the spin system, determines correlation length $\xi = 1/\sqrt{z\delta}$, and leads to the Curie law for the magnetic susceptibility of the spin liquid at high temperatures.

The spin liquid has a short-range order similar to the antiferromagnetic order with alternating spin correlation functions. The behavior of reciprocal susceptibility is also close to that characteristic of antiferromagnets (even to the existence of the paramagnetic Curie point).

The antiferromagnetic state can compete with the spin liquid state if there are stabilizing factors. The conclusion can be drawn that systems with a long-range magnetic order transform into the spin liquid state at temperatures above critical.

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