

Few-Dimensional Heisenberg Ferromagnets at Low Temperature

Minoru Takahashi

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

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A simple approximation for one- and two-dimensional Heisenberg ferromagnets is proposed. This is a modification of the spin-wave theory for a three-dimensional ferromagnet and is expected to give correct low-temperature properties. The free energy and susceptibility of the linear chain are expanded in powers of square root of temperature. At $S = \frac{1}{2}$ the results agree excellently with those of Bethe-*Ansatz* integral equations. The susceptibility of the two-dimensional square lattice diverges as $\exp(4\pi JS^2/T)$.

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One- and two-dimensional Heisenberg ferromagnets have a completely ordered ground state but no long-range order at finite temperature. The transition point is at zero temperature and the thermodynamic properties are of interest since they differ from the usual transition at finite temperature. Experimentally this is important for an understanding of quasi few-dimensional ferromagnetic substances such as $(C_6H_{11}NH_3)CuCl_3$ and K_2CuF_4 .¹ The Hamiltonian is

$$H = -J \sum_{\langle ij \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - S^2) - 2h \sum_i S_i^z, \quad J > 0. \quad (1)$$

Here, $\langle ij \rangle$ means that i and j sites are nearest neighbors. We assume that there are N spins and that S is the spin quantum number.

Low-temperature properties of the $S = \frac{1}{2}$ linear chain were recently analyzed by Takahashi and Yamada² and by Schlottmann^{3,4} using thermodynamic Bethe-*Ansatz* integral equations.⁵ Numerical calculation of integral equations gave $\alpha = -\frac{1}{2}$ and $\gamma = 2$. By application of the least-squares method to the numerical data at $0.004 \leq T/J \leq 1.00$, the following expansions were obtained for free energy f and susceptibility χ per site:

$$f = T[-1.042(T/J)^{1/2} + 1.00(T/J) - 0.9(T/J)^{3/2} + O(T^2)], \quad (2)$$

$$\chi = JT^{-2}[0.1667 + 0.581(T/J)^{1/2} + 0.68(T/J) + O(T^{3/2})]. \quad (3)$$

In contrast, the usual spin-wave theory⁶ gives

$$f = T[-1.0421869(T/J)^{1/2} - 0.0668971(T/J)^{3/2} - \dots]. \quad (4)$$

The fact that the first terms of (2) and (4) coincide with each other indicates that the spin-wave theory here applies to some degree. The second terms, however, are completely different and modification of the theory is necessary to obtain higher-order terms. In the spin-wave theory the magnetic field h serves as the chemical potential of bosons. At the limit $h \rightarrow 0$, the number of bosons becomes infinite. Actually, the number of spin waves should be SN because magnetization is zero at the limit. The chemical potential should be chosen so that the density of spin waves is S . With the modification of the spin-wave theory (1) can be treated at $h = 0$.

By use of the Holstein-Primakoff transformation $[S_j^+ = (2S - a_j^* a_j)^{1/2} a_j, S_j^- = a_j^* (2S - a_j^* a_j)^{1/2}, S_j^z = S - a_j^* a_j]$, the spin-pair operator $\mathbf{S}_i \cdot \mathbf{S}_j$ is represented by boson operators a_i^* and a_i :

$$\mathbf{S}_i \cdot \mathbf{S}_j = S^2 - S(a_i^* - a_j^*)(a_i - a_j) - \frac{1}{4}\{a_i^* a_j^*(a_i - a_j)^2 + (a_i^* - a_j^*)^2 a_i a_j\} + O(S^{-1}), \quad \text{for } i \neq j. \quad (5)$$

An ideal spin-wave state is given by a set of N non-negative integers $\{n_{\mathbf{k}}\}$:

$$| \{n_{\mathbf{k}}\} \rangle = \prod_{\mathbf{k}} (n_{\mathbf{k}}!)^{-1/2} (a_{\mathbf{k}}^*)^{n_{\mathbf{k}}} | 0 \rangle. \quad (6)$$

Here, \mathbf{k} varies over N wave vectors in the first Brillouin zone and $a_{\mathbf{k}}^*$ [$\equiv N^{-1/2} \sum_j \exp(i\mathbf{k} \cdot \mathbf{r}_j) a_j^*$] is the creation operator for a spin wave with wave vector \mathbf{k} . At finite temperature $n_{\mathbf{k}}$ is fluctuating and its average value is set at $\bar{n}_{\mathbf{k}}$. From (5) and (6) the expectation value of $\mathbf{S}_i \cdot \mathbf{S}_j$ is given as

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \{S - N^{-1} \sum_{\mathbf{k}} [1 - \cos \mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j)] \bar{n}_{\mathbf{k}}\}^2. \quad (7)$$

The entropy of the state is $\sum_{\mathbf{k}} \{(1 + \bar{n}_{\mathbf{k}}) \ln(1 + \bar{n}_{\mathbf{k}}) - \bar{n}_{\mathbf{k}} \ln \bar{n}_{\mathbf{k}}\}$. Then, conditions of free-energy minimum and zero magnetization yield the following self-consistent equations:

$$\bar{n}_{\mathbf{k}} = \{\exp[JS' \varepsilon(\mathbf{k})/T + v] - 1\}^{-1}, \quad (8)$$

$$\varepsilon(\mathbf{k}) \equiv \sum_{\delta} (1 - \cos \mathbf{k} \cdot \delta), \quad (9)$$

$$S = N^{-1} \sum_{\mathbf{k}} \bar{n}_{\mathbf{k}}, \quad (10)$$

$$S' = S - (Nz)^{-1} \sum_{\mathbf{k}} \varepsilon(\mathbf{k}) \bar{n}_{\mathbf{k}}.$$

Here, z is the number of nearest neighbors, δ 's are lattice vectors to the nearest neighbors, and v is the reduced chemical potential. v and S' should be solved self-consistently from (9) and (10). In this formulation f and χ become

$$f = -T[vS + N^{-1} \sum_{\mathbf{k}} \ln(1 + \tilde{n}_{\mathbf{k}})] - \frac{1}{2} Jz(S - S')^2, \quad (11)$$

$$\chi = (4/3TN) \sum_{\mathbf{k}} \tilde{n}_{\mathbf{k}}(\tilde{n}_{\mathbf{k}} + 1). \quad (12)$$

By use of the state-density function $w(x) = N^{-1} \sum_{\mathbf{k}} \delta(x$

$-\varepsilon(\mathbf{k}))$, the sums in Eqs. (9)–(12) are replaced by integrals. At low temperature we can put $S = S'$ in (8).

For the linear chain $w(x) = (2\pi)^{-1} x^{-1/2} (1 + x/8 \dots)$. Then the sums in (9)–(12) are represented by the Bose-Einstein integral function $F(\alpha, v) \equiv \sum_{n=1}^{\infty} e^{-nv} n^{-\alpha}$. If α is not a positive integer, F is expanded in a power series⁷ in v :

$$F(\alpha, v) = \Gamma(1 - \alpha) v^{\alpha-1} + \sum_{n=0}^{\infty} (n!)^{-1} (-v)^n \zeta(\alpha - n). \quad (13)$$

From Eq. (9) $v^{1/2}$ is obtained as a function of T :

$$v^{1/2} = (t^{1/2}/2S) + \pi^{-1/2} \zeta(\frac{1}{2})(t^{1/2}/2S)^2 + \pi^{-1} \zeta^2(\frac{1}{2})(t^{1/2}/2S)^3 + \dots, \quad t \equiv T/JS. \quad (14)$$

Substitution of this into (11) and (12) gives

$$f = T \left[\frac{\zeta(\frac{3}{2})}{(2\pi)^{1/2}} \left(\frac{T}{2SJ} \right)^{1/2} + \frac{T}{4S^2 J} + \left[\frac{1}{2S^2} \frac{\zeta(\frac{1}{2})}{(2\pi)^{1/2}} - \frac{1}{8} \frac{\zeta(\frac{5}{2})}{(2\pi)} \right] \left(\frac{T}{2SJ} \right)^{3/2} + O(T^2) \right], \quad (15)$$

$$\chi = \frac{8}{3} S^4 J T^{-2} \left[1 - \frac{3}{S} \frac{\zeta(\frac{1}{2})}{(2\pi)^{1/2}} \left(\frac{T}{2SJ} \right)^{1/2} + \frac{3}{S^2} \frac{\zeta^2(\frac{1}{2})}{2\pi} \frac{T}{2SJ} + O(T^{3/2}) \right]. \quad (16)$$

At $S = \frac{1}{2}$ these become

$$f = T[-1.042 186 9(T/J)^{1/2} + (T/J) - 1.232 091 9(T/J)^{3/2} + O(T^2)], \quad (17)$$

$$\chi = J T^{-2} [\frac{1}{6} + 0.582 597 4(T/J)^{1/2} + 0.678 839 6(T/J) + O(T^{3/2})]. \quad (18)$$

All coefficients except the third term of f coincide very well with (2) and (3).

In a recent paper Schlottmann⁴ proposed that χ diverges as $J/[T^2 \ln(J/T)]$. This contradicts my expansions (16) and (18). He reached this conclusion making some approximations for the Bethe-*Ansatz* integral equation and for this reason I do not believe that his derivation is analytical. Of course, I myself have not yet succeeded in making an analytical calculation from Bethe-*Ansatz* integral equations. In Fig. 1, therefore, I compare the numerical results of integral equations, my expansion (18), and Schlottmann's expansion⁴

$$\chi = 0.84 J T^{-2} \left[\frac{1}{\ln(J/T)} + \frac{\ln \ln(J/T)}{\ln^2(J/T)} \right]. \quad (19)$$

His expansion is apparently weaker than mine. From (7) and (8) we can see that the correlation function decays exponentially and correlation length is JS^2/T .

Kondo and Yamaji⁸ derived similar expressions for f and χ for the $S = \frac{1}{2}$ linear chain using the Green's-function decoupling method. Their coefficients are slightly different from mine. The first term of the free energy is $\frac{5}{6}$ times the spin-wave result. For susceptibility they derived the correct first term $\chi = J/6T^2$.

For the two-dimensional square lattice, the state density $w(x)$ is $(4\pi)^{-1} [1 + (x/8) + O(x^2)]$. From (9) I find $v = \exp[-4\pi JS^2 T^{-1} + O(T)]$; this is a very small quan-

tity. The effect of the chemical potential on the zero-field free energy is thus also very small. On the other hand, χ diverges as v^{-1} :

$$f = -(4\pi JS)^{-1} T^2 \{ \zeta(2) + \frac{1}{8} \zeta(3)(T/JS) + O(T^2) \}, \quad (20)$$

$$\chi = (3\pi JS)^{-1} \exp(4\pi JS^2/T) [1 + O(T)]. \quad (21)$$

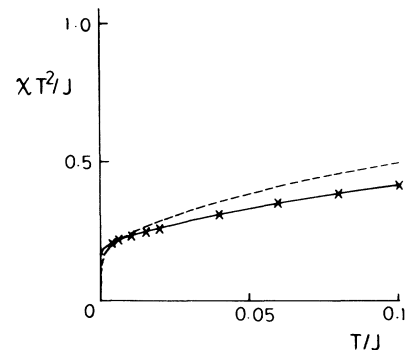


FIG. 1. $\chi T^2 J^{-1}$ as a function of $T J^{-1}$ for the $S = \frac{1}{2}$ Heisenberg linear chain. Crosses are results of the Bethe-*Ansatz* integral equation from Ref. 2. Solid line is my expansion (18). Dashed line is Schlottmann's susceptibility (19) taken from Ref. 4. My expansion formula coincides accurately with numerical results of the Bethe-*Ansatz* integral equation.

Similar expressions for free energy and susceptibility were obtained by Yamaji and Kondo and by Dalton and Wood,⁹ but the coefficients were different. I found that the correlation length is $(JS/T)^{1/2} \exp(2\pi JS^2/T)$. Details will be published elsewhere.

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