

### Classical Heisenberg ferromagnet in two dimensions

Minoru Takahashi

*Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo 106*

(Received 11 March 1987)

Modified spin-wave theory is applied to the classical Heisenberg ferromagnet on a square lattice:  $H_c = -J_0 \sum_{\langle ij \rangle} (\mathbf{s}_i \cdot \mathbf{s}_j - 1)$ . The energy, the correlation function, and the magnetic susceptibility are calculated at low temperatures. These agree excellently with the Monte Carlo results for a  $64 \times 64$  system. For an infinite system, the reduced susceptibility behaves as  $T^2 \exp(4\pi J_0/T)$  and the correlation length behaves as  $\exp(2\pi J_0/T)$ . The preexponential factors differ from those of renormalization-group Monte Carlo calculations.

#### I. INTRODUCTION

In previous papers<sup>1</sup> a modified spin-wave theory was proposed for calculating the low-temperature properties of a quantum Heisenberg ferromagnet in one and two dimensions with the arbitrary spin quantum number  $S$ :

$$H_q = -J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z - S^2). \tag{1.1}$$

Here,  $\langle ij \rangle$  means that the  $i$  and  $j$  sites are nearest neighbors. The free energy and susceptibility derived from this theory coincide very well with the results of Bethe-ansatz integral-equation calculations for an  $S = \frac{1}{2}$  ferromagnetic Heisenberg chain at low temperature.<sup>2</sup> In the limit of infinite  $S$  the system is equivalent to the classical Heisenberg ferromagnet. In this case Hamiltonian becomes

$$H_c = -J_0 \sum_{\langle ij \rangle} (\mathbf{s}_i \cdot \mathbf{s}_j - 1), \quad \mathbf{s}_i^2 = 1. \tag{1.2}$$

The modified spin-wave theory is also applicable to this model. For the one-dimensional classical Heisenberg model, Fisher's exact solution is known.<sup>3</sup> Therefore it is easy to validate the applicability of spin-wave theory. The two-dimensional (2D) case is very interesting not only for condensed-matter physics but also for field theory, because it is related to the  $O(3)$  nonlinear  $\sigma$  model and to the confinement of quarks. Many authors have investigated the 2D case using various methods such as high-temperature expansion,<sup>4</sup> renormalization-group approximations,<sup>5</sup> the Monte Carlo method,<sup>6,7</sup> instanton theory,<sup>8</sup> and so on. Nowadays it is believed that this system has no phase transition and that its magnetic susceptibility diverges strongly as temperature approaches zero.

By using spin-wave theory, the low-temperature expansions of the energy density  $e$ , the reduced susceptibility  $\chi_0$ , and the correlation length  $\xi$  for the square lattice are obtained as follows:

$$e = J_0 [t + t^2/8 + t^3/16 + O(t^4)], \tag{1.3}$$

$$\chi_0 \equiv \sum_r \langle \mathbf{s}_0 \cdot \mathbf{s}_r \rangle = \frac{t^2}{128\pi e^\pi} \exp\left[\frac{4\pi}{t}\right] \left[1 + (\frac{1}{2} - \pi/4)t + O(t^2)\right] \sim 1.075 \times 10^{-4} t^2 \exp(4\pi/t), \tag{1.4}$$

$$\xi = \frac{1}{8\sqrt{2}e^{\pi/2}} \exp\left[\frac{2\pi}{t}\right] \left[1 - \frac{\pi}{8}t + O(t^2)\right] \sim 0.01837 \exp(2\pi/t), \tag{1.5}$$

where

$$t \equiv T/J_0. \tag{1.6}$$

Equation (1.3) can be compared with the energy derived from Monte Carlo calculations. The spin-wave theory works well at  $t \leq 0.5$ . At these temperatures  $\xi$  becomes very long and exceeds the size of the model system used for Monte Carlo calculations. The reduced susceptibility  $\chi_0$  saturates at the value of the system size. Roughly speaking, at  $t = 0.5$ ,  $\xi$  is about  $6 \times 10^3$  and at  $t = 0.25$ ,  $\xi$  is about  $1.6 \times 10^6$ . To verify Eqs. (1.4) and (1.5) at such

temperatures, one needs Monte Carlo calculations for very large systems such as  $(6 \times 10^3)^2$  or  $(1.6 \times 10^6)^2$ . Thus it is almost impossible to verify Eqs. (1.4) and (1.5) by applying Monte Carlo calculations to a finite system. Spin-wave calculations of the susceptibility and the correlation function of a finite system such as  $64 \times 64$  are possible. Those results agree excellently with Monte Carlo calculations for the same system at  $t \leq 0.5$ . Therefore it can be concluded that (1.4) and (1.5) are valid for a sufficiently large system. The high-temperature expansions of  $e$  and  $\chi_0$  are available up to tenth orders.<sup>4</sup> For

the energy density  $e$ , the low-temperature expansion (1.3) and the high-temperature expansion connect smoothly at  $t \sim 0.5-0.75$ . For the susceptibility  $\chi_0$ , coincidence occurs near  $t \sim 0.5$ . But the connection is not as smooth as that of the energy density.

Shenker and Tobochnik<sup>6</sup> give the following formulas for  $\chi_0$  and  $\xi$ :

$$\begin{aligned} \chi_0 &= 0.018 \left[ \frac{t}{2\pi+t} \right]^4 \exp(4\pi/t) \\ &\simeq 1.1 \times 10^{-5} t^4 \exp(4\pi/t), \end{aligned} \quad (1.7)$$

$$\begin{aligned} \xi &\simeq 0.010 \left[ \frac{t}{2\pi+t} \right] \exp(2\pi/t) \\ &\simeq 1.6 \times 10^{-3} t \exp(2\pi/t). \end{aligned} \quad (1.8)$$

They used Monte Carlo data on a  $50 \times 50$  lattice. Several authors have confirmed these formulas using bigger lattices.<sup>7</sup> The exponential terms of these formulas are the same as in Eqs. (1.4) and (1.5). Preexponential factors, however, are different. Shenker and Tobochnik derived the functional form of  $\chi_0$  using a renormalization-group approximation and determined the amplitude of  $\chi_0$  by Monte Carlo calculation. Equation (1.7) is about one-fortieth of (1.4) at  $t \leq 0.5$ . Thus, modified spin-wave theory gives qualitatively the same but quantitatively different results from those of Shenker and Tobochnik. Fisher and Nelson<sup>5</sup> proposed that the susceptibility behaves as follows:

$$\chi_0 \simeq 0.00436t^2 \exp(4\pi/t). \quad (1.9)$$

This functional form is different from that of Shenker and Tobochnik, but the same as that of (1.4). I do not know which one is correct according to renormalization-group theory. But modified spin-wave theory supports functional form (1.9). Fisher and Nelson determined the amplitude from a high-temperature expansion. In contrast to (1.7), this is about 40 times larger than (1.4).

In Sec. II the modified spin-wave theory will be reviewed. Fundamental equations for the classical Heisenberg model are derived by taking the limit of  $S \rightarrow \infty$ . The spin-wave results for the linear chain are compared with Fisher's exact solution.<sup>3</sup> In Sec. III the energy, the correlation function, and the susceptibility of an infinite square lattice are derived. These quantities are calculated also for a  $64 \times 64$  system. The spin-wave results show

excellent agreement with Monte Carlo results for the same system. In Sec. IV the relations between the spin-wave theory and the renormalization-group method will be discussed. In the Appendix a direct derivation of fundamental equations for classical systems will be given.

## II. MODIFIED SPIN-WAVE THEORY FOR THE CLASSICAL SYSTEM

The Holstein-Primakoff transformation is applied to (1.1):

$$\begin{aligned} S_j^+ &= S_j^x + iS_j^y = \sqrt{2S} f_j(S) a_j, \\ S_j^- &= S_j^x - iS_j^y = \sqrt{2S} a_j^* f_j(S), \end{aligned} \quad (2.1)$$

$$S_j^z = S - a_j^* a_j,$$

$$f_j(S) = [1 - (2S)^{-1} a_j^* a_j]^{1/2} = 1 - (4S)^{-1} a_j^* a_j + O(S^{-2}). \quad (2.2)$$

Here,  $a_j^*$  and  $a_j$  are the creation and annihilation operators of bosons at the  $j$ th site. The pair product operator  $\mathbf{S}_i \cdot \mathbf{S}_j$  can be expressed as follows:

$$\begin{aligned} \mathbf{S}_i \cdot \mathbf{S}_j &= S^2 - S(a_i^* - a_j^*)(a_i - a_j) \\ &\quad - \frac{1}{4}[a_i^* a_j^*(a_i - a_j)^2 + (a_i^* - a_j^*)^2 a_i a_j] + O(S^{-1}). \end{aligned} \quad (2.3)$$

Let us consider the following ideal spin-wave density matrix:

$$\rho = C \exp \left[ - \sum_{\mathbf{k}} g(\mathbf{k}) a_{\mathbf{k}}^* a_{\mathbf{k}} \right]. \quad (2.4)$$

The expectation value of  $\mathbf{S}_i \cdot \mathbf{S}_j$  becomes

$$\begin{aligned} \text{Tr} \rho \mathbf{S}_i \cdot \mathbf{S}_j / \text{Tr} \rho &= \left| S - \frac{1}{N} \sum_{\mathbf{k}} (1 - e^{i\mathbf{k} \cdot \mathbf{r}_{ij}}) \bar{n}_{\mathbf{k}} \right|^2, \\ \bar{n}_{\mathbf{k}} &= \frac{1}{\exp[g(\mathbf{k})] - 1}. \end{aligned} \quad (2.5)$$

The entropy  $\mathcal{S}$  for this density matrix and magnetization are

$$\mathcal{S} = \sum_{\mathbf{k}} \frac{g(\mathbf{k})}{\exp[g(\mathbf{k})] - 1} - \ln \{ 1 - \exp[-g(\mathbf{k})] \}, \quad (2.6)$$

$$S_z = SN - \sum_{\mathbf{k}} \bar{n}_{\mathbf{k}}. \quad (2.7)$$

Factors  $g(\mathbf{k})$  should be chosen so that  $E-T\mathcal{S}$  is minimized under the condition  $S_z = 0$ :

$$W = \frac{JN}{2} \sum_{\delta} \left[ S^2 - \left| S - \frac{1}{N} \sum_{\mathbf{k}} (1 - e^{i\mathbf{k} \cdot \delta}) \bar{n}_{\mathbf{k}} \right|^2 \right] - T \sum_{\mathbf{k}} \left[ \frac{g(\mathbf{k})}{\exp[g(\mathbf{k})] - 1} - \ln \{ 1 - \exp[-g(\mathbf{k})] \} \right] - \mu \sum_{\mathbf{k}} \bar{n}_{\mathbf{k}}, \quad (2.8)$$

$$0 = \frac{\partial W}{\partial g(\mathbf{k})} = \frac{\exp[g(\mathbf{k})]}{\{\exp[g(\mathbf{k})] - 1\}^2} \left[ -JS' \sum_{\delta} [1 - \cos(\mathbf{k} \cdot \delta)] + Tg(\mathbf{k}) - \mu \right], \quad (2.9)$$

$$S' = S - \sum_{\mathbf{k}} [1 - \exp(i\mathbf{k} \cdot \delta)] \bar{n}_{\mathbf{k}}.$$

Here,  $\mu$  is the Lagrange multiplier and the  $\delta$ 's are lattice vectors to nearest neighbors. Then we have

$$\begin{aligned} g(\mathbf{k}) &= T^{-1}[JS'\epsilon(\mathbf{k}) - \mu], \\ \epsilon(\mathbf{k}) &\equiv \sum_{\delta} [1 - \cos(\mathbf{k} \cdot \delta)]. \end{aligned} \quad (2.10)$$

$S'$  and  $\mu$  are solutions of the following coupled equations:

$$S = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\exp\left[\frac{JS'\epsilon(\mathbf{k}) - \mu}{T}\right] - 1}, \quad (2.11)$$

$$S' = \frac{1}{N} \sum_{\mathbf{k}} \frac{\cos(\mathbf{k} \cdot \delta)}{\exp\left[\frac{JS'\epsilon(\mathbf{k}) - \mu}{T}\right] - 1}. \quad (2.12)$$

It is assumed that  $S'$  in (2.9) and (2.12) is independent of the  $\delta$ 's. The correlation function  $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$  is as follows:

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \begin{cases} \left| \frac{1}{N} \sum_{\mathbf{k}} \exp(i\mathbf{k} \cdot \mathbf{r}_{ij}) \bar{n}_{\mathbf{k}} \right|^2 & \text{for } i \neq j, \\ S(S+1) & \text{for } i = j. \end{cases} \quad (2.13)$$

Then the energy and the susceptibility become

$$e = \frac{Jz}{2}(S^2 - S'^2), \quad (2.14)$$

$$\chi_0 = \sum_j \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \frac{1}{N} \sum_{\mathbf{k}} (\bar{n}_{\mathbf{k}}^2 + \bar{n}_{\mathbf{k}}), \quad (2.15)$$

where  $z$  is the number of nearest neighbors.

The above is the main formulation given in Ref. 1 for the quantum Heisenberg model. By taking the limit of infinite  $S$ , one can treat the classical case. Setting  $JS^2 = J_0$  and  $\mathbf{S}_i/S = \mathbf{s}_i$ , we have Hamiltonian (1.2). We put that  $T \gg JS = J_0/S$ . Then Eqs. (2.11) and (2.12) become:

$$\frac{x}{t} = N^{-1} \sum_{\mathbf{k}} \frac{1}{\epsilon(\mathbf{k}) + v}, \quad (2.16)$$

$$\frac{x^2}{t} = N^{-1} \sum_{\mathbf{k}} \frac{\cos(\mathbf{k} \cdot \delta)}{\epsilon(\mathbf{k}) + v} = N^{-1} \sum_{\mathbf{k}} \frac{1 - z^{-1}\epsilon(\mathbf{k})}{\epsilon(\mathbf{k}) + v}, \quad (2.17)$$

$$x = S'/S, \quad v = -\mu S/(J_0 x), \quad t = T/J_0. \quad (2.18)$$

Here,  $x$  and  $v$  should be determined self-consistently. The correlation function, energy, and magnetic susceptibility are as follows:

$$\langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle = \left| \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_{ij}} \frac{t}{x[\epsilon(\mathbf{k}) + v]} \right|^2, \quad (2.19)$$

$$e = \frac{z}{2} J_0 (1 - x^2), \quad (2.20)$$

$$\chi_0 = \sum_{\mathbf{r}} \langle \mathbf{s}_0 \cdot \mathbf{s}_{\mathbf{r}} \rangle = N^{-1} \sum_{\mathbf{k}} \left[ \frac{t}{x[\epsilon(\mathbf{k}) + v]} \right]^2. \quad (2.21)$$

Equations (2.16)–(2.21) are the fundamental equations of modified spin-wave theory for the classical Heisenberg model defined by Eq. (1.2). Let us define the following

function  $G(v)$ :

$$G(v) \equiv N^{-1} \sum_{\mathbf{k}} \frac{1}{\epsilon(\mathbf{k}) + v}. \quad (2.22)$$

Equations (2.16) and (2.17) are written as follows:

$$x/t = G(v), \quad (2.23)$$

$$x^2/t = -\frac{1}{z} + \left[1 + \frac{v}{z}\right] G(v). \quad (2.24)$$

Thus  $t$ ,  $x$ , and  $\chi_0$  can be represented as functions of  $v$ :

$$t = \left[1 + \frac{v}{z}\right] / G(v) - \frac{1}{zG^2(v)}, \quad (2.25)$$

$$x = 1 + \frac{v}{z} - \frac{1}{zG(v)}, \quad (2.26)$$

$$\chi_0 = -G'(v)/G^2(v). \quad (2.27)$$

Thermodynamic quantities are calculated through parameter  $v$  and function  $G(v)$ .

For the linear chain we have  $z=2$ ,  $\epsilon(k) = 2 - 2\cos k$ , and

$$G(v) = 1/(v^2 + 4v)^{1/2}. \quad (2.28)$$

Substituting this into (2.25) gives

$$t = \left[1 + \frac{v}{2}\right] (v^2 + 4v)^{1/2} - \frac{v^2 + 4v}{2}. \quad (2.29)$$

From this one can eliminate parameter  $v$ :

$$v = \frac{2-t}{\sqrt{1-t}} - 2, \quad (2.30)$$

$$x = \sqrt{1-t}. \quad (2.31)$$

Energy and susceptibility become

$$e = J_0 t, \quad (2.32)$$

$$\chi_0 = 2/t - 1. \quad (2.33)$$

This may be compared with Fisher's exact solution, which gives

$$\begin{aligned} e &= J_0 \{1 - [\coth(1/t) - t]\} \\ &= J_0 [t + O(e^{-2/t})], \end{aligned} \quad (2.34)$$

$$\begin{aligned} \chi_0 &= \frac{1 + [\coth(1/t) - t]}{1 - [\coth(1/t) - t]} \\ &= \frac{2}{t} - 1 + O(t^{-2}e^{-2/t}). \end{aligned} \quad (2.35)$$

Thus spin-wave theory gives a very accurate solution at low temperatures. The discrepancy from the exact value is of the order of  $\exp(-2/t)$ . It is expected that the situation is the same also for the two-dimensional system.

### III. CLASSICAL SQUARE LATTICE

#### A. Infinite system

For the square lattice we have  $z=4$  and  $\epsilon(\mathbf{k}) = 4 - 2\cos k_x - 2\cos k_y$ . In the limit of infinite sys-

tem the sum in Eq. (2.22) is replaced by the first-kind complete elliptic integral  $K(k)$ :<sup>9</sup>

$$G(v) = \frac{1}{4\pi^2} \int_0^{2\pi} \int_0^{2\pi} dx dy \frac{1}{4+v-2\cos x - 2\cos y} \\ = (2\pi)^{-1} kK(k), \quad (3.1)$$

$$k \equiv \left[ 1 + \frac{v}{4} \right]^{-1}.$$

Then Eqs. (2.25)–(2.27) can be written as

$$t = k^{-2} \left[ \frac{2\pi}{K(k)} - \frac{\pi^2}{K^2(k)} \right], \quad (3.2)$$

$$x = k^{-1} \left[ 1 - \frac{\pi}{2K(k)} \right], \quad (3.3)$$

$$\chi_0 = \frac{\pi E(k)}{2(1-k^2)K^2(k)}, \quad (3.4)$$

where  $E(k)$  is the second-kind complete elliptic integral.<sup>9</sup> From Eq. (3.2) one has

$$K(k) = \pi \left[ \frac{1+(1-k^2t)^{1/2}}{k^2t} \right]. \quad (3.5)$$

Substituting this into (3.3), (3.4), and (2.20) gives

$$\langle \mathbf{s}_0 \cdot \mathbf{s}_r \rangle^{1/2} \simeq (2\pi)^{-2} \frac{t}{x} \int \int \frac{\exp(i\mathbf{k} \cdot \mathbf{r}) dk_x dk_y}{k_x^2 + k_y^2 + v} = \frac{t}{2\pi x} K_0(r/\sqrt{v}) \simeq \frac{t}{2\pi x} \left[ \frac{\pi}{2r\sqrt{v}} \right]^{1/2} \exp(-r\sqrt{v}). \quad (3.12)$$

Here,  $K_0$  is the modified Bessel function.<sup>9</sup> Then the two-point correlation function becomes a Yukawa function:

$$\langle \mathbf{s}_0 \cdot \mathbf{s}_r \rangle \simeq \frac{t^2}{8\pi x^2 \sqrt{v} r} \exp(-2\sqrt{v} r). \quad (3.13)$$

The correlation length  $\xi$  is  $1/(2\sqrt{v})$  and Eq. (1.5) is derived. In two dimensions the Ornstein-Zernike-type correlation function should be  $\exp(-r/\xi)/\sqrt{r}$ . But correlation function (3.13) is slightly different from the Ornstein-Zernike type.

### B. Comparison with Monte Carlo calculation and high-temperature expansion

Let us consider a finite  $64 \times 64$  square lattice. The modified spin-wave theory in Sec. II works also for finite systems with the periodic boundary condition. But one cannot replace the momentum sum in (2.22) by an integral. Solving (2.26) numerically we can determine  $v$  for a given temperature. We also carry out the Monte Carlo calculation of the  $64 \times 64$  classical Heisenberg lattice using the heat-bath algorithm. The two-point correlation function is calculated by the use of the fast Fourier transformation. Details of these numerical techniques are given in Ref. 10. As shown in Fig. 1, at  $t=0.5$  and  $0.25$  spin-wave results agree excellently with the Monte Carlo results for correlation functions.

The high-temperature expansions of  $e$  and  $\chi_0$  are known:<sup>4</sup>

$$e/J_0 = 2 - 0.666\,666\,666\,7t^{-1} - 0.103\,703\,7t^{-3} + 0.005\,643\,79t^{-5} \\ + 0.003\,595\,226t^{-7} + 0.001\,154\,507t^{-9} + O(t^{-11}), \quad (3.14)$$

$$\chi_0 = 1 + 1.333\,333\,333t^{-1} + 1.333\,333\,333\,3t^{-2} + 1.244\,444\,44t^{-3} \\ + 1.056\,790\,12t^{-4} + 0.851\,263\,96t^{-5} + 0.659\,564\,96t^{-6} \\ + 0.492\,710\,96t^{-7} + 0.358\,061\,79t^{-8} + 0.252\,923\,16t^{-9} + 0.174\,853\,908t^{-10} + O(t^{-11}). \quad (3.15)$$

Then the logarithm of  $\chi_0$  becomes

$$e = J_0 \{ 2 - [1 + (1 - k^2 t)^{1/2}] k^{-2} + t/2 \}, \quad (3.6)$$

$$\chi_0 = \frac{k^4 t^2 E(k)}{2\pi(1-k^2)[1+(1-k^2 t)^{1/2}]^2}. \quad (3.7)$$

Near  $k=1$ ,  $K(k)$  and  $E(k)$  are expanded by  $k' \equiv (1-k^2)^{1/2}$ :<sup>9</sup>

$$K(k) = \ln \left[ \frac{4}{k'} \right] \left[ 1 + \frac{k'^2}{4} \right] - \frac{k'^2}{4} + O(k'^4 \ln k'), \quad (3.8)$$

$$E(k) = 1 + \frac{1}{2} \left[ \ln \left[ \frac{4}{k'} \right] - \frac{1}{2} \right] k'^2 + O(k'^4 \ln k'). \quad (3.9)$$

Substituting (3.8) into (3.5) gives

$$1 - k^2 = 16 \exp \left[ -\frac{4\pi}{t} + \pi + \frac{\pi t}{4} + O(t^2) \right]. \quad (3.10)$$

This means that  $k$  is very near 1 at low temperature. Substituting this into (3.6) and (3.7) gives Eqs. (1.3) and (1.4). Equations (3.1) and (3.10) yield

$$v = 32e^\pi \exp(-4\pi/t) \left[ 1 + \frac{\pi t}{4} + O(t^2) \right]. \quad (3.11)$$

From Eq. (2.19) we have a correlation function at  $|\mathbf{r}| \gg 1$ :

$$\begin{aligned} \ln\chi_0 = & 1.333\,333\,33t^{-1} + 0.444\,444\,444t^{-2} + 0.256\,790\,12t^{-3} \\ & + 0.088\,888\,89t^{-4} + 0.047\,971\,782\,9t^{-5} + 0.021\,738\,846t^{-6} \\ & + 0.008\,938\,012\,0t^{-7} + 0.004\,238\,376t^{-8} + 0.000\,635\,384\,17t^{-9} + 0.000\,623\,154\,223t^{-10} + O(t^{-11}). \end{aligned} \quad (3.16)$$

In Figs. 2 and 3 these high-temperature expansions, the low-temperature expansions (1.3) and (1.4), and the results of Monte Carlo calculations are given as functions of  $1/t$ . With respect to the energy, the high-temperature expansion (3.14) and the low-temperature expansion (1.3) smoothly connect with each other near  $t=0.5-0.75$ . As shown in Fig. 3, the connection is not so smooth for the susceptibility. At  $t=0.75$ , spin-wave result (1.4) for susceptibility is several tens of times greater than the Monte Carlo result. This is because the spin-wave approximation is not good in this temperature region. It is expected that the coincidence becomes better at  $t \leq 0.5$ . To estimate the susceptibility of an infinite system at  $t=0.5$ , we need to treat the  $1000 \times 1000$  system. Unfortunately, the Monte Carlo calculation for the susceptibility of such a large system is not available. So it is very difficult to verify Eq. (1.4) using the Monte Carlo calculation.

#### IV. SUMMARY AND DISCUSSION

In previous papers<sup>1</sup> the reduced susceptibility and correlation length were obtained for the quantum system described by Eq. (1.1):

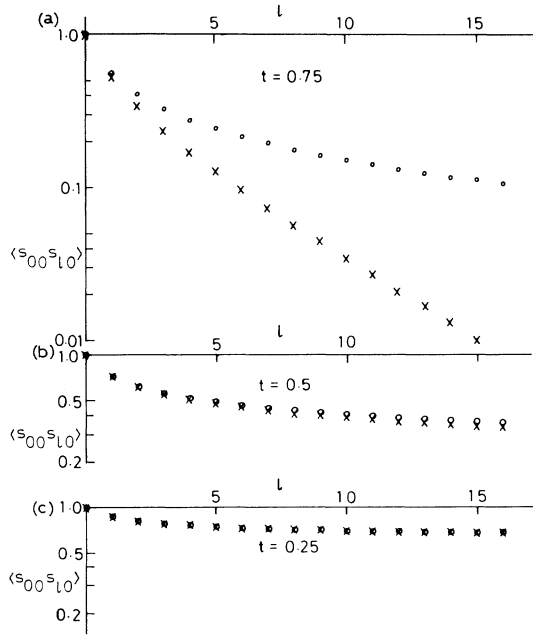


FIG. 1. Two-point correlation function  $\langle s_{00} s_{l0} \rangle$  along a column of a  $64 \times 64$  square lattice at various temperatures. (a)  $t=0.75$ , (b)  $t=0.5$ , and (c)  $t=0.25$ . Crosses are the Monte Carlo results and circles are the spin-wave results. At  $t \leq 0.5$  both results agree excellently.

$$\chi_0 \simeq \frac{T}{\pi JS} \exp(4\pi JS^2/T)$$

and (4.1)

$$\xi \simeq (JS/T)^{1/2} \exp(2\pi JS^2/T).$$

On the other hand, Eqs. (1.4) and (1.5) give the following formulas for a sufficiently large spin quantum number  $S$ :

$$\chi_0 \simeq \frac{1}{128\pi e^\pi} \left[ \frac{T}{JS} \right]^2 \exp(4\pi JS^2/T)$$

and (4.2)

$$\xi \simeq \frac{1}{8\sqrt{2}e^{\pi/2}} \exp(2\pi JS^2/T).$$

The prefactors for exponentials are slightly different in Eqs. (4.1) and (4.2). Equations (4.2) are valid at  $JS^2 \gg T \gg JS$ . However, the expansion formulas (4.1) are valid at  $T \ll JS$ . Thus we can say that the quantum-classical crossover occurs near  $T \sim JS$  for actual systems with large spin quantum number  $S$ . Below this temperature the system is quantum mechanical. The specific heat is proportional to  $T$  and Eqs. (4.1) are valid. But above this temperature the system is classical and Eqs. (4.2) are valid and specific heat is nearly a constant. It should be noted that the preexponential factor changes between the classical case and the quantum case in two dimensions. In one dimension  $\chi_0$  behaves as  $2JS^2/T$  both for classical and quantum cases.

Renormalization-group methods<sup>5-7</sup> have succeeded in describing qualitatively the critical behavior of magnetic susceptibility of the two-dimensional Heisenberg model. They have been able to show that  $\chi_0$  diverges as  $\exp(4\pi/t)$ . However, they were not able to determine the amplitude of the divergent term by themselves. They estimated it with the aid of high-temperature ex-

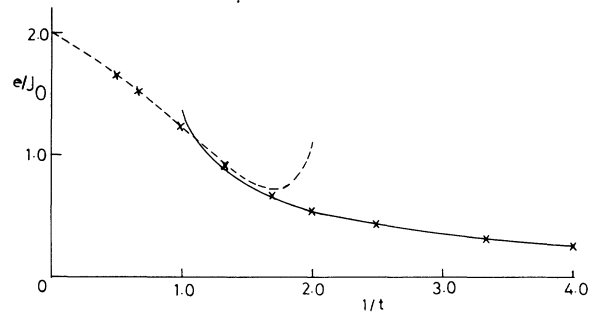


FIG. 2. Energy per site as a function of  $1/t$ . Dashed line is the result of high-temperature expansion (3.14). Solid line is the spin-wave result (1.3). Crosses are results of the Monte Carlo calculation for the  $64 \times 64$  system.

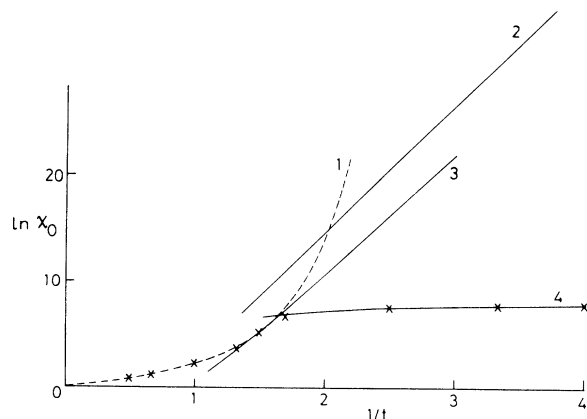


FIG. 3. Logarithm of susceptibility as a function of  $1/t$ . Line 1 is the result of high-temperature expansion (3.16). Line 2 shows the spin-wave results for an infinite system (1.4). Line 3 is the result of the Shenker-Tobochnik formula (1.7). Line 4 shows the spin-wave results for the  $64 \times 64$  lattice. Crosses are the Monte Carlo results for the  $64 \times 64$  lattice.

pansion or Monte Carlo calculations as shown in Eqs. (1.7) and (1.9). It seems that these attempts<sup>6,7</sup> failed to determine the correct preexponential factors of  $\chi_0$  and  $\xi$  because the system size of the Monte Carlo calculation is not sufficiently large. To get the numerical factors they used lattices such as  $50 \times 50$ – $200 \times 200$ . Then,  $\chi_0$  and  $\xi$  were estimated only at  $t \geq 0.7$ . Spin-wave theory, however, can calculate the magnetic susceptibility quantitatively by itself. It is expected that formulas (1.4) and (1.5) become better than (1.7) and (1.8) at sufficiently low temperatures such as  $t \leq 0.5$ . Moreover, spin-wave theory gives the correlation function (3.13), which is different from the Ornstein-Zernike type.

Quantitative spin-wave calculations for the O(2) planar model have already been done by many authors.<sup>11</sup> The correlation function at low temperature has been calculated and it decays algebraically on a two-dimensional lattice. I believe that this paper derives the quantitative calculation for O(3) classical Heisenberg model at low temperature. It is expected that the same kind of quantitative calculation is possible for the O( $n$ ) ( $n \geq 4$ ) Heisenberg model, although its calculation becomes complicated.

#### ACKNOWLEDGMENT

The author thanks Dr. S. Miyashita for informing him of Ref. 11.

#### APPENDIX: DIRECT DERIVATION OF FUNDAMENTAL EQUATIONS FOR CLASSICAL SYSTEMS

In Sec. II equations were derived for the classical system by taking the limit of  $S \rightarrow \infty$  in a quantum system. Of course, we can also derive them in the regime of classical mechanics.

Let us consider the following transformation for classical spin  $s_j$ :

$$\begin{aligned} s_j^x &= (2 - x_j^2 - y_j^2)^{1/2} x_j, \\ s_j^y &= (2 - x_j^2 - y_j^2)^{1/2} y_j, \\ s_j^z &= 1 - x_j^2 - y_j^2. \end{aligned} \quad (\text{A1})$$

The region of  $(x_j, y_j)$  is in a circle with radius  $\sqrt{2}$ :  $x_j^2 + y_j^2 \leq 2$ . The advantage of this representation is that the weight function of the phase-space integral is a constant. The partition function of the classical system defined by (1.2) can be written as follows:

$$Z = \int \prod_j dx_j dy_j \exp \left[ T^{-1} \sum_{\langle ij \rangle} (\mathbf{s}_i \cdot \mathbf{s}_j - 1) \right]. \quad (\text{A2})$$

The pair product  $\mathbf{s}_i \cdot \mathbf{s}_j$  is expanded as follows:

$$\begin{aligned} \mathbf{s}_i \cdot \mathbf{s}_j &= 1 - (\bar{z}_i - \bar{z}_j)(z_i - z_j) \\ &\quad - \frac{1}{4} [\bar{z}_i \bar{z}_j (z_i - z_j)^2 + (\bar{z}_i - \bar{z}_j)^2 z_i z_j] + \cdots, \\ z_j &= x_j + iy_j, \end{aligned} \quad (\text{A3})$$

and the ellipsis represents higher-order terms in  $z$  and  $\bar{z}$ . A classical state is described by a set of  $N$  complex numbers  $z_j$ 's. We apply the self-consistent harmonic approximation for this problem and assume that the distribution function of  $z_j$ 's is

$$\begin{aligned} \rho(\{z_j\}) &= \prod_{\mathbf{k}} \left[ \frac{1}{\pi h(\mathbf{k})} \right] \exp \left[ - \sum_{\mathbf{k}} \bar{z}_{\mathbf{k}} z_{\mathbf{k}} / h(\mathbf{k}) \right], \\ z_{\mathbf{k}} &\equiv \frac{1}{\sqrt{N}} \sum_j \exp(i\mathbf{k} \cdot \mathbf{r}_j) z_j. \end{aligned} \quad (\text{A4})$$

Parameters  $h(\mathbf{k})$  should be determined by conditions of zero magnetization and minimum free energy. We assume that  $x_{\mathbf{k}}$  and  $y_{\mathbf{k}}$  move from plus infinity to minus infinity. The expectation values of  $\mathbf{s}_i \cdot \mathbf{s}_j$ ,  $\sum_j s_j^z$ , and entropy are

$$\langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle = \left| 1 - N^{-1} \sum_{\mathbf{k}} [1 - \exp(i\mathbf{k} \cdot \mathbf{r}_{ij}) h(\mathbf{k})] \right|^2, \quad (\text{A5})$$

$$\sum_{\mathbf{k}} s_j^z = N - \sum_{\mathbf{k}} h(\mathbf{k}), \quad (\text{A6})$$

$$\mathcal{S} = \sum_{\mathbf{k}} 1 + \ln h(\mathbf{k}). \quad (\text{A7})$$

We must minimize the following quantity  $W$ :

$$\begin{aligned} W &\equiv (J_0 N / 2) \sum_{\delta} \left[ 1 - \left| 1 - N^{-1} \sum_{\mathbf{k}} (1 - e^{i\mathbf{k} \cdot \delta}) h(\mathbf{k}) \right|^2 \right] \\ &\quad - T \sum_{\mathbf{k}} \ln h(\mathbf{k}) - \mu' \sum_{\mathbf{k}} h(\mathbf{k}). \end{aligned} \quad (\text{A8})$$

Here,  $\mu'$  is the Lagrange multiplier. Then we have

$$h(\mathbf{k}) = T / [J_0 x \varepsilon(\mathbf{k}) - \mu'], \quad (\text{A9})$$

$$x = 1 - N^{-1} \sum_{\mathbf{k}} (1 - e^{i\mathbf{k} \cdot \delta}) h(\mathbf{k}), \quad (\text{A10})$$

$$1 = N^{-1} \sum_{\mathbf{k}} h(\mathbf{k}). \quad (\text{A11})$$

Then, if we read  $v = -\mu' / J_0 x$ , we get Eqs. (2.16), (2.17), and (2.19)–(2.21).

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