

MAGNETISM AND FERROELECTRICITY

Two-Dimensional Heisenberg Model with Spin $s = 1/2$ and Antiferromagnetic Exchange Treated as a Spin Liquid

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Abstract—The spin system of the Heisenberg model ($s = 1/2$) on a square lattice with antiferromagnetic (AFM) exchange between nearest neighbors (in which there is no long-range magnetic order at any $T \neq 0$) is treated as a spatially homogeneous isotropic spin liquid. The double-time temperature Green's function method is used in the framework of a second-step decoupling scheme. It is shown that, as $T \rightarrow 0$, the spin liquid goes over (without any change in symmetry) to a singlet state with energy (per bond) $\varepsilon_0 = -0.352$ and the correlation length diverges as $\xi \propto T^{-1} \exp(T_0/T)$. The spatial spin correlators oscillate in sign with distance, as in the AFM state. The theory allows one to calculate the main characteristics of the system in all temperature ranges. © 2002 MAIK "Nauka/Interperiodica".

1. INTRODUCTION

The objective of this paper is to discuss the problem of the ground state and the main thermodynamic properties of the $s = 1/2$ spin system described by the isotropic Heisenberg model on a square lattice with antiferromagnetic (AFM) exchange interaction between nearest neighbors ($J > 0$). The Hamiltonian H and the total spin S are

$$H = \frac{1}{2} J \sum_{\mathbf{f}\mathbf{a}} \mathbf{s}_{\mathbf{f}} \mathbf{s}_{\mathbf{f}+\mathbf{a}}, \quad S = \sum_{\mathbf{f}} \mathbf{s}_{\mathbf{f}}. \quad (1)$$

We will consider the general case of the Hamiltonian (1) on an alternant lattice¹ of N sites with periodic boundary conditions. In Eq. (1), \mathbf{f} specifies the lattice sites, D is the lattice dimensionality, z is the number of nearest neighbors, and \mathbf{a} are the vectors connecting nearest neighbors. The ground state and the thermodynamic properties of the system essentially depend on its dimensionality D .

The problem of the ground state (at $T = 0$) for the two-dimensional model ($D = 2$, $z = 4$) still remains unsolved. Marshall [1, 2] argued that the ground state of the Hamiltonian (1) on alternant lattices is a nondegenerate singlet with total spin $S = 0$ (this statement has been rigorously proved only for a one-dimensional chain). On the other hand, on alternant lattices of $D = 2$ and 3, the spin distribution can have a chessboard pattern described by the Néel wave function of an antiferromagnet with two equivalent sublattices which are

mirror images of each other. It is generally agreed that at $T = 0$, the two-sublattice AFM state with long-range order is the closest approximation to the ground state of the system [3]. However, Anderson [4] assumed that the ground state of the Hamiltonian (1) on a square lattice can be disordered and described by a wave function with resonant valence bonds (RVBs). Later [5], the energy of the disordered (singlet) state was calculated numerically with RVB wave functions on 128×128 and 256×256 lattices and was found to be -0.3344 per bond, which is equal, within 0.1%, to the best result for the energy of the ordered AFM state. However, in [6], using exact diagonalization for a small (4×4) cluster, the energy of the singlet state was calculated to be -0.3509 . Different methods for solving this problem are reviewed in [3].

The thermodynamic properties are also of fundamental importance. According to the Mermin–Wagner theorem [7], long-range magnetic order can exist at $T \neq 0$ only on three-dimensional (or quasi-two-dimensional) lattices ($D = 3$) up to the critical temperature T_c . Therefore, the AFM state on a square ($D = 2$) lattice is represented by the “pricked-out” temperature point and the problem arises of describing the system at $T \neq 0$. In a sense, the case of dimensionality $D = 2$ is critical or intermediate between a one-dimensional system (in which the long-range magnetic order can never occur) and three-dimensional systems with a long-range magnetic order at temperatures below the critical point.

The theory of the thermodynamic properties of this system was developed in [8–11], where the long-range AFM order of the Néel type was postulated to occur at $T = 0$.

¹ A lattice is termed alternant if it is made up of two interpenetrating equivalent sublattices A and B , such that the nearest neighbors of a site of sublattice A are sites of sublattice B alone and *vice versa*.

In this paper, the two-dimensional system is assumed to be in a nonmagnetic state with a well-developed short-range AFM order. This state is referred to as the spin liquid (SL). In describing the thermodynamic properties of the SL, we make some assumptions and follow the method used in [8–11]. As $T \rightarrow 0$, the SL goes over, without any change in symmetry, to a singlet state with an energy per bond ε_0 . However, it is not known in advance whether or not this state is the ground state, because the AFM state with energy ε_{AF} can also arise. Only a comparison between ε_0 and ε_{AF} will allow one to draw a conclusion as to the type of the ground state.

2. SPIN LIQUID: CORRELATION FUNCTIONS AND GREEN'S FUNCTIONS

We define the spin liquid as a spatially homogeneous state (with the short-range order symmetry unbroken) in which (i) the spin correlation functions are isotropic, i.e.,

$$\begin{aligned} \frac{1}{N} \sum_{\mathbf{f}} \langle s_{\mathbf{f}}^x s_{\mathbf{f}+\mathbf{r}}^x \rangle &= \frac{1}{N} \sum_{\mathbf{f}} \langle s_{\mathbf{f}}^y s_{\mathbf{f}+\mathbf{r}}^y \rangle \\ &= \frac{1}{N} \sum_{\mathbf{f}} \langle s_{\mathbf{f}}^z s_{\mathbf{f}+\mathbf{r}}^z \rangle \equiv \frac{1}{4} K_r, \end{aligned} \quad (2)$$

and depend only on the magnitude $r = |\mathbf{r}|$ of the space vector, with $K_0 = 1$ and, hence, $\langle s_{\mathbf{f}}^2 \rangle = 3/4$ (here and henceforth, $\langle \dots \rangle$ is a thermodynamic average at $T \neq 0$ or the expectation value in the singlet state $|\Psi_0\rangle$ at $T = 0$), and (ii) the following averages are zero:

$$\langle s_{\mathbf{f}}^{\alpha} \rangle = 0, \quad \langle S^{\alpha} \rangle = 0, \quad (3a)$$

$$\langle s_{\mathbf{f}}^{\alpha} s_{\mathbf{m}}^{\beta} s_{\mathbf{n}}^{\gamma} \rangle = 0, \quad \mathbf{f} \neq \mathbf{m} \neq \mathbf{n}; \quad (3b)$$

the averages of any other odd products of the operators at different sites are also zero ($\alpha = x, y, z$ or $+, -, z$).

The properties of the SL state are mainly determined by the temperature dependence of the spin correlation functions. The SL state energy per bond (in units of J) is

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

where $K_a = -K_1$ ($K_1 > 0$) is the correlation function for nearest neighbors (a is the lattice parameter). At $T = 0$, Eq. (4) gives the energy of the singlet state ε_0 .

To describe the SL state, we go over to the Fourier transforms of the spin operators and introduce the Fourier

transform of the correlation function

$$\begin{aligned} K(\mathbf{q}) &= \sum_{\mathbf{r}} e^{-i\mathbf{q}\mathbf{r}} K_r = 4 \langle s^z(\mathbf{q}) s^z(-\mathbf{q}) \rangle \\ &= 2 \langle s^+(\mathbf{q}) s^-(\mathbf{q}) \rangle, \end{aligned} \quad (5)$$

$$K_r = \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} K(\mathbf{q})$$

with evident properties $K(\mathbf{q}) = K(-\mathbf{q})$ and $K_r = K_{-r}$. Given the Fourier transform $K(\mathbf{q})$, one can calculate any space correlators K_r . We follow the method applied in [8–11] and calculate $K(\mathbf{q})$ using the double-time retarded temperature Green's functions [12]. Below, we calculate the function $\langle\langle s^z(\mathbf{q}) | s^z(-\mathbf{q}) \rangle\rangle_{\omega} \equiv G(\mathbf{q}, \omega)$. Since the spin correlators are isotropic, we have $\langle\langle s^+(\mathbf{q}) | s^-(\mathbf{q}) \rangle\rangle_{\omega} = 2G(\mathbf{q}, \omega)$.

3. EQUATIONS OF MOTION

It is convenient to go over to the dimensionless Hamiltonian $h = H/zJ$; all energetic parameters will also be measured in units of zJ . The equations of motion have the form ($\hbar = 1$)

$$i\dot{s}_{\mathbf{f}}^+ = \frac{1}{z} \sum_{\mathbf{a}} (s_{\mathbf{f}+\mathbf{a}}^z s_{\mathbf{f}}^+ - s_{\mathbf{f}}^z s_{\mathbf{f}+\mathbf{a}}^+), \quad (6)$$

$$i\dot{s}_{\mathbf{f}}^z = \frac{1}{2z} \sum_{\mathbf{a}} (s_{\mathbf{f}}^+ s_{\mathbf{f}+\mathbf{a}}^- - s_{\mathbf{f}+\mathbf{a}}^+ s_{\mathbf{f}}^-),$$

$$\frac{\partial^2 s_{\mathbf{f}}^z}{\partial t^2} = \frac{1}{2z^2} \sum_{\mathbf{a}} (s_{\mathbf{f}}^z - s_{\mathbf{f}+\mathbf{a}}^z) + R_{\mathbf{f}}, \quad (7)$$

where

$$\begin{aligned} R_{\mathbf{f}} &= \frac{1}{2} \sum_{\mathbf{a} \neq \mathbf{a}'} \left[s_{\mathbf{f}}^z s_{\mathbf{f}+\mathbf{a}}^+ s_{\mathbf{f}+\mathbf{a}'}^- + s_{\mathbf{f}+\mathbf{a}}^z s_{\mathbf{f}+\mathbf{a}'}^- \frac{1}{2} (s_{\mathbf{f}}^+ s_{\mathbf{f}+\mathbf{a}}^- + s_{\mathbf{f}+\mathbf{a}}^+ s_{\mathbf{f}}^-) \right. \\ &\quad \left. - s_{\mathbf{f}+\mathbf{a}}^z \frac{1}{2} (s_{\mathbf{f}}^+ s_{\mathbf{f}+\mathbf{a}}^- + s_{\mathbf{f}+\mathbf{a}}^+ s_{\mathbf{f}}^-) \right. \\ &\quad \left. - s_{\mathbf{f}+\mathbf{a}'}^z \frac{1}{2} (s_{\mathbf{f}}^+ s_{\mathbf{f}+\mathbf{a}}^- + s_{\mathbf{f}+\mathbf{a}}^+ s_{\mathbf{f}}^-) \right]. \end{aligned} \quad (8)$$

In the second-order differential equation, the kinematic properties of spin operators at one site are exactly taken into account, which is of fundamental importance.

The chain of equations is cut off at the second step by linearizing the operator $R_{\mathbf{f}}$ ($\mathbf{a} \neq \mathbf{a}'$) according to the scheme [8–11]

$$s_{\mathbf{f}}^z s_{\mathbf{f}+\mathbf{a}}^+ s_{\mathbf{f}+\mathbf{a}'}^- \approx \alpha_2 \langle s_{\mathbf{f}+\mathbf{a}}^+ s_{\mathbf{f}+\mathbf{a}'}^- \rangle s_{\mathbf{f}}^z = \frac{1}{2} \alpha_2 K_{\mathbf{a}-\mathbf{a}'} s_{\mathbf{f}}^z, \quad (9)$$

$$s_{\mathbf{f}+\mathbf{a}}^z s_{\mathbf{f}}^+ s_{\mathbf{f}+\mathbf{a}'}^- \approx \alpha_1 \langle s_{\mathbf{f}}^+ s_{\mathbf{f}+\mathbf{a}'}^- \rangle s_{\mathbf{f}+\mathbf{a}}^z = \frac{1}{2} \alpha_1 K_{\mathbf{a}} s_{\mathbf{f}+\mathbf{a}}^z,$$

where α_1 is a factor which corrects the decoupling approximation for nearest neighbors ($K_a = -K_1$) and

α_2 is an analogous factor for the correlators at distances $r = d = \sqrt{2}a$ (along a diagonal) and $r = 2a$ (in what follows, we put $a = 1$). Thus, we have

$$(R_f)_{\text{lin}} = \frac{1}{2} \frac{1}{z^2} \sum_{a \neq a'} [\alpha_2 K_{a-a'} (s_{\mathbf{f}}^z - s_{\mathbf{f}+a}^z) + \alpha_1 K_1 (s_{\mathbf{f}+a'}^z - s_{\mathbf{f}+a'-a}^z)], \quad (10)$$

$$K_2 = \frac{1}{2} \sum_{a, a'} K_{a-a'} = \frac{1}{z} [1 + (z-2)K_d + K_{2a}]. \quad (11)$$

Using Eqs. (6) and linearized equation (7), the Fourier transform of the Green's function in the second-step decoupling scheme is routinely found to be

$$G(\mathbf{q}, \omega) = \frac{A(\mathbf{q})}{\omega^2 - \Omega_{\mathbf{q}}^2}, \quad A(\mathbf{q}) = \frac{K_1}{2} (1 - \gamma_{\mathbf{q}}) \quad (12)$$

with the excitation spectrum

$$\Omega_{\mathbf{q}} = \lambda E_{\mathbf{q}}(\Delta), \quad E_{\mathbf{q}}(\Delta) = \sqrt{(1 - \gamma_{\mathbf{q}})(1 + \gamma_{\mathbf{q}} + \Delta)},$$

$$\gamma_{\mathbf{q}} = \frac{1}{D} \sum_j \cos q_j, \quad (13)$$

where λ is the hardness parameter of the excitation spectrum,

$$\lambda^2 = \alpha_1 K_1 / 2, \quad (14)$$

and the pseudogap Δ at $\mathbf{q} = \mathbf{Q} = (\pi, \pi)$ (where $\gamma_{\mathbf{Q}} = -1$) is given by

$$1 + \Delta = \frac{1}{2\lambda^2} \left[\frac{1 + 2\lambda^2}{z} + \alpha_2 \left(K_2 - \frac{1}{z} \right) \right]. \quad (15)$$

The spectrum $\Omega_{\mathbf{q}} \geq 0$ describes collective triplet excitations from the singlet state. All parameters of the spectrum are temperature-dependent and should be calculated self-consistently.

4. SELF-CONSISTENCY EQUATIONS

The imaginary part of the Green's function (12) is equal to

$$-\frac{1}{\pi} \text{Im} G(\mathbf{q}, \omega + i0) = \frac{A(\mathbf{q})}{2\Omega_{\mathbf{q}}} [\delta(\omega - \Omega_{\mathbf{q}}) - \delta(\omega + \Omega_{\mathbf{q}})] \equiv n(\mathbf{q}, \omega); \quad (16)$$

therefore, the spectral density for the z components is

$$J(\mathbf{q}, \omega; \tau) = \frac{e^{\omega/\tau}}{e^{\omega/\tau} - 1} n(\mathbf{q}, \omega), \quad (17)$$

where $\tau = T/zJ$ is the dimensionless temperature. Using a spectral theorem [12], the equal-time correlation

function can be written as

$$\langle s^z(\mathbf{q}) s^z(-\mathbf{q}) \rangle \equiv \frac{1}{4} K(\mathbf{q}) = \frac{A(\mathbf{q})}{2\Omega_{\mathbf{q}}} \coth\left(\frac{\Omega_{\mathbf{q}}}{2\tau}\right) \quad (18)$$

or

$$K(\mathbf{q}) = \frac{K_1}{\lambda} \frac{1 - \gamma_{\mathbf{q}}}{E_{\mathbf{q}}(\Delta)} \coth\left(\frac{\lambda E_{\mathbf{q}}(\Delta)}{2\tau}\right). \quad (19)$$

Using the definition of the space correlators K_r of Eq. (5), one can derive the relations

$$K_n = \frac{1}{N} \sum_{\mathbf{q}} (-\gamma_{\mathbf{q}})^n K(\mathbf{q}) = \frac{K_1}{\lambda} I_n(\Delta, \tau), \quad K_0 = 1, \quad (20)$$

where

$$I_n(\Delta, \tau) = \frac{1}{N} \sum_{\mathbf{q}} \frac{(1 - \gamma_{\mathbf{q}})(-\gamma_{\mathbf{q}})^n}{E_{\mathbf{q}}(\Delta)} \coth\left(\frac{\lambda E_{\mathbf{q}}(\Delta)}{2\tau}\right), \quad (21)$$

$$n = 0, 1, 2.$$

These equations should be solved self-consistently in combination with Eq. (15) for the pseudogap and Eq. (14).

As in [8–11], there are five parameters ($K_1, K_2, \alpha_1, \alpha_2, \Delta$) to be found from three equations (20) ($n = 0, 1, 2$) and Eq. (15). The needed fifth equation can be chosen arbitrarily to some extent. Shimahara and Takada [8] put $r_{\alpha} = (\alpha_1 - 1)/(\alpha_2 - 1) = \text{const}$ and found this parameter from the condition that the AFM state with sublattice magnetization $m = 0.3$ exist at $T = 0$; that is, the ground state is postulated to be antiferromagnetic. We will refer to this as the Shimahara–Takada (ST) condition.

In this paper, the needed fifth equation for closing the set of equations is chosen on the basis of Eq. (3b). Using the rules for calculating the products of spin operators at one site and Eq. (3b), one can exactly calculate the average:

$$\langle R_f s_{\mathbf{f}}^z \rangle = \frac{1}{4z^2} \sum_{a \neq a'} \langle s_{\mathbf{f}+a}^+ s_{\mathbf{f}+a'}^- \rangle = \frac{1}{8} \tilde{K}_2, \quad (22)$$

$$\tilde{K}_2 = K_2 - 1/z,$$

which allows one to find

$$\left\langle \left(-\frac{\partial^2 s_{\mathbf{f}}^z}{\partial t^2} \right) s_{\mathbf{f}}^z \right\rangle = \frac{1}{8} \left(K_2 + \frac{1}{z} K_1 \right). \quad (23)$$

In the framework of the linear theory used here, we have

$$\begin{aligned} & \left\langle \left(-\frac{\partial^2 s_{\mathbf{f}}^z}{\partial t^2} \right)_{\text{lin}} s_{\mathbf{f}}^z \right\rangle \\ &= \frac{1}{8} \left(\frac{1+K_1}{z} + [\alpha_2(1+K_1) - \alpha_1 K_1] \tilde{K}_2 - \frac{z-1}{z} \alpha_1 K_1^2 \right). \end{aligned} \quad (24)$$

From the condition that exact equation (23) and approximate equation (24) be the same, we obtain the fifth equation needed to close the set of equations.

Equation (24) is conveniently represented in an equivalent form by expressing it in terms of the second moment. Using the spectral theorem, the single-site average can be written as

$$\begin{aligned} \langle s_{\mathbf{f}}^z(t) s_{\mathbf{f}}^z(0) \rangle &= \int_{-\infty}^{\infty} e^{-i\omega t} J_0(\omega) d\omega, \\ J_0(\omega) &= \frac{1}{N} \sum_{\mathbf{q}} J(\mathbf{q}, \omega; \tau), \end{aligned} \quad (25)$$

where $J_0(\omega)$ is the spectral density of the single-site Green's function $G_{\mathbf{ff}}(\omega) \equiv G_0(\omega)$.

The zeroth moment is defined as the average in Eq. (25) at $t=0$:

$$\begin{aligned} M_0 &= \langle s_{\mathbf{f}}^z(0) s_{\mathbf{f}}^z(0) \rangle = \langle s_{\mathbf{f}}^z s_{\mathbf{f}}^z \rangle = \frac{1}{4} \\ &= \int_{-\infty}^{\infty} J_0(\omega) d\omega = \frac{1}{N} \sum_{\mathbf{q}} \frac{A(\mathbf{q})}{2\Omega_{\mathbf{q}}} \coth\left(\frac{\Omega_{\mathbf{q}}}{2\tau}\right). \end{aligned} \quad (26)$$

This relation is a sum rule and reproduces the expression for the correlator K_0 . Differentiating Eq. (25) with respect to time and putting $t=0$, we obtain the first moment

$$M_1 = \left\langle \left(i \frac{\partial s_{\mathbf{f}}^z(t)}{\partial t} \right) s_{\mathbf{f}}^z(0) \right\rangle_{t=0} = \int_{-\infty}^{\infty} \omega J_0(\omega) d\omega. \quad (27)$$

The left-hand side of Eq. (27) can be exactly calculated using Eq. (6), which gives $K_1/4$. The same is obtained by calculating the right-hand side; that is, we have an identity. The second moment is defined as

$$M_2 = \left\langle \left(-\frac{\partial^2 s_{\mathbf{f}}^z(t)}{\partial t^2} \right) s_{\mathbf{f}}^z(0) \right\rangle_{t=0} = \int_{-\infty}^{\infty} \omega^2 J_0(\omega) d\omega. \quad (28)$$

The left-hand side of Eq. (28) is given by exact

expression (23). Calculating the right-hand side, we represent Eq. (28) in the form

$$\frac{1}{8} (K_2 + K_1/z) = \frac{1}{4} \lambda K_1 P(\Delta, \tau), \quad (29)$$

$$P(\Delta, \tau) = \frac{1}{N} \sum_{\mathbf{q}} (1 - \gamma_{\mathbf{q}}) E_{\mathbf{q}}(\Delta) \coth\left(\frac{\Omega_{\mathbf{q}}}{2\tau}\right).$$

Equation (29) is equivalent to the requirement that $\langle R_{\mathbf{f}} s_{\mathbf{f}}^z \rangle = \langle (R_{\mathbf{f}})_{\text{lin}} s_{\mathbf{f}}^z \rangle$ and, therefore, that Eq. (23) be identical to Eq. (24). Thus, instead of the ST condition used in [8], we derived a new self-consistency condition in the form of Eq. (29). Therefore, the self-consistent second-step decoupling scheme can be based on the requirement that the first three moments (M_0, M_1, M_2) be calculated exactly.

5. SELF-CONSISTENT SOLUTION OF THE EQUATIONS

In what follows, the set of equations (20), (15), and (29) with $\Omega_{\mathbf{q}} = \lambda E_{\mathbf{q}}(\Delta)$ and $\lambda^2 = \alpha_1 K_1/2$ will be solved analytically and numerically. For this purpose, we represent Eq. (21) in the form

$$\begin{aligned} I_n(\Delta, \tau) &= I_n(\Delta) + B_n(\Delta, \tau), \\ I_n(\Delta) &= \frac{1}{N} \sum_{\mathbf{q}} \frac{(1 - \gamma_{\mathbf{q}})(-\gamma_{\mathbf{q}})^n}{E_{\mathbf{q}}(\Delta)}, \end{aligned} \quad (30)$$

$$\begin{aligned} B_n(\Delta, \tau) &= \frac{1}{N} \sum_{\mathbf{q}} \frac{(1 - \gamma_{\mathbf{q}})(-\gamma_{\mathbf{q}})^n}{E_{\mathbf{q}}(\Delta)} \\ &\times \frac{2}{\exp(\lambda E_{\mathbf{q}}(\Delta)/\tau) - 1}. \end{aligned} \quad (31)$$

The integrals $I_n(\Delta)$ correspond to zero temperature ($\tau=0$); therefore, we put $\Delta = \Delta(0)$ in them. The energy of the system given by Eq. (4) is minimal when K_1 reaches its maximum and, as can be easily shown, when $\Delta(0) = 0$. In this case, the integrals take the form

$$\begin{aligned} I_n(0) \equiv I_n &= \frac{1}{N} \sum_{\mathbf{q}} \sqrt{\frac{1 - \gamma_{\mathbf{q}}}{1 + \gamma_{\mathbf{q}}}} (-\gamma_{\mathbf{q}})^n \\ &= \int_{-1}^1 D(\gamma) \sqrt{\frac{1 - \gamma}{1 + \gamma}} (-\gamma)^n d\gamma. \end{aligned} \quad (32)$$

Here, $D(\gamma)$ is the density of states (on the square lattice) for the dispersion law $\gamma_{\mathbf{q}} = 0.5(\cos q_x + \cos q_y)$; this den-

sity of states is expressed through the complete elliptic integral of the first kind $\mathbf{K}(x)$ as

$$D(\gamma) = \frac{2}{\pi^2} \mathbf{K}(\sqrt{1-\gamma^2}) \approx \frac{1}{\pi} - \left(\frac{1}{2} - \frac{1}{\pi}\right) \ln|\gamma|, \quad (33)$$

$$\int_{-1}^1 D(\gamma) d\gamma = 1.$$

A calculation gives the following values: $I_0 = 1.396$ and $I_1 = I_2 = 0.555$. The integrals $B_n(\Delta, \tau)$ can also be expressed through the density of states.

5.1. Low-Temperature Regime

In the case of $\tau \rightarrow 0$, we calculate the integrals B_n following the procedure employed in [8, 13]. When $\tau \rightarrow 0$, the vicinity of the point $\mathbf{q} = \mathbf{Q}$ is the most important, because this region can lead not only to power-law terms but also to anomalous terms that do not vanish as $\tau \rightarrow 0$. Calculations give

$$B_0(t) = C(t) + \frac{D(1)}{2} t^3, \quad (34)$$

$$B_1(t) = B_2(t) = C(t) - \frac{3}{2} D(1) t^3$$

to within terms $O(t^5)$. Here, $D(1) = 1/\pi$ and

$$C(t) = \frac{2}{\pi} \ln\left(\frac{t^2}{2\Delta}\right), \quad t = \tau/\lambda(0). \quad (35)$$

We represent the low-temperature dependence of the energy gap parameter in the most general form,

$$\Delta(t) = \Delta_0 t^{2\beta} \exp\left(-\frac{2t_0}{t}\right), \quad (36)$$

which allows us to consider two scenarios: we will have power-law behavior ($\beta > 0$) if $t_0 = 0$ and exponential behavior if $t_0 \neq 0$. As in [8–11], we will say that condensation occurs in the vicinity of the point $\mathbf{q} = \mathbf{Q} = (\pi, \pi)$ (where $\gamma_{\mathbf{Q}} = -1$) if the function given by Eq. (35) tends to a nonzero value as $\tau \rightarrow 0$:

$$C(0) = \lim_{t \rightarrow 0} C(t) = \frac{4t_0}{\pi} \equiv C, \quad (37)$$

which is independent of the preexponential factor in Eq. (36).

5.2. The Ground State of the System on a Square Lattice

The set of equations (20), (15), and (22), which allows the parameters of the system to be determined self-consistently, possesses the following solution for $\tau = 0$, $\Delta = 0$, and $P(0, 0) = 0.84$:

$$\lambda = 0.744, \quad K_1 = 0.469, \quad (38)$$

$$\alpha_1 = 2.236, \quad \alpha_2 = 2.65, \quad C = 0.189.$$

The energy of the system per bond (in units of J) is

$$\varepsilon_0 = -(3/4)K_1 = -0.352, \quad (39)$$

which is lower than the energy of the AFM state $\varepsilon_{\text{AF}} = -0.335$ (the best result of the spin-wave theory [3]). An energy very close to this numerical value was found in [8] ($\varepsilon_{\text{AF}} = -0.3508$) for the sublattice magnetization $m = 0.3$ and in [9, 10] ($\varepsilon_{\text{AF}} = -0.345$). We will show that the solution found is a singlet. A singlet state at $\tau = 0$ must satisfy the condition $\langle \mathbf{S}^2 \rangle = 0$. Let us consider the function

$$S^2(\tau) \equiv \frac{1}{N} \langle \mathbf{S}^2 \rangle = \frac{1}{N} \sum_{\text{fm}} \langle \mathbf{s}_f \mathbf{s}_m \rangle \quad (40)$$

$$= \frac{1}{N} \sum_{\text{fr}} \langle \mathbf{s}_f \mathbf{s}_{f+\mathbf{r}} \rangle = \frac{3}{4} \sum_{\mathbf{r}} K_{\mathbf{r}} = \frac{3}{4} K(0).$$

From Eq. (19), it follows that

$$K(0) = \lim_{\mathbf{q} \rightarrow 0} K(\mathbf{q})$$

$$= \frac{K_1}{\lambda} \lim_{\mathbf{q} \rightarrow 0} \frac{1 - \gamma_{\mathbf{q}}}{E_{\mathbf{q}}(\Delta)} \coth\left(\frac{\Omega_{\mathbf{q}}}{2\tau}\right) = \frac{4\tau}{\alpha_1(2 + \Delta)}, \quad (41)$$

which gives $K(0) = 0$ and $\langle \mathbf{S}^2 \rangle = 0$ at $\tau = 0$. Thus, according to the approximate analytical theories developed to date, the ground state of the spin system on a square lattice is a singlet. This conclusion is supported by the result $\varepsilon_0 = -0.3509$ [6] obtained by the exact-diagonalization method for a cluster.

5.3. The Equation for Δ

The solution with $C \neq 0$ obtained above implies an exponential $\Delta(\tau)$ dependence, according to Eq. (36), and allows one to find the parameter $\tau_0 = \lambda t_0 = (\pi\lambda/4)C = 0.11$. In the case of a pure power-law $\Delta(\tau)$ dependence (for which $C = 0$), the set of equations has no self-consistent solution. It should be noted that in the three-dimensional case, the condensate does not occur ($C = 0$) because of the square-root dependence of the density of states near the limits of the spectrum.

In the low-temperature range, Eq. (15) for the energy gap Δ has a solution

$$2\Delta(\tau) \approx \left(\frac{\tau}{\lambda}\right)^2 \exp(-2\tau_0/\tau). \quad (42)$$

It follows from Eq. (42) that in this temperature range, the parameters λ , α_1 , and α_2 show a pure power-law dependence (as was found in [8]) with the main contribution $\propto \tau^3$:

$$\lambda(\tau) = \lambda - \frac{3}{2\pi} (\tau/\lambda)^3, \quad (43)$$

$$\alpha_1(\tau) = \alpha_1 - A_1 \tau^3, \quad \alpha_2(\tau) = \alpha_2 - A_2 \tau^3.$$

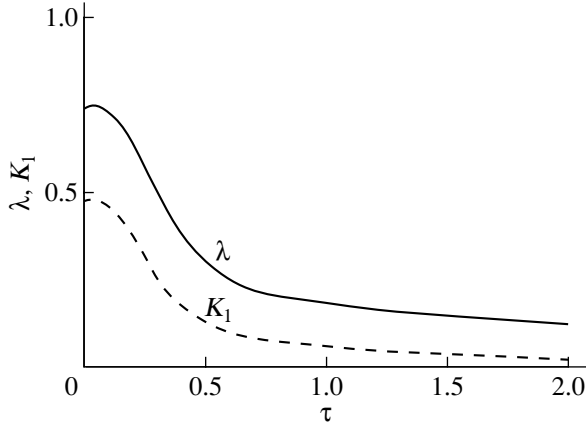


Fig. 1. Dependence of the hardness parameter of the excitation spectrum $\lambda(\tau)$ (solid curve) and the modulus of the correlator for nearest neighbors $K_1(\tau)$ (dashed curve) on dimensionless temperature $\tau = T/zJ$ for a square lattice ($z = 4$).

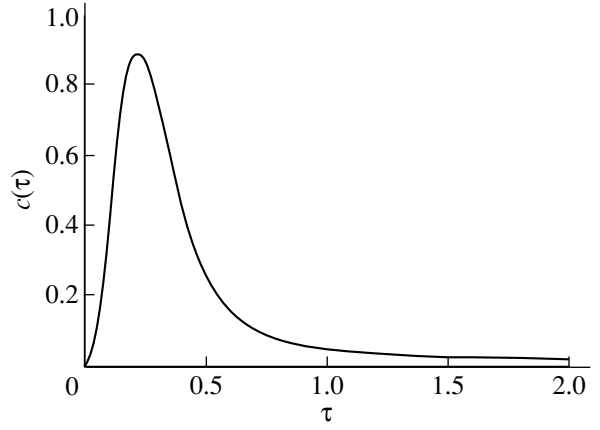


Fig. 2. Specific heat $c(\tau)$ (in dimensionless units) of the spin liquid on a square lattice.

Since $K_1(\tau) = K_1 - \kappa\tau^3$ in this temperature range, the energy of the system behaves as

$$\varepsilon(\tau) = -(3/4)K_1(\tau) = \varepsilon_0 + (3/4)\kappa\tau^3 \quad (44)$$

and the specific heat $c(\tau) \propto \tau^2$.

5.4. Thermodynamic Properties of the Spin Liquid

The replacement of the ST condition by Eq. (29) does not affect the character of the temperature dependence of the model parameters; however, the numerical values of the coefficients are changed insignificantly. For this reason, we will only discuss the main results and will not present details concerning self-consistent calculations of the thermodynamic SL characteristics.

Self-consistent calculations of the hardness parameter $\lambda(\tau)$ of the excitation spectrum and the modulus of the correlation function for nearest neighbors $K_1(\tau)$ are represented in Fig. 1. Their asymptotic temperature dependence (for $\tau > 2$) is described by a power law: $\lambda(\tau) \approx 0.18/\tau^{1/2}$ and $K_1(\tau) \approx 0.06/\tau$.

The specific heat (in dimensionless units) is $c(\tau) = \partial\varepsilon(\tau)/\partial\tau$; its temperature dependence is shown in Fig. 2. For $\tau \rightarrow 0$, we have $c(\tau) \propto \tau^2$ in accordance with Eq. (44); the maximum is reached at the temperature $\tau^* \approx 0.2 \approx 2\tau_0$, and the asymptotic high-temperature dependence is $c(\tau) \propto 1/\tau^2$, because $K_1(\tau) \propto 1/\tau$.

The dynamic susceptibility of the spin system (in dimensionless units) is given by [12]

$$\chi^{\alpha\beta}(\mathbf{q}, \omega) = -\langle\langle s^\alpha(\mathbf{q}) | s^\beta(-\mathbf{q}) \rangle\rangle_\omega. \quad (45)$$

In the SL state, the correlation functions are isotropic and, therefore, $\chi^+(\mathbf{q}, \omega) = 2\chi^{zz}(\mathbf{q}, \omega)$. The static sus-

ceptibility (at $\omega = 0$), in accordance with Eq. (12), has the form

$$\begin{aligned} \chi^{zz}(\mathbf{q}, 0) &= \frac{K_1(1 - \gamma_{\mathbf{q}})}{2 \Omega_{\mathbf{q}}^2} = \frac{K_1}{2\lambda^2} \frac{1}{1 + \gamma_{\mathbf{q}} + \Delta} \\ &= \frac{1}{\alpha_1} \frac{1}{1 + \gamma_{\mathbf{q}} + \Delta}. \end{aligned} \quad (46)$$

From Eq. (46), it follows that

$$\begin{aligned} \chi^{zz}(\mathbf{q} = 0, 0) &= 1/2\alpha_1 = 0.212, \quad \tau \rightarrow 0, \\ \chi^{zz}(\mathbf{q} = \mathbf{Q}, 0) &= \frac{1}{\alpha_1 \Delta} = \frac{2\lambda^2 \exp(2\tau_0/\tau)}{\alpha_1 \tau^2}, \end{aligned} \quad (47)$$

with the latter expression diverging as $\tau \rightarrow 0$ (as in the AFM state).

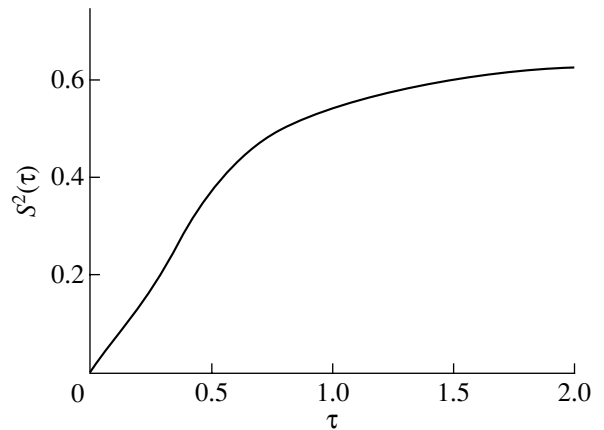


Fig. 3. Temperature dependence of the mean square of the total spin of the system (per lattice site) $S^2(\tau) = N^{-1}\langle S^2 \rangle$.

The thermodynamic longitudinal susceptibility, by definition, is [12]

$$\chi^{zz} = \frac{1}{T} [\langle (S^z(0))^2 \rangle - \langle S^z(0) \rangle^2] \equiv \frac{1}{T} \tilde{\chi}_0, \quad (48)$$

$$\tilde{\chi}_0 = \frac{1}{N} \langle (S^z)^2 \rangle = \frac{1}{3} S^2(\tau) = \frac{1}{4} K(0)$$

and equals the dynamic susceptibility for $\omega \rightarrow 0$, $\mathbf{q} \rightarrow 0$. At low temperatures, we have $\tilde{\chi}^{zz}(\tau) = \tilde{\chi}^{zz}(0) + a_1 \tau^3$, in accordance with the temperature dependence of $\alpha_1(\tau)$; the numerical value of $\tilde{\chi}^{zz}(0) = 1/2\alpha_1 = 0.212$ agrees with the result obtained in [8] if the normalization to $z = 4$ is taken into account ($T/J = z\tau$, $0.212/4 = 0.053$, as in [8]). The susceptibility $\tilde{\chi}^{zz}(\tau)$ reaches a maximum at $\tau \approx 0.1 \approx \tau_0$ and then decreases, with the asymptotic high-temperature dependence being $1/4\tau$. The temperature dependence of the mean square of the total spin of the system $S^2(\tau)$ is shown in Fig. 3.

The coefficients characterizing the asymptotic temperature dependence of the functions considered above (in the case of $\tau \rightarrow \infty$, where there are no correlations) can be found analytically under the following assumptions: (i) the excitation spectrum is limited, $\Omega_{\mathbf{q}} \rightarrow \lambda\sqrt{\Delta(1-\gamma_{\mathbf{q}})}$, i.e., $\lambda\sqrt{\Delta} \rightarrow \text{const} \equiv \bar{c}$; (ii) $S^2(\tau) \rightarrow 3/4$; and (iii) the decoupling parameters $\alpha_1(\tau) \rightarrow 1$ and $\alpha_2(\tau) \rightarrow 1$ and $K_2 \rightarrow 1/4$. Condition (ii) is equivalent to $K(0) \rightarrow 1$. Using the strong inequality $\Delta \gg 2$, we find that $\Delta(\tau) \rightarrow 4\tau$ and condition (i) reduces to $\lambda(\tau) = \bar{c}/2\sqrt{\tau}$. Asymptotically, $I_0 \rightarrow 2\tau/\lambda\Delta$, $I_2 \rightarrow (1/z)2\tau/\lambda\Delta$, and Eq. (15) for the energy gap takes the form $\Delta = 1/8\lambda^2$, from which it follows that $\bar{c}^2 = 1/2z = 1/8$ and $c = 0.354$. Thus, we have the following asymptotic ($\tau \rightarrow \infty$) temperature dependence of the parameters of the system:

$$\Delta(\tau) = 4\tau, \quad \lambda(\tau) = \frac{0.177}{\sqrt{\tau}}, \quad K_1(\tau) = \frac{0.063}{\tau}, \quad (49)$$

$$\bar{c} = \lambda(\tau)\sqrt{\Delta(\tau)} = 0.354, \quad \tilde{\chi}^{zz}(\tau) = \frac{1}{4\tau}.$$

These expressions are identical to the numerical calculations to within less than one percent.

6. SPACE CORRELATIONS

Let $\mathbf{r} = (x, y)$ be the vector connecting two arbitrary sites of a square lattice ($a = 1$). According to Eqs. (5) and (19), the space correlators have the form

$$K_r = \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} K(\mathbf{q})$$

$$= \frac{K_1}{\lambda} \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{q}\mathbf{r}} \frac{1-\gamma_{\mathbf{q}}}{E_{\mathbf{q}}(\Delta)} \coth\left(\frac{\lambda E_{\mathbf{q}}(\Delta)}{2\tau}\right), \quad (50)$$

$$e^{i\mathbf{Q}\mathbf{r}} = (-1)^{x+y}$$

and oscillate in sign with distance, as in the AFM state.

By definition, $K(\mathbf{q}) = \sum_{\mathbf{r}} \exp(-i\mathbf{q}\mathbf{r}) K_r$; therefore, at $\mathbf{q} = 0$ and $\mathbf{q} = \mathbf{Q}$, we have

$$K(0) = \sum_{\mathbf{r}} K_r, \quad K(\mathbf{Q}) = \sum_{\mathbf{r}} |K_r|. \quad (51)$$

We note that $\langle \mathbf{S}^2 \rangle = N(3/4)K(0)$, i.e., $\langle \mathbf{S}^2 \rangle = 0$ at $\tau = 0$ (the ground state is a singlet); therefore, as can be seen from the expressions for $K(0)$, the correlations of alternating sign cancel out at $\tau = 0$. It follows from the general expression for $K(\mathbf{q})$ at $\mathbf{q} = \mathbf{Q}$ that

$$K(\mathbf{Q}) = \frac{K_1}{\lambda} \frac{2}{\sqrt{2\Delta}} \coth\left(\frac{\lambda\sqrt{2\Delta}}{2\tau}\right). \quad (52)$$

Substituting the solution for Δ at low temperatures given by Eq. (42), we obtain

$$K(\mathbf{Q}) = 2K_1\tau^{-1} \exp(2\tau_0/\tau), \quad (53)$$

which diverges as $\tau \rightarrow 0$.

Now, we discuss the behavior of the correlation functions at large distances r of the order of the linear dimensions of the system \sqrt{N} ($D = 2$). At $\tau \equiv 0$, $\Delta = 0$, we obtain from Eq. (50)

$$K_r = \frac{K_1}{\lambda} \frac{1}{(2\pi)^2} \int e^{i\mathbf{q}\mathbf{r}} \sqrt{\frac{1-\gamma_{\mathbf{q}}}{1+\gamma_{\mathbf{q}}}} d^2\mathbf{q}. \quad (54)$$

In this integral, the main contribution comes from the region (of radius $k_0 \ll \pi$) of the point $\mathbf{q} = \mathbf{Q}$ of the Brillouin zone. Substituting $\mathbf{q} = \mathbf{Q} - \mathbf{k}$, we obtain

$$K_r \approx e^{i\mathbf{Q}\mathbf{r}} \frac{K_1}{\lambda} \frac{\sqrt{2}}{\pi} \int_0^{k_0 r} J_0(x) dx \frac{1}{r}, \quad (55)$$

$$|K_r| \approx \frac{0.284}{r}, \quad r \rightarrow \infty,$$

which is indicative of the absence of long-range order in the ground state. Integrating Eq. (55) over the two-dimensional lattice volume, we find $K(\mathbf{Q}) \propto \sqrt{N}$; that is, we have a divergence in the thermodynamic limit

($N \rightarrow \infty$). The staggered magnetization m is defined as [3]

$$m^2 = \left\langle \left(\frac{1}{N} \sum_{\mathbf{f}} (-1)^{x+y} \mathbf{s}_{\mathbf{f}} \right)^2 \right\rangle \quad (56)$$

$$= \frac{1}{N^2} \sum_{\mathbf{r}} |K_{\mathbf{r}}|^2 = \frac{1}{N^2} K(\mathbf{Q}).$$

In this definition, the factor $1/N$ is of importance; since $K(\mathbf{Q}) \propto \sqrt{N}$ at $\tau = 0$, we have $m^2 \propto 1/\sqrt{N} \rightarrow 0$ in the thermodynamic limit.

At low temperatures, the dominant contribution in Eq. (50) also comes from the vicinity of the point $\mathbf{q} = \mathbf{Q}$; this equation can be written as

$$K_r(\tau) \approx e^{i\mathbf{Q}\mathbf{r}} \frac{4\tau}{\alpha_1 \pi^2} \int \frac{e^{i\mathbf{k}\mathbf{r}}}{k^2 + 4\Delta} d^2\mathbf{k}. \quad (57)$$

The correlation length ξ is commonly defined by the equation $4\Delta(\tau) = \kappa^2 = \xi^{-2}$. For large values of r , we find

$$|K_r(\tau)| = \frac{4\tau}{\alpha_1} \frac{1}{2\pi} \int_0^{k_0 r} \frac{x J_0(x)}{x^2 + \kappa^2 r^2} dx \quad (58)$$

$$= \frac{4\tau}{\alpha_1} \frac{\sqrt{2}}{\sqrt{\kappa r}} \exp(-\kappa r) \left(1 - \frac{1}{8\kappa r} + \dots \right).$$

It follows from Eq. (42) that $\xi/a \propto \tau^{-1} \exp(\tau_0/\tau)$, as in [8, 13, 14]. Despite the fact that there are regions of large values of r , such that $\kappa r = r/\xi \sim 1$, the correlation function possesses the property $|K_r| \rightarrow 0$ as $\tau \rightarrow 0$ (there is no long-range order).

It was shown in [14] that the behavior of the two-dimensional Heisenberg model with AFM exchange in the long-wavelength and low-temperature regions can be described in terms of the quantal nonlinear σ model using the renormalization group method. The results obtained above correspond to the classical renormalization regime; however, in a higher order approximation, we have $\xi/a = C_\xi \exp(2\pi\rho_s/T)$, where $C_\xi \approx 1$; that is, the preexponential factor is temperature-independent [3, 14]. Thus, the low-temperature dependence of ξ can be different, but there is always an exponential divergence as $T \rightarrow 0$ in both AFM and SL singlet states.

7. CONCLUSION

Thus, we have described the Heisenberg model with Hamiltonian (1) on a square lattice as a thermodynamically stable homogeneous isotropic nonmagnetic spin liquid at any temperature T . In the limit as $T \rightarrow 0$, its

state is a singlet (with the total spin $S = 0$) with an energy per bond $\epsilon_0 = -0.352$. At $T = 0$, the AFM state with energy ϵ_{AF} can compete with the singlet state. For the best result obtained analytically within the spin-wave theory, we have $\epsilon_0 \leq \epsilon_{\text{AF}}$; that is, the ground state is a singlet. It should be noted that the results of numerical calculations at $T = 0$ are contradictory, because the difference in energy of these states is very small. In the SL state, there is a well-defined short-range AFM order with spin correlators oscillating in sign according to distance. At high temperatures ($T \gg J$), the system asymptotically goes over to the paramagnetic state ($K_1 \rightarrow 0, N^{-1}\langle \mathbf{S}^2 \rangle \rightarrow 3/4$) with susceptibility $\chi \propto 1/T$.

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REFERENCES

1. W. Marshall, Proc. R. Soc. London, Ser. A **232**, 48 (1955).
2. D. C. Mattis, *The Theory of Magnetism* (Harper and Row, New York, 1965; Mir, Moscow, 1967).
3. E. Manousakis, Rev. Mod. Phys. **63** (1), 1 (1991).
4. P. W. Anderson, Mater. Res. Bull. **8**, 153 (1973).
5. S. Liang, B. Doucot, and P. W. Anderson, Phys. Rev. Lett. **61** (10), 365 (1988).
6. K. Fabricius, U. Low, and K.-H. Mutter, Phys. Rev. B **44** (18), 9981 (1991).
7. N. Mermin and G. Wagner, Phys. Rev. Lett. **17** (22), 1136 (1966).
8. H. Shimahara and S. Takada, J. Phys. Soc. Jpn. **60**, 2394 (1991).
9. A. F. Barabanov and V. M. Berezovskii, Zh. Éksp. Teor. Fiz. **106**, 1156 (1994) [JETP **79**, 627 (1994)].
10. A. F. Barabanov and V. M. Beresovsky, Phys. Lett. A **186**, 175 (1994).
11. A. F. Barabanov, V. M. Beresovsky, and E. Zasinias, Phys. Rev. B **52** (14), 10177 (1995).
12. S. V. Tyablikov, *Methods in the Quantum Theory of Magnetism* (Nauka, Moscow, 1975, 2nd ed.; Plenum, New York, 1967).
13. M. Takahashi, Phys. Rev. B **40** (4), 2494 (1989).
14. S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B **39** (4), 2344 (1989).

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