Quantum Heisenberg Ferromagnets in One and Two Dimensions at Low Temperature

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Modifying the spin-wave theory in the three-dimensional Heisenberg ferromagnet, we propose a simple approximation to investigate the low-temperature thermodynamics of one- and two-dimensional Heisenberg ferromagnets $H = -J\sum_{\langle ij \rangle} (S_i S_j - S^2)$, where S is the spin quantum number. We regard that the system is an ideal Bose gas with density S. For one-dimensional chain we get the free energy and the susceptibility per site:

$$f = -T^{3/2} \frac{\zeta\left(\frac{3}{2}\right)}{\sqrt{4\pi JS}} + \frac{T^2}{4JS^2} + O(T^{5/2}),$$

$$\chi = \frac{8S^4 J}{3T^2}\left\{1 - \frac{3}{S}\sqrt{\frac{T}{2JS}} \cdot \frac{\zeta\left(\frac{1}{2}\right)}{\sqrt{2\pi}} + O(T)\right\}.$$

At $S = 1/2$ these coincide with the numerical results of the Bethe-ansatz integral equation. The susceptibility has not logarithmic correction contrary to a recent proposal by Schlottmann. For two-dimensional square lattice we get:

$$f = -\frac{T^2}{4\pi JS}\left\{\frac{\pi^2}{6} + \frac{\zeta(3)}{8} \cdot \frac{T}{JS} + O(T^2)\right\},$$

$$\chi = \frac{1}{3\pi JS}\exp\left(\frac{4\pi JS^2}{T}\right)(1 + O(T)).$$

§ 1. Introduction

In this paper we investigate the low-temperature thermodynamics of one- and two-dimensional Heisenberg ferromagnets with general spin quantum number S:

$$H = -J \sum_{\langle ij \rangle} (S_i S_j - S^2), \quad J > 0. \tag{1.1}$$

Here $\langle ij \rangle$ means that i and j sites are nearest neighbors. We assume that there are N sites. Recently the one-dimensional $S = 1/2$ case was analyzed by us [1],[2] and Schlottmann [3],[4] by the use of thermodynamic Bethe-ansatz integral equations. [5] From the numerical result of the integral equations we obtained free energy per site f as follows: [1]

$$\frac{f}{T} = -1.042\left(\frac{T}{J}\right)^{1/2} + 1.00\left(\frac{T}{J}\right) - 0.9\left(\frac{T}{J}\right)^{3/2} + O(T^2). \tag{1.2}$$

On the other hand the spin-wave theory [6]~[8] gives

$$\frac{f}{T} = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk \ \ln(1 - \exp(T^{-1}J(1-\cos k)))$$

$$= -1.0421869\left(\frac{T}{J}\right)^{1/2} - 0.0668971\left(\frac{T}{J}\right)^{3/2} - O(T^{5/2}) \ . \tag{1·3}$$

The first term of Eq. (1·2) coincides with that of Eq. (1·3). This means that the spin-wave theory stands in the one-dimensional system also. This is very surprising because one- and two-dimensional systems have not long range order and spin-wave theory is expected to lose its validity. The second terms of (1·2) and (1·3) are completely different. Then conventional spin-wave theory should be modified to get higher order terms.

In one- and two-dimensional systems at low temperature the correlation length becomes very long and the system is nearly ordered. The spin-wave theory regards that an eigenstate of Eq. (1·1) is an excited state of non-interacting spin waves. In zero magnetic field the number of spin waves becomes infinite and the magnetization should be minus infinity. Actually the magnetization is zero and the density of spin waves is S. Restriction on the particle number is a natural result of the fact that a site cannot have more than $2S$ bosons. This is well known as kinematical interaction.[8] Then we calculate the free energy of an ideal Bose gas on the condition that the number of bosons is SN. Corresponding to this constraint condition a Lagrange multiplier appears which is equivalent to the chemical potential. In three-dimensional system this chemical potential is equal to the external magnetic field. In one- and two-dimensional system the chemical potential is not zero even in zero magnetic field. Then we determine the chemical potential so that the average number of bosons is SN. At low temperature it is a very small negative quantity. The introduction of non-zero chemical potential is the essentials of this paper. Strictly speaking this should be derived from kinematical and dynamical interactions of spin waves. But we have not such a systematic way to calculate the effective chemical potential.

In §2 we formulate our approximation for one- and two-dimensional Heisenberg ferromagnets. The expressions of the free energy, energy, two-point correlation function and magnetic susceptibility are given. The results at high-temperature limit are given. In §3 we investigate low-temperature properties of one-dimensional chain and the two-dimensional square lattice. In §4 the two-point correlation function is calculated. For the one-dimensional chain chemical potential is of the order of T^2, where T is the temperature. It is shown that specific heat behaves as $\sqrt{T}$ and the susceptibility diverges as $1/T^2$. The free energy and the magnetic susceptibility are expanded for general S. At $S=1/2$ our formulas coincide with the results of Bethe-ansatz integral equations in the first and second orders. Then our approximation is better than the conventional spin-wave theory. The two-point correlation function decays as $\exp(-r/\xi)$. The correlation length ξ is JS^2/T. In the two-dimensional square lattice the chemical potential is of the order of $-\exp(-4\pi JS^2/T)$. The free energy is expanded by power series of T. The coefficients coincide with those of the conventional spin-wave theory. The low-temperature specific heat behaves as T. The susceptibility diverges as $\exp(4\pi JS^2/T)$. The two-point correlation function decays like the Yukawa function $r^{-1}\exp(-r/\xi)$, where ξ is $(JS/T)^{1/2}\exp(2\pi JS^2/T)$. In §5 we discuss about Schlottmann's susceptibility[4] for $S = 1/2$ linear chain which diverges as $J/(T^2 \ln(J/T))$. We compare our results with

various approximations[9]~[12] which were made for the low-dimensional Heisenberg ferromagnet.

§ 2. Spin-wave theory with fixed number of bosons

2.1. *Holstein-Primakoff expansion up to S^0*

For Hamiltonian (1·1) we apply the Holstein-Primakoff transformation:[7]

$$S_j{}^+ = S_j{}^x + iS_j{}^y = \sqrt{2S}\, f_j(S)\, a_j\,,$$

$$S_j{}^- = S_j{}^x - iS_j{}^y = \sqrt{2S}\, a_j{}^* f_j(S)\,,$$

$$S_j{}^z = S - a_j{}^* a_j\,,$$

$$f_j(S) = \sqrt{1 - (2S)^{-1} a_j{}^* a_j} = 1 - (4S)^{-1} a_j{}^* a_j - O(S^{-2})\,, \tag{2·1}$$

where $a_j{}^*$ and a_j are the creation and annihilation operators of bosons of the j-th site. Expanding with respect to S^{-1} we have

$$H = J \sum_{\langle ij \rangle} \left[S(a_j{}^* - a_i{}^*)(a_j - a_i) + \frac{1}{4}\{a_i{}^* a_j{}^*(a_i - a_j)^2 + (a_i{}^* - a_j{}^*)^2 a_i a_j\} \right] + O(S^{-1})\,. \tag{2·2}$$

We change from the site representation to the momentum representation:

$$a_j = (N)^{-1/2} \sum_k e^{i k r_j} a_k\,, \quad a_j{}^* = (N)^{-1/2} \sum_k e^{-i k r_j} a_k{}^*\,.$$

For simplicity we assume that the lattice has only one magnetic site in a unit cell. Then, for example, the honeycomb lattice is excluded. In the momentum representation (2·2) is

$$H = H_0 + H_1\,, \tag{2·3}$$

$$H_0 = \sum_k JS\varepsilon(k) a_k{}^* a_k\,, \quad \varepsilon(k) \equiv \sum_\delta (1 - \cos k\delta)\,, \tag{2·4}$$

$$H_1 = (8N)^{-1} J \sum_{kk'q} \sum_\delta \{ e^{-i(k'-q)\delta}(1 - e^{i k'\delta})(1 - e^{i k\delta})$$

$$+ e^{i k\delta}(1 - e^{-i(k+q)\delta})(1 - e^{-i(k'-q)\delta})\} a_{k+q}^* a_{k'-q}^* a_{k'} a_k\,. \tag{2·5}$$

Here δ's are the lattice vectors to nearest neighbors. We neglect the terms of $O(S^{-1})$.

2.2. *Eigenstate of H_0*

An eigenstate of H_0 is given by

$$|\{n_k\}\rangle = \prod_k (n_k!)^{-1/2} (a_k{}^*)^{n_k} |0\rangle\,. \tag{2·6}$$

A state is characterized by a set of N non-negative integers $\{n_k\}$. The expectation value of H_1 for this state is as follows:

$$\langle\{n_k\}|H_1|\{n_k\}\rangle = -\frac{J}{2N}\sum_\delta\{\sum_{k\neq k'}(1-e^{ik\delta})(1-e^{-ik'\delta})n_k n_{k'}$$

$$+\sum_k(1-e^{ik\delta})(1-e^{-ik\delta})(n_k^2-n_k)\} . \qquad (2\cdot7)$$

The operator $S_i S_j$ is written by the Bose operators:

$$S_i S_j = S^2 - S(a_i^*-a_j^*)(a_i-a_j)-\frac{1}{4}\{a_i^* a_j^*(a_i-a_j)^2$$

$$+(a_i^*-a_j^*)^2 a_i a_j\}+O(S^{-1}) \quad \text{at } i\neq j . \qquad (2\cdot8)$$

In the momentum representation this becomes

$$S_i S_j = S^2 - N^{-1}S\sum_{k_1 k_2}(e^{-ik_1 r_i}-e^{-ik_1 r_j})(e^{ik_2 r_i}-e^{ik_2 r_j})a_{k_1}^* a_{k_2}$$

$$-\frac{1}{4}N^{-2}\sum_{k_1 k_2 k_3 k_4}\{e^{-ik_1 r_i-ik_2 r_j}(e^{ik_3 r_i}-e^{ik_3 r_j})(e^{ik_4 r_i}-e^{ik_4 r_j})$$

$$+(e^{-ik_1 r_i}-e^{-ik_1 r_j})(e^{-ik_2 r_i}-e^{-ik_2 r_j})e^{ik_3 r_i+ik_4 r_j}\}a_{k_1}^* a_{k_2}^* a_{k_3} a_{k_4}+O(S^{-1}) . \qquad (2\cdot9)$$

Then we have the expectation value of $S_i S_j$ at $i\neq j$:

$$\langle\{n_k\}|S_i S_j|\{n_k\}\rangle = S^2 - 2SN^{-1}\sum_k(1-\cos k(r_i-r_j))n_k$$

$$+N^{-2}\sum_{kk'}(1-e^{ik(r_i-r_j)})(1-e^{-ik'(r_i-r_j)})(n_k n_{k'}-\delta_{kk'}n_k) . \qquad (2\cdot10)$$

For $i=j$ we have $S_i S_j = S(S+1)$.

2.3. Density matrix and thermodynamic quantities

We assume that the density matrix is approximately given by

$$\rho = \sum_{\{n_k\}}\prod_k P_k(n_k)|\{n_k\}\rangle\langle\{n_k\}| . \qquad (2\cdot11)$$

Here $P_k(n)$ is the probability that the k momentum state has n bosons. It stands

$$\sum_{n=0}^\infty P_k(n)=1 \quad \text{for all } k\text{'s} . \qquad (2\cdot12)$$

Entropy for this density matrix is

$$\text{entropy}=-\sum_k\sum_{n=0}^\infty P_k(n)\ln P_k(n) .$$

Unperturbed free energy for H_0 is

$$F_0 = JS\sum_k\varepsilon(k)\sum_{n=0}^\infty n P_k(n)+T\sum_k\sum_{n=0}^\infty P_k(n)\ln P_k(n) . \qquad (2\cdot13)$$

Magnetization in the z-direction is given by $SN-\sum_k a_k^* a_k$. Then the condition of zero magnetization is

$$SN = \sum_{k} \sum_{n=0}^{\infty} nP_k(n) \ . \tag{2.14}$$

We should minimize Eq. (2·13) under constraint conditions (2·12) and (2·14). Then we introduce $N+1$ Lagrange multipliers μ_k's and μ and minimize the following quantity W:

$$W = F_0 - \sum_{k} \mu_k \sum_{n=0}^{\infty} P_k(n) - \mu \sum_{k} \sum_{n=0}^{\infty} nP_k(n) \ . \tag{2.15}$$

From $\partial W/\partial P_k(n) = 0$ we have

$$P_k(n) = \exp(\mu_k T^{-1} - 1)\exp(-nT^{-1}(JS\varepsilon(\boldsymbol{k}) - \mu)) \ . \tag{2.16}$$

Using Eq. (2·12) we have

$$\exp(\mu_k T^{-1} - 1) = 1 - \exp(-T^{-1}(JS\varepsilon(\boldsymbol{k}) - \mu)) \ .$$

Then we get the self-consistent equation for μ:

$$S = N^{-1} \sum_{k} \tilde{n}_k \ , \tag{2.17}$$

$$\tilde{n}_k \equiv \sum_{n=0}^{\infty} nP_k(n) = \frac{1}{\exp(T^{-1}(JS\varepsilon(\boldsymbol{k}) - \mu)) - 1} \ . \tag{2.18}$$

Unperturbed free energy is given by

$$F_0 = \mu SN - T\sum_{k} \ln(1 + \tilde{n}_k) \ .$$

The expectation value of $n_k{}^2$ is as follows:

$$\langle n_k{}^2 \rangle = \sum_{n=0}^{\infty} n^2 P_k(n) = \tilde{n}_k{}^2 + \tilde{n}_k \ . \tag{2.19}$$

Using (2·7) and (2·19) we get the expectation value of H_1:

$$\langle H_1 \rangle = -\frac{J}{2N} \sum_{\delta} (\sum_{k}(1 - e^{i\boldsymbol{k}\boldsymbol{\delta}})\tilde{n}_k)(\sum_{k'}(1 - e^{-i\boldsymbol{k}'\boldsymbol{\delta}})\tilde{n}_{k'})$$

$$= -\frac{J}{2N} \sum_{\delta} (\sum_{k}(1 - \cos\boldsymbol{k}\boldsymbol{\delta})\tilde{n}_k)^2 \ . \tag{2.20}$$

In the same way we get the expectation value of $S_i S_j$ from (2·10) and (2·19):

$$\langle S_i S_j \rangle = (S - N^{-1}\sum_{k}(1 - \cos\boldsymbol{k}(\boldsymbol{r}_i - \boldsymbol{r}_j))\tilde{n}_k)^2 \ . \tag{2.21}$$

Substituting (2·17) we have

$$\langle S_i S_j \rangle = (N^{-1}\sum_{k}\cos\boldsymbol{k}(\boldsymbol{r}_i - \boldsymbol{r}_j)\tilde{n}_k)^2 \ . \tag{2.22}$$

The free energy per site with the first order correction is given as follows:

$$f = N^{-1}(F_0 + \langle H_1 \rangle) = \mu S - TN^{-1}\sum_{k}\ln(1 + \tilde{n}_k) - \frac{Jz}{2}(S - S')^2 \ . \tag{2.23}$$

Here S' is defined by

$$S' \equiv S - N^{-1} \sum_k (1 - \cos k\delta) \tilde{n}_k = S - (Nz)^{-1} \sum_k \varepsilon(k) \tilde{n}_k , \tag{2.24}$$

z is the number of the nearest neighbors. S'^2 is the correlation of nearest neighbors. The energy per site e is:

$$e = N^{-1}(\langle H_0 \rangle + \langle H_1 \rangle) = \frac{1}{2} zJ(S^2 - S'^2) . \tag{2.25}$$

Consider the case where the Zeeman term $H' = -2h \sum S_i^z$ is added to Hamiltonian (1.1). The susceptibility per site χ is given by the correlation functions:

$$\chi = \frac{4}{TN} \sum_{i,j} \langle S_i^z S_j^z \rangle = \frac{4}{3TN} \{ \sum_{i \neq j} \langle S_i S_j \rangle + NS(S+1) \} . \tag{2.26}$$

Here we used $S_i S_i = S(S+1)$. Substitution of (2.22) into (2.26) yields

$$\chi = \frac{4}{3TN} \{ \sum_k \tilde{n}_k^2 \} + \frac{4S}{3T} = \frac{4}{3TN} \{ \sum_k \tilde{n}_k^2 + \tilde{n}_k \} . \tag{2.27}$$

In the same way the magnetic form factor $S(q)$ is as follows:

$$S(q) \equiv N^{-1} \sum_{i,j} \langle S_i S_j \rangle e^{iq(r_i - r_j)} = N^{-1} \sum_k \tilde{n}_{k+q} \tilde{n}_k + S . \tag{2.28}$$

2.4. Solution at $T \to \infty$

We consider the limit of infinite temperature. In this case $\tilde{n}_k$ is a constant which equals to S. Self-consistent equation (2.17) gives

$$\mu/T = \ln(1 + S^{-1}) . \tag{2.29}$$

Then we have S', e, χT, $\langle S_i S_j \rangle$ from (2.24), (2.25), (2.27), (2.22):

$$S' = 0 ,$$

$$e = \frac{1}{2} zJS^2 ,$$

$$\chi T = 4S(S+1)/3 ,$$

$$\langle S_i S_j \rangle = S(S+1)\delta_{ij} . \tag{2.30}$$

These are trivial but correct results. From (2.23) we have

$$-\lim_{T \to \infty} \frac{f}{T} = \ln(1+S)\left(1 + \frac{1}{S}\right)^S . \tag{2.31}$$

This value of entropy per site is bigger than the correct value $\ln(2S+1)$. For $S = 1/2$ our theory gives $\ln(2.598)$ corresponding to the correct value $\ln 2$. Thus our approximation is not very bad even at $T \to \infty$.

2.5. Rotational symmetry

The true density matrix should have a rotational symmetry in the spin space. But approximate density matrix (2.11) is far from rotationally symmetric. Actually we have

completely different expectation values of $S_i{}^z S_j{}^z$ and $S_i{}^x S_j{}^x$ if we use density matrix (2·11) and the Holstein-Primakoff transformation (2·1). Then in real calculation of expectation value of an operator, it should be averaged by the following rotational symmetrization. The average is taken over angle 2π around a fixed axis. About the direction of axis we average the operator over solid angle 4π. By this averaging, an operator A is replaced by the following $\bar{A}$:

$$\bar{A} = \frac{1}{8\pi^2} \int_0^\pi d\theta \int_0^{2\pi} d\phi \int_0^{2\pi} d\psi \ \sin\theta \ U^\dagger(\theta, \phi, \psi) A U(\theta, \phi, \psi) ,$$

where

$$U = \exp i\psi(\cos\theta \ S^z + \sin\theta\cos\phi \ S^x + \sin\theta\sin\phi \ S^y) . \tag{2·32}$$

By this rotational symmetrization we have

$$\overline{S_i{}^z S_j{}^z} = \overline{S_i{}^x S_j{}^x} = \overline{S_i{}^y S_j{}^y} = \frac{1}{3}(\boldsymbol{S}_i \boldsymbol{S}_j) , \tag{2·33}$$

$$\overline{S_i{}^z S_j{}^z S_k{}^z S_l{}^z} = \frac{1}{15}((\boldsymbol{S}_i \boldsymbol{S}_j)(\boldsymbol{S}_k \boldsymbol{S}_l) + (\boldsymbol{S}_i \boldsymbol{S}_k)(\boldsymbol{S}_j \boldsymbol{S}_l) + (\boldsymbol{S}_i \boldsymbol{S}_l)(\boldsymbol{S}_j \boldsymbol{S}_k)) . \tag{2·34}$$

It seems that the rotational symmetrization of any operator is expressed in terms of inner products of spin pair. Then we only need to calculate expectation values of the quantities as appeared on the right-hand side of (2·33) and (2·34). It is dangerous and misleading to calculate expectation value of an operator without this symmetrization.

2.6. *Relation with the usual spin-wave theory*

As Dyson[8] formulated, the usual spin-wave theory considers the problem of Hamiltonian (1·1) with finite magnetic field:

$$H' = -2h\sum_i S_i{}^z .$$

The zero-field case is derived by taking the limit $h \to 0+$. In the case of three dimensions at low temperature this limit is easily calculated. But in one and two dimensions this procedure is difficult because number of spin waves diverges. Therefore many approximations were invented for the low-dimensional Heisenberg model. Our theory formulated in this section is a kind of such approximations. But as will be shown in the next section, it gives the correct low-temperature expansion for the one-dimensional $S=1/2$ Heisenberg ferromagnet. Our theory is applied also to the three-dimensional system. At low temperature we get zero-momentum condensation with $\mu = 0-$. The quantity of zero momentum condensate is equal to the spontaneous magnetization. It is equivalent to the spin-wave theory for three-dimensional system at low temperature in the limit of zero field. Our theory is restricted to zero external magnetic field. If we want the free energy with finite field we should use the conventional spin-wave theory. For a very weak magnetic field, we can expand the free energy with powers of h^2. The first expansion coefficient is the susceptibility given by (2·27). The second coefficient is given by four-point correlation functions. This may be calculated by rotational symmetrization (2·34) and substitution of (2·9).

2.7. *Improvement of approximation*

In § 2.3 we minimize $\langle H_0 \rangle - T \cdot entropy$ and obtain a self-consistent equation for μ. But this is improved if we minimize $\langle H_0 + H_1 \rangle - T \cdot entropy$. In this approximation (2·18) should be replaced by

$$\tilde{n}_k = \frac{1}{\exp(T^{-1}(JS'\varepsilon(k) - \mu)) - 1} .$$
(2·35)

It should be noted that S is replaced by S' defined in (2·24). So we have two parameters S' and μ which should be determined self-consistently by coupled equations (2·35), (2·17) and (2·24). Equations (2·19)~(2·28) still stand in this improvement. At the lowest few orders of the low-temperature expansion this improvement does not change the coefficients because $S' = S - O(T^{3/2})$ or $S' = S - O(T^2)$. In this paper we do not adopt this improvement because the formulas become too complicated.

§ 3. Free energy and susceptibility at low temperature $T \ll JS$

3.1. *State density and Bose-Einstein integral function*

It is convenient to define the state density function:

$$w(x) = \frac{1}{N}\sum_k \delta(x - \varepsilon(k)) .$$
(3·1)

Equations (2·17), (2·24), (2·23) and (2·27) are written as follows:

$$S = \int_0^\infty \frac{w(x)dx}{\exp(xt^{-1} + v) - 1} ,$$
(3·2)

$$S' = S - \frac{1}{z}\int_0^\infty \frac{xw(x)dx}{\exp(xt^{-1} + v) - 1} ,$$
(3·3)

$$\frac{f}{T} = -vS + \int_0^\infty \ln(1 - \exp(-xt^{-1} - v))w(x)dx - \frac{zJ}{2T}(S - S')^2 ,$$
(3·4)

$$\chi = \frac{4}{3T}\int_0^\infty \frac{\exp(xt^{-1} + v)w(x)dx}{(\exp(xt^{-1} + v) - 1)^2} ,$$
(3·5)

where we define reduced temperature t and reduced chemical potential v by

$$t \equiv T/(JS) , \qquad v \equiv -\mu/T .$$
(3·6)

Thus in our approximation thermodynamic quantities are determined by state density $w(x)$. For the one-dimensional chain, $w(x)$ is as follows:

$$w(x) = \frac{1}{2\pi}\int_0^{2\pi} \delta(x - 2 + 2\cos k)dk = \begin{cases} \frac{1}{2\pi} \cdot \left(x\left(1 - \frac{x}{4}\right)\right)^{-1/2} & \text{at } 0 \le x \le 4 , \\ 0 & \text{at } x > 4 . \end{cases}$$
(3·7)

For the square lattice we have

$$w(x) = \frac{1}{4\pi^2} \int_0^{2\pi} dk_1 \int_0^{2\pi} dk_2 \delta(x - 4 + 2\cos k_1 + 2\cos k_2)$$

$$= \begin{cases} \dfrac{8}{\pi^2(8-x)} K\left(\dfrac{x}{8-x}\right) & \text{at } 0 \le x \le 4, \\[2mm] \dfrac{8}{\pi^2 x} K\left(\dfrac{8-x}{x}\right) & \text{at } 4 \le x \le 8, \\[2mm] 0 & \text{at } x \ge 8. \end{cases} \tag{3.8}$$

Here $K(k)$ is the complete elliptic integral of the first kind with modulus k. For the calculation of $(3\cdot2) \sim (3\cdot5)$ we need Bose-Einstein integral function:

$$F(\alpha, v) = \frac{1}{\Gamma(\alpha)} \int_0^\infty \frac{u^{\alpha-1} du}{e^{u+v} - 1} = \frac{e^{-v}}{1^\alpha} + \frac{e^{-2v}}{2^\alpha} + \cdots. \tag{3.9}$$

Analytical property of this function near $v=0$ is known.[13] If α is not a positive integer we have

$$F(\alpha, v) = \Gamma(1-\alpha)v^{\alpha-1} + \sum_{n=0}^\infty (n!)^{-1}(-v)^n \zeta(\alpha-n). \tag{3.10}$$

When α is a positive integer, we have

$$F(\alpha, v) = (-v)^{\alpha-1}((\alpha-1)!)^{-1}\left\{\sum_{r=1}^{\alpha-1}\frac{1}{r} - \ln v\right\} + \sum_{n \ne \alpha-1} (n!)^{-1}(-v)^n \zeta(\alpha-n). \tag{3.11}$$

Here $\zeta(\alpha)$ is Riemann's zeta function. For the integrals in $(3\cdot4)$ and $(3\cdot5)$ the following identities are useful:

$$\int_0^\infty u^{\alpha-1}\ln(1 - e^{-u-v})du = \Gamma(\alpha)F(\alpha+1, v), \tag{3.12}$$

$$\int_0^\infty u^{\alpha-1}e^{u+v}(e^{u+v} - 1)^{-2}du = \Gamma(\alpha)F(\alpha-1, v). \tag{3.13}$$

3.2. One-dimensional chain

From $(3\cdot7)$, $w(x)$ is expanded at small x:

$$w(x) = (2\pi)^{-1} x^{-1/2}\left(1 + \frac{1}{8}x + \frac{3}{128}x^2 + \cdots\right). \tag{3.14}$$

Equations $(3\cdot2) \sim (3\cdot5)$ are expanded by Bose-Einstein integral function. Using Eq. $(3\cdot10)$, these are written as series of v and t:

$$S = \frac{t^{1/2}}{2\sqrt{\pi}}\left\{\sqrt{\pi}v^{-1/2} + \zeta\left(\frac{1}{2}\right) + \frac{1}{16}\zeta\left(\frac{3}{2}\right)t - \zeta\left(-\frac{1}{2}\right)v + \cdots\right\}, \tag{3.15}$$

$$S' = S - \frac{1}{8\sqrt{\pi}}\zeta\left(\frac{3}{2}\right)t^{3/2} + \cdots, \tag{3.16}$$

$$\frac{f}{T} = -vs - \frac{t^{1/2}}{2\sqrt{\pi}}\left\{\zeta\left(\frac{3}{2}\right) - 2\sqrt{\pi}v^{1/2} - \zeta\left(\frac{1}{2}\right)v + \frac{t}{16}\zeta\left(\frac{5}{2}\right) + \cdots\right\}, \tag{3.17}$$

$$\chi = \frac{t^{1/2}v^{-3/2}}{3T}(1 + O(v^{3/2})). \tag{3.18}$$

From Eq. $(3\cdot15)$ we should determine v as a function of t. We transform Eq. $(3\cdot15)$ as follows:

$$v^{1/2} = \frac{t^{1/2}}{2S}\left\{1 + \pi^{1/2}\zeta\left(\frac{1}{2}\right)v^{1/2} + \frac{1}{16}\pi^{-1/2}\zeta\left(\frac{3}{2}\right)tv^{1/2} - \pi^{-1/2}\zeta\left(-\frac{1}{2}\right)v^{3/2} + \cdots\right\}. \tag{3.19}$$

By iteration we get $v^{1/2}$ as a power series of $t^{1/2}$:

$$v^{1/2} = \frac{t^{1/2}}{2S}\left(1 + \pi^{-1/2}\zeta\left(\frac{1}{2}\right)\left(\frac{t^{1/2}}{2S}\right) + \pi^{-1}\zeta^2\left(\frac{1}{2}\right)\frac{t}{4S^2} + O(t^{3/2})\right). \tag{3.20}$$

Substituting this into (3·17) and (3·18) we get

$$\frac{f}{T} = -\frac{\zeta(3/2)}{\sqrt{2\pi}}\left(\frac{T}{2SJ}\right)^{1/2} + \frac{T}{4S^2J} + \left\{\frac{1}{2S^2}\cdot\frac{\zeta(1/2)}{\sqrt{2\pi}} - \frac{1}{8}\cdot\frac{\zeta(5/2)}{\sqrt{2\pi}}\right\}\left(\frac{T}{2SJ}\right)^{3/2} + O(T^2). \tag{3.21}$$

$$\chi = \frac{8S^4J}{3T^2}\left(1 - \frac{3}{S}\cdot\frac{\zeta(1/2)}{\sqrt{2\pi}}\left(\frac{T}{2SJ}\right)^{1/2} + \frac{3}{S^2}\cdot\frac{\zeta^2(1/2)}{2\pi}\left(\frac{T}{2SJ}\right) + O(T^{3/2})\right). \tag{3.22}$$

We substitute the following values into the above equations:

$$\frac{\zeta(1/2)}{\sqrt{2\pi}} = -0.582597455, \qquad \frac{\zeta(3/2)}{\sqrt{2\pi}} = 1.0421869,$$

$$\frac{\zeta(5/2)}{\sqrt{2\pi}} = 0.53517597 \tag{3.23}$$

and get the expansions for $S = 1/2$:

$$\frac{f}{T} = -1.0421869\left(\frac{T}{J}\right)^{1/2} + \frac{T}{J} - 1.2320919\left(\frac{T}{J}\right)^{3/2} + O(T^2), \tag{3.24}$$

$$\chi = \frac{J}{6T^2} + 0.5825974\frac{J^{1/2}}{T^{3/2}} + 0.6788396\frac{1}{T} + O(T^{1/2}). \tag{3.25}$$

These equations should be compared with the result of the Bethe-ansatz integral equations :[1],[2]

$$\frac{f}{T} = -1.042\left(\frac{T}{J}\right)^{1/2} + 1.00\left(\frac{T}{J}\right) - 0.9\left(\frac{T}{J}\right)^{3/2} + O(T^2), \tag{3.26}$$

$$\chi = 0.1667\frac{J}{T^2} + 0.581\frac{J^{1/2}}{T^{3/2}} + 0.68\frac{1}{T} + O(T^{1/2}). \tag{3.27}$$

All the coefficients except the third term of f coincide very well. Anyway it is possible that Eqs. (3·21) and (3·22) give exact coefficients of the low-temperature expansions for arbitrary spin quantum number at least up to the second term.

3.3. *Two-dimensional square lattice*

From Eq. (3·8), $w(x)$ is expanded at small x:

$$w(x) = \frac{1}{4\pi}\left(1 + \frac{x}{8} + \frac{3}{128}x^2 + \cdots\right). \tag{3.28}$$

Then the integrals in Eqs. (3·2)~(3·5) are expanded by Bose-Einstein integral function with integer a. Using Eqs. (3·10) and (3·11), we have

$$S = \frac{t}{4\pi}\left\{ -\ln v + \frac{v}{2} + \frac{\zeta(2)}{8}t + \cdots \right\},$$

(3·29)

$$S' = S - \frac{\zeta(2)}{16\pi}t^2 + \cdots,$$

(3·30)

$$\frac{f}{T} = -\frac{\zeta(2)}{4\pi}t - \frac{\zeta(3)}{32\pi}t^2 - \frac{27\zeta(4)}{256\pi}t^3\cdots - \frac{2J}{T}(S-S')^2,$$

(3·31)

$$\chi = \frac{t}{3\pi T}\left(\frac{1}{v} + O(1)\right).$$

(3·32)

From Eq. (3·29) we get

$$v = \exp\left(-\frac{4\pi S}{t} + O(t)\right).$$

(3·33)

At low temperature v is a very small quantity. Substituting this into (3·31)~(3·32) we have

$$f = -\frac{T^2}{4\pi JS}\left\{\zeta(2) + \frac{\zeta(3)}{8}\cdot\frac{T}{JS} + O(T^2)\right\},$$

(3·34)

$$\chi = \frac{1}{3\pi JS}\exp\left(\frac{4\pi JS^2}{T}\right)(1 + O(T)).$$

(3·35)

The susceptibility diverges strongly as $\exp(4\pi JS^2/T)$. The free energy behaves as the conventional spin-wave theory predicts. Unfortunately for the two-dimensional Heisenberg ferromagnet we have no exact solution to compare with our theory. But it is possible that Eqs. (3·34) and (3·35) give the correct low-temperature expansion of the free energy and the susceptibility.

§ 4. Asymptotic behavior of two-point correlation function at low temperature and long distance

As shown in Eq. (2·22) the two-point correlation function is the square of the Fourier transform of the Bose momentum distribution (2·18). At long distances it is determined by $\tilde{n}_k$ at small $|k|$. From Eq. (2·18) we have

$$\tilde{n}_k = \frac{2dt/z}{k^2 + (2\xi)^{-2}}, \qquad \xi \equiv \frac{1}{2}(2dtv/z)^{-1/2}.$$

(4·1)

The Fourier transform of this function is well known both in one and two dimensions. In one dimension we have

$$\langle S_0 S_r \rangle = S^2\exp(-r/\xi), \qquad \xi \simeq JS^2/T.$$

(4·2)

In two dimensions we have

$$\langle S_0 S_r \rangle^{1/2} = (2dt/z)\frac{1}{(2\pi)^2}\int_0^\infty dk\, k \int_0^{2\pi} d\theta\frac{\exp(ikr\cos\theta)}{k^2 + (2\xi)^{-2}}$$

$$= (2dt/z)\frac{1}{2\pi}\int_0^\infty dk\frac{kJ_0(kr)}{k^2 + (2\xi)^{-2}} = \frac{dt}{\pi z}K_0(r/2\xi)$$

$$\simeq \frac{dt}{\pi z}\sqrt{\frac{\pi\xi}{r}}\exp(-r/2\xi),$$

(4·3)

where K_0 is the modified Bessel function. Then for the square lattice we have

$$\langle S_0 S_r \rangle = \frac{T^2}{4\pi J^2 S^2} \cdot \frac{e^{-r/\xi}}{(r/\xi)}, \qquad \xi \simeq \left(\frac{JS}{T}\right)^{1/2} \exp\left(\frac{2\pi JS^2}{T}\right). \tag{4.4}$$

Thus we find that ξ defined in (4·1) gives the correlation length. Reduced chemical potential v determines the correlation length and the magnetic susceptibility.

§ 5. Summary and discussion

As shown in § 2 we can construct modified spin-wave theory which calculates low-temperature properties of one- and two-dimensional Heisenberg ferromagnets. We reproduced the low-temperature expansions of free energy and susceptibility of the $S=1/2$ Heisenberg chain which was previously obtained by the Bethe-ansatz method.

Recently Schlottmann[4] proposed that the susceptibility diverges as $J/(T^2\ln(J/T))$. He claims that this susceptibility is derived analytically from the Bethe-ansatz integral equation. Apparently it contradicts with our expansion (3·25) which diverges as J/T^2. Here we review his derivation briefly. The Bethe-ansatz integral equations[5] contain infinite number of unknowns $\eta_n(\Lambda)$ ($n=1, 2, \cdots, -\infty < \Lambda < \infty$). At very large n or $|\Lambda|$, $\eta_n(\Lambda)$ approaches to the free spin solution. At sufficiently low temperature, $T\ln\eta_n(\Lambda)$ approaches to its zero-temperature solution. He assumes that one can define crossover point $\Lambda_c(n)$ and n_c for given temperature T. Using matching condition for two solutions he determined n_c and $\Lambda_c(n)$ and got expressions of the free energy and the susceptibility. In our opinion the crossover region is very wide and the behavior of $\eta_n(\Lambda)$ in this region is essential. His assumption is too crude for the calculation of the susceptibility. His derivation cannot be regarded as an analytical one. Of course we have not succeeded in deriving analytically that χ behaves as J/T^2 from the Bethe-ansatz integral equations. In Fig. 1 we compare numerical results of the integral equations, our expansion (3·25) and Schlottmann's expansion:[4]

$$\chi = \frac{0.84J}{T^2} \left\{ \frac{1}{\ln(J/T)} + \frac{\ln\ln(J/T)}{\ln^2(J/T)} \right\}. \tag{5.1}$$

Apparently his expansion is worse than ours. Thus we can say that there is not logarithmic correction in the susceptibility. The correlation length is proportional to T^{-1} and has not logarithmic correction.

We can understand the reason why thermodynamic quantities of the linear chain are expanded by $\sqrt{T}$. It is because the chemical potential is expanded by $\sqrt{T}$
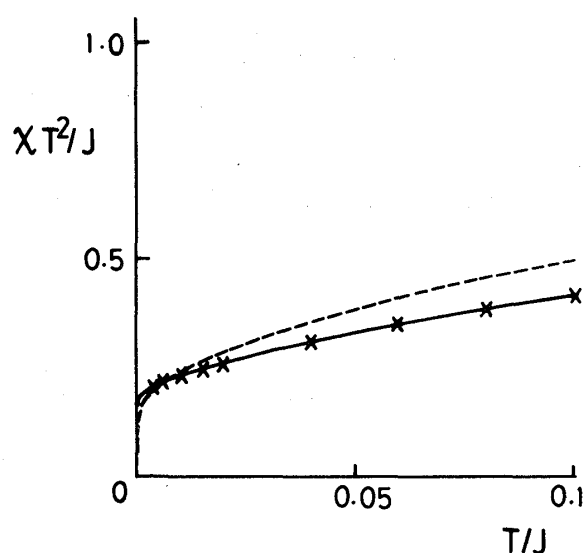

Fig. 1. $\chi T^2 J^{-1}$ as a function of TJ^{-1} for the $S=1/2$ Heisenberg ferromagnet. Crosses are the results of the Bethe-ansatz integral equation from Ref. 1). The solid line is our expansion Eq. (3·25). The dashed line is Schlottmann's susceptibility (5·1) taken from Ref. 4). Our expansion formula coincides accurately with that of the Bethe-ansatz integral equation.

as shown in (3·20). We can explain the mysterious second term of free energy expansion (1·2) by the effect of chemical potential.

Kondo and Yamaji[9] were the first to find that the energy and the free energy of the $S=1/2$ linear chain is expanded by power series of $\sqrt{T}$. They used the Green function decoupling approximation. Their coefficients are slightly different from ours. The first term of the free energy is $5/6$ times of the spin-wave result. This discrepancy comes from their decoupling approximation. For the susceptibility they gave the correct first term $\chi = J/(6T^2)$.

From Eq. (3·21) we get the expansion of the specific heat per site:

$$C = \frac{3}{4}\frac{\zeta(3/2)}{\sqrt{2\pi}}\left(\frac{T}{2SJ}\right)^{1/2} - \frac{T}{2S^2J} + O(T^{3/2}). \tag{5·2}$$

This formula does not contradict with Blöte's numerical result[10] for the finite linear chain with large spin quantum number S. He got that the specific heat is smaller than the spin-wave result which is the first term of r.h.s. of (5·2). Unfortunately detailed comparison is difficult because the length of chain is short.

For the two-dimensional Heisenberg ferromagnet the free energy is expanded as a power series of T and the first and the second terms are the same with those of the conventional spin-wave theory. It is because in two dimensions chemical potential effect is of the order of $\exp(-4\pi JS^2/T)$ and the situation is different from that in one dimension. We show that the susceptibility diverges as $\exp(4\pi JS^2/T)$. This result apparently denies Stanley and Kaplan's conjecture[11] that the susceptibility diverges at finite temperature. The following formula for the susceptibility was derived by several authors:[12]

$$\chi = CT^l\exp(a/T).$$

The values of C, l and a are dependent on approximations. Our result is $a=4\pi JS^2$ and $l=0$.

Our spin-wave approximation can be applied to the classical Heisenberg model by taking an appropriate limit.

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