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PHYSICAL REVIEW A VOLUME 6, NUMBER 4 OCTOBER 1972

Low-Temperature Thermodynamics of the $|\Delta| \geq 1$ Heisenberg-Ising Ring*

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(Received 20 March 1972)

We use the equations proposed by Gaudin for the free energy of the Heisenberg-Ising ring for $|\Delta| \geq 1$ to obtain the first temperature-dependent term in a systematic low-temperature expansion of the free energy.

I. INTRODUCTION

We consider the Hamiltonian

$$H = \delta \sum_{n=1}^{N} [S_n{}^x S_{n+1}{}^x + S_n{}^y S_{n+1}{}^y + \Delta(S_n{}^z S_{n+1}{}^z - \tfrac{1}{4})] - H_0 \sum_{n=1}^{N} S_n{}^z, \quad (1.1)$$

where $S_i{}^\mu = \frac{1}{2}\sigma_i{}^\mu$ and the σ_i^μ are Pauli spin matrices for site i. H_0 is the external magnetic field, N is the number of lattice sites and is even, $\Delta = \cosh\Phi \geq 1$, and δ equals $+1$ or -1 for the antiferromagnetic or ferromagnetic regions, respectively. We impose periodic boundary conditions.

Gaudin[1] has recently obtained a solution for the free energy per site, $F(T, \sigma)$, in terms of the solutions of an infinite set of coupled nonlinear integral equations. (σ is the magnetization per spin.) In this paper we perform a systematic expansion of $F(T, \sigma)$ in both T and T^{-1} for T small and large, respectively. Our reasons for such computations are threefold. First, Gaudin in deriving his formalism made two principal assumptions. One concerned the general character of the zeros of a set

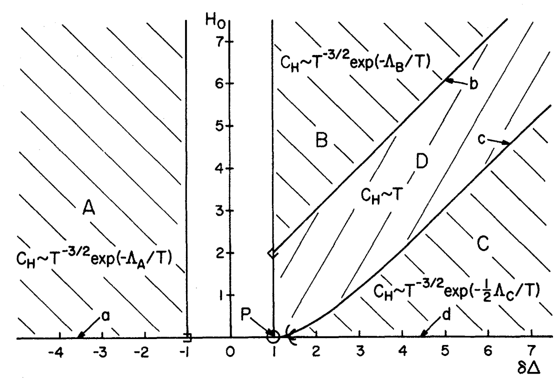

FIG. 1. Regions of various low-temperature characteristics. The lines b and c are determined in Sec. IV by setting the gaps between the ground states and first excited states of regions B and C, respectively, equal to zero. Lines a and b include their $\Delta = 1$ end points while lines c and d do not. Regions A, B, C, and D do not include the lines a, b, c, and d nor point P. The low temperature behavior of the specific heat C_H is shown.

of transcendental equations; in particular, the allowed values of the imaginary part of the zeros were needed. The second was an assumption on the movement of these zeros as Δ was varied. These are standard assumptions repeatedly made for the one-dimensional δ-function quantum gases and the one-dimensional nearest-neighbor spin systems. The agreement of the high-T expansion (made in Sec. II) of Gaudin's formalism with standard high-temperature expansions gives a check on the validity of these assumptions. A weaker verification consists of looking at the low-temperature expansion and examining its agreement with results obtained by arguments of the spin-wave variety.

Secondly, by reversing the direction of the logic, the systematic low-temperature expansion is useful to justify naive constructions (where such arguments can be made) of the first-order terms from a knowledge of the low-lying excitations of the system. Moreover, our expansions in principle can be extended to higher-order terms (although it is expected that such expansions will usually be asymptotic rather than convergent).

Our third reason for studying Gaudin's integral equations is that there are several cases, in particular the isotropic antiferromagnet and isotropic ferromagnet at $H_0 = 0$, where it is not apparent that the "spin-wave" arguments give even the leading term as $T \to 0$.

The Hamiltonian given by Eq. (1.1) is not without physical importance in itself. One-dimensional spin systems whose interactions are principally nearest neighbor do exist in nature; for example, $MCl_2 \cdot 2NC_5H_5$ (M; Co, Cu) are probably described by such a Hamiltonian.[2]

Finally, while previous numerical work is sufficiently accurate to give a good description of the thermodynamics at higher temperatures, the existing extrapolations toward zero temperature suffer from the standard questions of the validity of such extrapolations.[3] Therefore, the analytic expressions for $T \to 0$, available only through our expansions, are interesting in that they provide a firmer result for the low-temperature thermodynamics.

Our low-temperature results are best presented by referring to Fig. 1. The division of the low-temperature characteristics into several regions is indicated by the change in the ground state as a function of H_0 and Δ. Region C has a doubly degenerate ground state with the z component of total spin S^z equal to zero, region B has a totally aligned ground state, and region D has a ground state whose S^z varies from the $S^z = 0$ for C to the $S^z = \frac{1}{2}N$ of B. The ferromagnetic region A has a unique totally aligned ground state while line a has a doubly degenerate ground state.

We can obtain some idea of the expected low-temperature behavior of $F(T, \sigma)$ from the Ising model. Take

$$H^I = \delta J \sum_{n=1}^{N} (S_n^z S_{n+1}^z - \tfrac{1}{4}) - B_0 \sum_{n=1}^{N} S_n^z$$

and obtain

$$F_A^I = \sigma B_0 - \tfrac{1}{2} B_0 - T\, e^{-(B_0 + J)/T} + \cdots ,$$

$$F_B^I = \sigma B_0 - \tfrac{1}{2} B_0 - T\, e^{(J - B_0)/T} + \cdots ,$$

and

$$F_C^I = \sigma B_0 - \tfrac{1}{2} J - \tfrac{1}{2} T\, e^{1/2(B_0 - J)/T} + \cdots .$$

Region D is not present in the Ising limit. Note that the exponentials in F_A^I and F_B^I are dependent on the full gap between the ground state and first excited states, while F_C^I is a function of one-half the gap.

In general, we find that in regions A, B, and C there is an energy gap $\Lambda_{A,B,C}$ between the ground state of the system and the first excited states. In regions A and B the temperature-dependent term of the free energy $F_T(T, \sigma)$ is given for $T \sim 0$ by $F_T = K T^{3/2} e^{-\Lambda_{A,B}/T}$, where K is constant in T. In region C, $F_T = K T^{3/2} e^{-\Lambda_C/2T}$. All constants for the preceding are evaluated in closed form in Sec. IV. In region D there is no gap, and $F_T = K T^2$ with the constants obtained from the solutions of two integral equations. Near lines b and c we approximate and solve these equations for the constants.

When the lines a, b, c, and d are approached from the interiors of the various regions, the above F_T become invalid. However, from a theorem of Araki[4] one knows that for $T \neq 0$ the free energy is analytic in T. Therefore, one is led to consider interpolating among the various regions by expanding the scale of the H_0 axis in the vicinity of a line. Then for $O(T)$ near lines b or c, F_T is equal to the functions of regions B or C, respectively, evaluated on the boundaries and multiplied by $-F_0(-e^{-\Lambda_B/T}, \frac{3}{2})$ for b and by $-F_0(-e^{-\Lambda_C/2T}, \frac{3}{2})$ for c. $\Lambda_{B,C}$ is an $O(T)$ number and

$$F_0(z, \tfrac{3}{2}) = -\pi^{-1/2}\int_{-\infty}^{\infty} dx \ln(1 - z\, e^{-x^2}).$$

For $O(T)$ near line d, F_T is equal to F_T from region C evaluated on d and multiplied by $2\cosh(\frac{1}{2}H_0/T)$, where $H_0 = O(T)$. [This behavior is also exhibited by the Ising model where

$$F_d^I = \sigma B_0 - \tfrac{1}{2}J - T\cosh(\tfrac{1}{2}B_0/T)\, e^{-J/2T} + \cdots .\ ]$$

In A, B, and D and on line b one can let $\Delta = 1$, but in C and on lines c and d, $\Delta \to 1$ is not allowed. Therefore, the $O(T)$ neighborhood of point P is treated separately to obtain $F_T = KT^2$, where the constant is given by the solution of an infinite set of nonlinear integral equations.

Another summary in terms of the susceptibility χ is given by Fig. 2. The deviation of χ from its $T = 0$ value in regions A, B, and C has an exponential character, whereas in region D it has a T^2 behavior. The $O(T)$ neighborhoods of lines b and c interpolate among the various regions.

A comparison can be made with the numerical work of Bonner and Fisher.[3] They anticipated the possibility of the half-gap in C but were unaware that the area covered by C and D is two regions.

Finally in the course of our calculation we obtained as excitations from the ferromagnetic ground state the zero-temperature multimagnon bound-state dispersion curves and as excitations from the antiferromagnetic ground state a set of spin-wave excitations. The magnon curves agree with the expression Torrance and Tinkham[5-7] have found for Δ large.

The organization of the paper is outlined by the following: Section II consists of those results of Gaudin which we use. In the last part of the section we solve for the first three terms of the free energy in the high-temperature expansion. In Sec. III we obtain the multimagnon bound-state dispersion curves for regions A and B and a set of spin-wave excitations for region C by solving for the energies of a class of eigenstates of H. In Sec. IV the derivation of the low-temperature thermodynamics is given. The presentation is organized around the divisions given in Fig. 1. In Sec. V the results of Sec. IV are discussed in terms of spin-wave arguments using the dispersion curves of Sec. III.

II. FORMULATION

The energy levels of the Hamiltonian expressed by Eq. (1.1) are given by the coupled equations[8,9]

$$E = \delta \sum_{\alpha=1}^{M} (\cos k_\alpha - \Delta) - H_0 S^z \qquad (2.1)$$

and

$$N k_\alpha = 2\pi\lambda_\alpha + \sum_{\beta=1;\beta\neq\alpha}^{M} \psi_{\alpha\beta}, \quad \alpha = 1, 2, \ldots, M. \qquad (2.2)$$

It is easier to manipulate the above equations if one parametrizes[10] the k_α and $\psi_{\alpha\beta}$ by

$$\cot(\tfrac{1}{2}k_\alpha) = \coth(\tfrac{1}{2}\Phi)\tan(\tfrac{1}{2}\phi_\alpha), \quad \Delta = \cosh\Phi, \qquad (2.3)$$

and

$$\cot(\tfrac{1}{2}\psi_{\alpha\beta}) = \coth\Phi \tan[\tfrac{1}{2}(\phi_\alpha - \phi_\beta)] \qquad (2.4)$$

with

$$0 \le k_\alpha \le 2\pi, \quad -\pi \le \psi_{\alpha\beta} \le \pi, \quad \text{and} \quad -\pi \le \phi_\alpha \le \pi.$$

The integer M is related to the z component of the total spin by $S^z = \frac{1}{2}N - M$, and the k_α give the total momentum of the system via

$$K_T = \sum_{\alpha=1}^{M} k_\alpha = 2\pi m/N, \quad m \text{ an integer}.$$

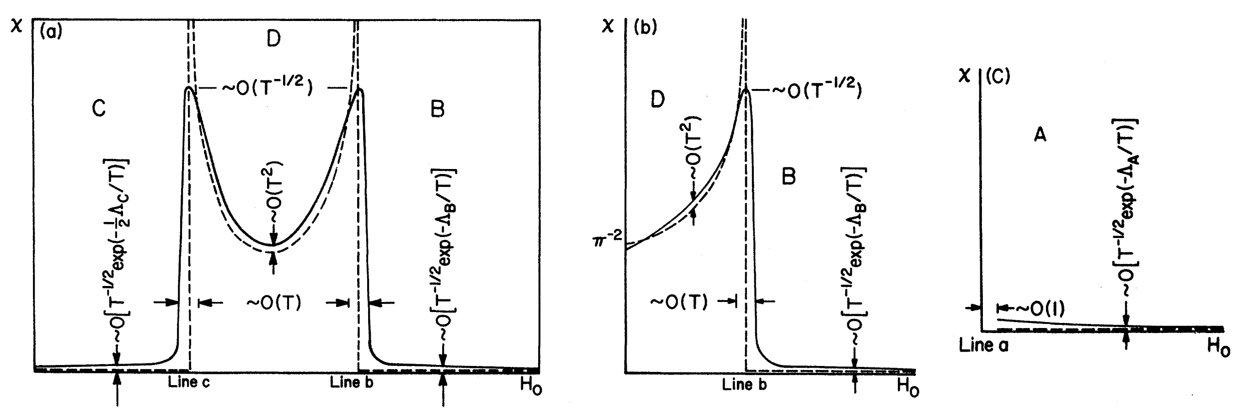

FIG. 2. (a) Susceptibility vs external magnetic field for $\delta = 1$, $\Delta \neq 1$; (b) susceptibility vs external magnetic field for $\delta = 1$, $\Delta = 1$; (c) susceptibility vs external magnetic field for $\delta = -1$. H_0 must not be equal to zero. For all three graphs the dashed line is the $T = 0$ curve, while the continuous line is the curve for T small but not equal to zero.

For N large Gaudin showed that for any particular solution of Eq. (2.2) the ϕ_α are grouped in strings characterized by an order p and common real value ϕ; that is,

$$\phi_\mu = \phi + i\,\mu\Phi, \quad \mu = -(p-1), -(p-3), \ldots, p-1 \tag{2.5}$$

to order e^{-N}.

One continues from this point to derive the equations for the thermodynamics. One finds

$$F(T,\sigma) = \delta E_0(\Delta)/N + \sigma H_0 - T(2\pi)^{-1}\int_{-\pi}^{\pi} dn(\phi)\ln(1+e^{\epsilon_1/T})d\phi, \tag{2.6}$$

where

$$\epsilon_n(\phi)/T = dn(\phi) * \ln[(1+e^{\epsilon_{n+1}/T})(1+e^{\epsilon_{n-1}/T})], \quad n \geq 2 \tag{2.7a}$$

$$\epsilon_1(\phi)/T = dn(\phi) * \ln(1+e^{\epsilon_2/T}) - \delta T^{-1}\sinh\Phi\, dn(\phi), \tag{2.7b}$$

and the boundary condition on the pseudoenergies is $\lim_{n\to\infty}\epsilon_n(\varphi)/n = H_0$. $dn(\phi)$ is given by $dn(\phi) = (K/\pi)\,\mathrm{dn}(K\phi/\pi, k)$, with $K'/K = \Phi/\pi$. $K(K')$ is the complete elliptic integral of the first kind with modulus $k(k')$ and $\mathrm{dn}(\phi,k)$ is one of the Jacobian elliptic functions as given by Bateman.[11] The * notation indicates for any function $f(\phi)$,

$$f(\phi) * g \equiv (2\pi)^{-1}\int_{-\pi}^{\pi} f(\phi-\phi')g(\phi')d\phi'.$$

$E_0(\Delta)$ is the energy of the antiferromagnetic ground state.[12] When $\Delta \to 1\,(\Phi \to 0)$, the above expressions tend to the proper limit if ϕ is rescaled by $x = \phi/\Phi$. To obtain σ, χ, and C_H, the magnetization per spin, the susceptibility, and the specific heat at constant magnetic field, respectively, one uses the thermodynamic relations

$$\sigma = \frac{-\partial}{\partial H_0}(F/N - \sigma H_0)\Big|_T, \tag{2.8a}$$

$$\chi = \frac{\partial \sigma}{\partial H_0}\Big|_T, \tag{2.8b}$$

and

$$C_H = \frac{-T\partial^2}{\partial T^2}(F/N - \sigma H_0)\Big|_{H_0}. \tag{2.8c}$$

In the derivation of Eqs. (2.6) and (2.7) several assumptions were made whose validity has not been rigorously investigated, and to strengthen one's confidence in them, it is desirable to check the high-temperature expansion obtained from the above equations against the standard high-temperature expansion,

$$F(T,\sigma) = -T\ln[2\cosh(\tfrac{1}{2}H_0/T)] + \sigma H_0 - [\tfrac{1}{4}\delta\Delta + (16T)^{-1}][\cosh(\tfrac{1}{2}H_0/T)]^{-2} - \Delta^2[\tfrac{1}{2} + \tanh^2(\tfrac{1}{2}H_0/T) - \tfrac{3}{2}\tanh^4(\tfrac{1}{2}H_0/T)](16T)^{-1} + \cdots, \tag{2.9}$$

obtained by expanding the exponential in $\mathrm{Tr}\,e^{-\beta H}$. One lets $\eta_n = e^{\epsilon_n/T}$ and expands $\eta_n = \eta_n^{(1)} + \eta_n^{(2)}/T + \eta_n^{(3)}/T^2 + \cdots$. To first order one drops the second term in (2.7b) and observes that the $\eta_n^{(1)}$ are independent of ϕ. The integrals in Eqs. (2.7) can be performed to obtain

$$\ln\eta_1^{(1)} = \tfrac{1}{2}\ln(1+\eta_2^{(1)}) \tag{2.10a}$$

and

$$\ln\eta_n^{(1)} = \tfrac{1}{2}\ln[(1+\eta_{n+1}^{(1)})(1+\eta_{n-1}^{(1)})], \quad n \geq 2 \tag{2.10b}$$

with

$$\lim_{n\to\infty}\ln\eta_n^{(1)}/n = H_0/T\ .$$

Note that we are not necessarily assuming that H_0/T is small but are including the case where H_0 is also large, both here and in Eq. (2.9). The solution to Eqs. (2.10) is

$$\eta_n^{(1)} = \sinh^2[\tfrac{1}{2}(n+1)H_0/T]\sinh^{-2}(\tfrac{1}{2}H_0/T) - 1 \tag{2.11}$$

for all n. The second-order equations are obtained by expanding the various logarithms to obtain linear integral equations. They are

$$\eta_1^{(2)}/\eta_1^{(1)} = dn(\phi) * \eta_2^{(2)}/(1+\eta_2^{(1)}) - \delta\sinh(\Phi)dn(\phi) \tag{2.12a}$$

and

$$\eta_n^{(2)}/\eta_n^{(1)} = dn(\phi) * [\eta_{n+1}^{(2)}/(1+\eta_{n+1}^{(1)}) + \eta_{n-1}^{(2)}/(1+\eta_{n-1}^{(1)})], \quad n \geq 2 \tag{2.12b}$$

with

$$\lim_{n\to\infty}\eta_n^{(2)}/(n\eta_n^{(1)}) = 0\ .$$

One solves Eqs. (2.12) by taking the finite Fourier transform of these equations, solving the resulting difference equations, and transforming back. The conventions we take for the Fourier transform are such that

$$\hat{dn}(l) = (2\pi)^{-1}\int_{-\pi}^{\pi} dn(\phi)e^{il\phi}\,d\phi = (2\cosh l\Phi)^{-1}\ .$$

The solution to Eqs. (2.12) is

$$\eta_n^{(2)} = \delta\sinh(\Phi)\sinh[\tfrac{1}{2}(n+1)H_0/T] \times [\sinh(\tfrac{1}{2}H_0/T)\sinh(H_0/T)]^{-1} \times\{\sinh(\tfrac{1}{2}nH_0/T)\sinh[(n+2)\Phi][\cosh(n+2)\Phi - \cos\phi] - \sinh[\tfrac{1}{2}(n+2)H_0/T]\sinh(n\Phi)(\cosh n\Phi - \cos\phi)^{-1}\}\ . \tag{2.13}$$

If

$$\eta_n^{(3)} = \xi_n + (\eta_n^{(2)})^2/[2(1+\eta_n^{(1)})]\ ,$$

the third-order equations, obtained similarly to the second-order ones, are

$$\xi_n/\eta_n^{(1)} + A_n = dn(\phi) * [\xi_{n+1}/(1+\eta_{n+1}^{(1)}) + \xi_{n-1}/(1+\eta_{n-1}^{(1)})], \quad n \geq 1 \tag{2.14}$$

with

$$\lim_{n\to\infty} \xi_n/(n\eta_n^{(1)}) = 0, \quad \xi_0 = 0,$$

and

$$A_n = -(\eta_n^{(2)})^2/[2(\eta_n^{(1)})^2(1+\eta_n^{(1)})] \ .$$

The homogeneous solutions to the resulting difference equations in Fourier space are

$$\hat{\xi}_n^{\pm} = \sinh[\tfrac{1}{2}(n+1)H_0/T]e^{\pm n|l|\Phi}\{\sinh(\tfrac{1}{2}nH_0/T)e^{\pm|l|\Phi} - \sinh[\tfrac{1}{2}(n+2)H_0/T]e^{\pm|l|\Phi}\} \ . \quad (2.15)$$

Using variation of parameters and imposing boundary conditions, the solution to Eqs. (2.14) is

$$\hat{\xi}_n = \hat{\xi}_n^{+}\sum_{m=n}^{\infty} g_m \hat{\xi}_{m+1}^{-} + \hat{\xi}_n^{-}\left(\sum_{m=0}^{n-1} g_m \hat{\xi}_{m+1}^{+} - e^{-2|l|\Phi}\sum_{m=0}^{\infty} g_m \hat{\xi}_{m+1}^{-}\right) , \quad (2.16a)$$

where

$$g_m(l) = 2\cosh(l\Phi)(\eta_{m+2}^{(1)}+1)\hat{A}_{m+1} \times \begin{vmatrix} \hat{\xi}_{m+1}^{+} & \hat{\xi}_{m+1}^{-} \\ \hat{\xi}_{m+2}^{+} & \hat{\xi}_{m+2}^{-} \end{vmatrix}^{-1} . \quad (2.16b)$$

One substitutes the preceding expressions for η_1 into Eq. (2.6), expands the logarithm, and performs the various integrals to obtain

$$F(T,\sigma) = -T\ln[2\cosh(\tfrac{1}{2}H_0/T)] + \sigma H_0 - [\tfrac{1}{4}\delta\Delta + (16T)^{-1}][\cosh(\tfrac{1}{2}H_0/T)]^{-2} - \Delta^2[\tfrac{1}{2} + \tanh^2(\tfrac{1}{2}H_0/T) - \tfrac{3}{2}\tanh^4(\tfrac{1}{2}H_0/T)](16T)^{-1} + \cdots . \quad (2.17)$$

This is the same as Eq. (2.9).

III. MULTIMAGNON BOUND STATES AND EVEN SPIN-WAVE EXCITATIONS

Regions A and B of the system have a ferromagnetic set of states in that the ground state has all spins aligned in the direction of the magnetic field and the excitations are grouped according to their spin deviation from the totally aligned state. For such a spectrum it is felt that the zero-temperature dispersion curves of the elementary excitations are equal to the energies of the magnon bound states. These states are characterized by taking p of Eq. (2.5) equal to M, the number of overturned spins from the ground state; i.e., all the zeros ϕ_α are in a single string with common real value fixed by the total momentum of the state.

First it is convenient to rewrite Eq. (2.3) as

$$e^{ik_\alpha} = (1 - e^{\Phi - i\phi_\alpha})(e^{\Phi} - e^{-i\phi_\alpha})^{-1} \ . \quad (3.1)$$

To obtain the relation between the total momentum K_T^M of the bound state and the real value ϕ_M of the ϕ_α, one forms

$$e^{i\Sigma_\alpha k_\alpha} = \prod_{\mu=-p+1}^{p-1}(1 - e^{\Phi+\mu\Phi-i\phi_M})(e^{\Phi} - e^{\mu\Phi - i\phi_M})^{-1} , \quad (3.2)$$

and, in performing the product, gets

$$e^{iK_T^M} = (1 - e^{M\Phi - i\phi_M})(e^{M\Phi} - e^{-i\phi_M})^{-1} \ . \quad (3.3)$$

To extract the energies of the bound states, one expresses the $\cos k_\alpha$ in Eq. (2.1) by its exponential form, substitutes Eq. (3.1) for the $e^{\pm ik_\alpha}$, sums the resulting expression over the string, and, using Eq. (3.3), writes the resulting expression in terms of K_T^M. The result is

$$E_M - E_{gr}^F = H_0 M - \delta(\cosh M\Phi - \cos K_T^M) \times \sinh(\Phi)(\sinh M\Phi)^{-1} , \quad (3.4)$$

where $E_{gr}^F = -\tfrac{1}{2}H_0 N$ and K_T^M is restricted to the first Brillouin zone, $0 \le K_T^M = 2\pi n/N \le 2\pi$. For $M \gtrsim 3$ and Δ large, Eq. (3.4) can be expanded to give $E_M - E_{gr}^F = H_0 M - \delta\cosh\Phi + \delta e^{-\Phi} + O(e^{-2\Phi})$. This is the same expression obtained by Torrance and Tinkham. Also, we can recover Bethe's results for $\Delta = 1$.[8]

In region C we are interested in excitations from the $S^z = 0$ antiferromagnetic ground state. To understand a little of the character of the low-lying excitations, the antiferromagnetic Ising model serves as a guide. One notes that the first excitations of the Ising model are two-particle (boundary) states and all higher ones are even excitations. Generalizing this away from the Ising limit, we seek the low-lying two spin-wave excitations. Equation (2.2), written as a function of the ϕ_α, gives the coupling among the ϕ_α. The energy as a function of the ϕ_α is expressed by Eq. (2.1), where the momenta as a function of the ϕ_α are taken from Eq. (2.3). The excitation energies of the system are found by the procedure of Yang and Yang,[13] where the effect of exciting ϕ_α's from their ground-state distribution ($\tfrac{1}{2}N$ real ϕ_α's) is calculated.

The $S^z = 1$ low-lying excitations are derived by eliminating one ϕ_α from position ϕ_1 and changing another from ϕ_2 to $\pm\pi$. The $\pm\pi$ apparently labels a doubly degenerate $S^z = 1$ dispersion curve. The difference between the ground-state and excited-state momentum $q_2(S^z, \phi_1, \phi_2)$ and the difference between the ground-state and excited-state energy $E_2(S^z, \phi_1, \phi_2)$ are

$$q_2(S^z, \phi_1, \phi_2) = \int_0^{\phi_1} dn(\phi)d\phi + \int_0^{\phi_2} dn(\phi)d\phi - \tfrac{1}{2}\pi \mp \tfrac{1}{2}\pi \quad (3.5a)$$

and

$$E_2(S^z, \phi_1, \phi_2) = \sinh(\Phi)[dn(\phi_1) + dn(\phi_2)] - S^z H_0 \quad (3.5b)$$

for $\pm\pi$. If one lets

$$q_{1,2}^{\pm}=\int_{\pm\pi}^{\phi_{1,2}} dn(\phi)d\phi \quad ,$$

the energy difference is

$$E_2(S^z, q_1^{\pm}, q_2^{\pm}) = \sinh(\Phi)K\pi^{-1}[(1-k^2\cos^2 q_1^{\pm})^{1/2} + (1-k^2\cos^2 q_2^{\pm})^{1/2}] - S^z H_0 \ , \quad (3.6)$$

with $0 \leq \mp q_{1,2}^{\pm} \leq \pi$. Note that the $q^{\pm}$ have only one-half the normal range of 2π and assume $\frac{1}{2}N$ values. This corresponds to the labeling by boundary positions in the Ising limit. Because of the symmetry between $S^z = +1$ and $S^z = -1$, the above expressions apply equally well to $S^z = -1$.

For the first excited states of $S^z = 0$ one considers the excitations that take two ϕ_α, ϕ_1 and ϕ_2, into a complex conjugate pair; i.e., $p = 2$ in Eq. (2.5). The q_2 and E_2 that result are independent of the real value of the pair, ϕ_r. Also, again built into the calculation are the above $\pm$ regions of the momentum. From an inspection of the Ising limit one suspects that ϕ_r takes on only two values and provides, in conjunction with the $\pm$ label, a labeling of four degenerate dispersion curves. The energy and momentum differences between the first excited and ground states are

$$E_2(S^z, q_1^{\pm}, q_2^{\pm}) = \sinh(\Phi)K\pi^{-1}[(1-k^2\cos^2 q_1^{\pm})^{1/2} + (1-k^2\cos^2 q_2^{\pm})^{1/2}] - S^z H_0 \quad (3.7a)$$

and

$$q_2(S^z, q_1^{\pm}, q_2^{\pm}) = q_1^{\pm} + q_2^{\pm} - \tfrac{1}{2}\pi \pm \tfrac{1}{2}\pi \ , \quad (3.7b)$$

with $0 \leq \mp q_{1,2}^{\pm} \leq \pi$. The four dispersion curves are distinguished from one another by the $\pm$ and the two values of ϕ_r. One can obtain a set of higher excitations by linearly combining the above momenta and energies. One must remember when adding the two particle states together that the q's satisfy an exclusion principle that is the same as the boundaries in the Ising limit.

IV. LOW-TEMPERATURE THERMODYNAMICS

A. Region A; $\delta = -1$ (Ferromagnetic), $H_0 \geq \rho > 0$, ρ Independent of T

One expands ϵ_n as $\epsilon_n = \epsilon_n^{(1)} + \epsilon_n^{(2)} + \cdots$. From Eqs. (2.7) it is observed that $\epsilon_n > 0$ for all n and ϕ. Therefore, in Eqs. (2.7) for small temperature the exponentials are large and the 1's inside the logarithms can be dropped to obtain

$$\epsilon_n^{(1)} = dn(\phi)*(\epsilon_{n+1}^{(1)} + \epsilon_{n-1}^{(1)}), \quad n \geq 2 \quad (4.1a)$$

and

$$\epsilon_1^{(1)} = dn(\phi)*\epsilon_2^{(1)} + \sinh(\Phi)dn(\phi) \ , \quad (4.1b)$$

with $\lim_{n\to\infty}\epsilon_n^{(1)}/n = H_0$. One extracts the solution by Fourier transforming, solving the resulting algebraic equations, and transforming back to the ϕ variable. We perform this operation often enough to make it worthwhile to label it as procedure A in the remainder of the paper. The solution is

$$\epsilon_n^{(1)} = H_0 n + \sinh(\Phi) j_{n+1}(\phi), \quad n \geq 1 \quad (4.2a)$$

where

$$j_n(\phi) = \sinh[(n-1)\Phi]\{\cosh[(n-1)\Phi] - \cos\phi\}^{-1} \ . \quad (4.2b)$$

The $\epsilon_n^{(2)}$ and the solution for the $\epsilon_n^{(1)}$ are substituted into Eqs. (2.7). Since the $\epsilon_n^{(2)}$ are observed to be exponentially small in T and the $\epsilon_n^{(1)}$ for $n \geq 2$ do not contribute to the $\epsilon_n^{(2)}$, the exponentials and logarithms can be expanded to derive

$$\epsilon_n^{(2)} = dn(\phi)*(\epsilon_{n+1}^{(2)} + \epsilon_{n-1}^{(2)}), \quad n \geq 3 \quad (4.3a)$$

$$\epsilon_2^{(2)} = dn(\phi)*(\epsilon_3^{(2)} + \epsilon_1^{(2)} + T e^{-\epsilon_1^{(1)}/T}) \ , \quad (4.3b)$$

and

$$\epsilon_1^{(2)} = dn(\phi)*\epsilon_2^{(2)} \ , \quad (4.3c)$$

with $\lim_{n\to\infty}\epsilon_n^{(2)}/n = 0$. (In this and later sets of equations we refer to the $e^{-\epsilon_1^{(1)}/T}$ term and similar terms as the driving term.) In applying procedure A one has

$$\epsilon_n^{(2)} = T h_n(\phi)*e^{-\epsilon_1^{(1)}/T} \quad \text{for} \quad n \geq 1 \quad (4.4a)$$

and with

$$h_1(\phi) = j_3(\phi) \quad (4.4b)$$

and

$$h_n(\phi) = j_{n+2}(\phi) + j_n(\phi) \ . \quad (4.4c)$$

The next term $\epsilon_n^{(3)}$ is exponentially smaller in T than the above expression for $\epsilon_n^{(2)}$; i.e., $\epsilon_n^{(3)}$ is of order $e^{-(\mathrm{const})/T}\epsilon_n^{(2)}$.

The integral in Eq. (4.4a) may be estimated by steepest descent. This simplifies $\epsilon_1^{(2)}$ to

$$\epsilon_1^{(2)}(\phi) = (2\pi)^{-1/2}(\Delta+1)j_3(\phi-\pi)(\sinh\Phi)^{-1}e^{(1-H_0-\Delta)/T} \times [T^{3/2} + O(T^{5/2})] \ . \quad (4.5)$$

One substitutes ϵ_1 into the free energy and performs expansions of the logarithm and exponential. After several cancellations the resulting, rather complicated, form reduces to

$$F(T,\sigma) = \sigma H_0 - \tfrac{1}{2}H_0 - (2\pi)^{-1/2}e^{(1-H_0-\Delta)/T} \times [T^{3/2} + O(T^{5/2})] \ . \quad (4.6a)$$

The magnetization, susceptibility, and specific heat are, respectively,

$$\sigma = \tfrac{1}{2} - (2\pi)^{-1/2}e^{(1-H_0-\Delta)/T}[T^{1/2} + O(T^{3/2})] \ , \quad (4.6b)$$

$$\chi = (2\pi)^{-1/2}e^{(1-H_0-\Delta)/T}[T^{-1/2} + O(T^{1/2})] \ , \quad (4.6c)$$

and

$$C_H = (2\pi)^{-1/2}(H_0 + \Delta - 1)^2 e^{(1-H_0-\Delta)/T}$$

$$\times [T^{-3/2}+O(T^{-1/2})] \quad . \quad (4.6d)$$

By rescaling ϕ the $\Delta\to 1$ limit can be performed on all the expressions in this subsection. Without a study of the higher-order terms it is not obvious why one cannot take $H_0\to 0$. However, for $\Delta\neq 1$, take $H_0\to 0$; then $T\to 0$ to obtain $\sigma=\frac{1}{2}$. Since the correct answer is $\sigma=0$, one concludes that $H_0\geq\rho>0$ is necessary.

B. Region B; $\delta=1$ (Antiferromagnetic), $\epsilon_1^{(1)}\geqslant\rho>0$, ρ Independent of T

So that we may use some of our results to obtain the free energy near line b, we will derive $\epsilon_n^{(1)}$ and $\epsilon_n^{(2)}$ valid for $\epsilon_1^{(1)}\gtrsim -\tau T$, τ an arbitrary positive number independent of T. [In the remainder of the paper ρ and τ will always be as described in this subsection; i.e., both are arbitrary positive numbers independent of T. Also, in Secs. IV B, IV C, IV G–IV J "near" to a line means that H_0 is such that the point $(\delta\Delta, H_0)$ is an $O(T)$ distance from the line along a constant $\delta\Delta$ curve. Throughout the paper "$O(T)$ near" refers to this definition of "near."] Let $\epsilon_n=\epsilon_n^{(1)}+\epsilon_n^{(2)}+\cdots$. The $\epsilon_n^{(1)}$ are found by an identical procedure to that for region A. The $\epsilon_n^{(1)}$ are

$$\epsilon_n^{(1)}=H_0 n-\sinh(\Phi)\, j_{n+1}(\phi), \quad n\geq 1 \; . \qquad (4.7)$$

The $\epsilon_n^{(2)}$ are also obtained as in region A except, since $\epsilon_1^{(1)}$ can be of order T, logarithms containing $e^{-\epsilon_1^{(1)}/T}$ cannot be expanded. This changes Eq. (4.4a) to

$$\epsilon_n^{(2)}=Th_n(\phi)*\ln(1+e^{-\epsilon_1^{(1)}/T}) \quad . \qquad (4.8)$$

$\epsilon_n^{(3)}$ is exponentially smaller than $\epsilon_n^{(2)}$ if $\epsilon_1^{(1)}\geq\rho$ and is of order T^2 if $\epsilon_1^{(1)}\gtrsim -\tau T$ and $\epsilon_1^{(1)}=O(T)$ in some region.

By taking $\epsilon_1^{(1)}\gtrsim\rho$ one is allowed to expand the logarithm and obtain an expression for $\epsilon_n^{(2)}$ in terms of $\epsilon_1^{(1)}$ identical to Eq. (4.4a). Therefore, in region B,

$$\epsilon_1^{(2)}=(2\pi)^{-1/2}(\Delta-1)j_3(\phi)\,e^{G/T}(\sinh\Phi)^{-1}$$
$$\times[T^{3/2}+O(T^{5/2})], \qquad (4.9)$$

where $G=\Delta+1-H_0$ and the restriction $\epsilon_1^{(1)}\geq\rho$ translates to $H_0-\Delta-1\geq\rho$. The free energy, magnetization, susceptibility, and specific heat are, respectively,

$$F(T,\ \sigma)=\sigma H_0-\tfrac{1}{2}H_0-(2\pi)^{-1/2}e^{G/T}$$
$$\times[T^{3/2}+O(T^{5/2})], \qquad (4.10a)$$

$$\sigma=\tfrac{1}{2}-(2\pi)^{-1/2}e^{G/T}[T^{1/2}+O(T^{3/2})], \qquad (4.10b)$$

$$\chi=(2\pi)^{-1/2}e^{G/T}[T^{-1/2}+O(T^{1/2})], \qquad (4.10c)$$

and

$$C_H=(2\pi)^{-1/2}G^2e^{G/T}[T^{-3/2}+O(T^{-1/2})]. \qquad (4.10d)$$

The $\Delta\to 1$ limit is allowed on all quantities if ϕ is rescaled.

C. Region C; $\delta=1$ (Antiferromagnetic), $\epsilon_1^{(1)}\leqslant-\rho_1<0$, $H_0\geqslant\rho_2>0$, $\Delta\neq 1$

As in Sec. IV B, we first assume $\epsilon_1^{(1)}\leq\tau T$ in obtaining $\epsilon_n^{(1)}$ and $\epsilon_n^{(2)}$, where $\epsilon_n=\epsilon_n^{(1)}+\epsilon_n^{(2)}+\cdots$. By examining Eqs. (2.7) it is seen that $\epsilon_n>0$ for $n\geq 2$. Therefore, in Eqs. (2.7) the 1's inside those logarithms whose arguments do not contain ϵ_1 can be dropped. Since $\epsilon_1^{(1)}\leq\tau T$, the logarithm containing ϵ_1 can be eliminated. The resulting equations are

$$\epsilon_n^{(1)}=dn(\phi)*(\epsilon_{n+1}^{(1)}+\epsilon_{n-1}^{(1)}), \quad n\geq 3 \qquad (4.11a)$$

$$\epsilon_2^{(1)}=dn(\phi)*\epsilon_3^{(1)}, \qquad (4.11b)$$

$$\epsilon_1^{(1)}=dn(\phi)*\epsilon_2^{(1)}-\sinh(\Phi)\,dn(\phi), \qquad (4.11c)$$

with $\lim_{n\to\infty}\epsilon_n^{(1)}/n=H_0$. By applying procedure A the solution is

$$\epsilon_n^{(1)}=H_0(n-1), \quad n\geq 2 \qquad (4.12a)$$

and

$$\epsilon_1^{(1)}=\tfrac{1}{2}H_0-\sinh(\Phi)dn(\phi) \; . \qquad (4.12b)$$

To extract the first temperature-dependent term of the free energy, the $\epsilon_n^{(2)}$ are not needed. However, for completeness they are included. One proceeds to solve for the $\epsilon_n^{(2)}$ in the manner outlined in Sec. IV A with the difference that either $\epsilon_1^{(1)}$ or $\epsilon_2^{(1)}$ contributes to the $\epsilon_n^{(2)}$ depending on whether $|\epsilon_1^{(1)}|$ or $\epsilon_2^{(1)}$ is the smaller. Since the minimum value of $|\epsilon_1^{(1)}|$ is at $\phi=\pi$, if $|\epsilon_1^{(1)}(\pi)|<H_0$, one obtains equations for the $\epsilon_n^{(2)}$ identical to Eqs. (4.3), except in Eq. (4.3b) the $\epsilon_1^{(2)}$ term is eliminated, and $\epsilon_1^{(1)}$ is changed to $-\epsilon_1^{(1)}$. In using procedure A the $\epsilon_n^{(2)}$ are

$$\epsilon_n^{(2)}=Tj_n(\phi)*\ln(1+e^{\epsilon_1^{(1)}/T}), \quad n\geq 2 \qquad (4.13a)$$

and

$$\epsilon_1^{(2)}=Th(\phi)*\ln(1+e^{\epsilon_1^{(1)}/T}) \quad , \qquad (4.13b)$$

where

$$h(\phi)=\sum_{m=-\infty}^{\infty}[2\cosh(m\Phi)]^{-1}\exp(-im\phi-|m|\Phi) \, . \qquad (4.13c)$$

If $H_0<|\epsilon_1^{(1)}(\pi)|$, the equations whose solution is Eqs. (4.13) are modified to have driving terms dependent on $\epsilon_2^{(1)}$. The $\epsilon_n^{(2)}$ are

$$\epsilon_n^{(2)}=2T\,e^{-H_0/T}, \quad n\geq 3 \qquad (4.14a)$$

and

$$\epsilon_n^{(2)}=Te^{-H_0/T}, \qquad n=1,2 \; . \qquad (4.14b)$$

The $\epsilon_n^{(3)}$ are exponentially smaller than the $\epsilon_n^{(2)}$ given in either Eqs. (4.13) or (4.14) if $\epsilon_1^{(1)}\lesssim-\rho_1$. If $\epsilon_1^{(1)}\leq\tau T$ and $\epsilon_1^{(1)}=O(T)$ is some region, the $\epsilon_n^{(3)}$ can only be restricted to $O(T^2)$.

Now one takes $\epsilon_1^{(1)} \lesssim -\rho_1$; i.e., region C. Since $e^{\epsilon_1^{(1)}/T}$ is then exponentially small in T, $\epsilon_1^{(1)}$ can be substituted in Eq. (2.6) for the free energy, and the logarithm can be expanded. After doing the asymptotic analysis of the resulting integral one derives

$$F(T,\sigma)=E_0/N+\sigma H_0-A^{1/2}e^{-B/T}\times[T^{3/2}+O(T^{5/2})] \ , \quad (4.15a)$$

$$\sigma=\tfrac{1}{2}A^{1/2}e^{-B/T}[T^{1/2}+O(T^{3/2})] \ , \quad (4.15b)$$

$$\chi=\tfrac{1}{4}A^{1/2}e^{-B/T}[T^{-1/2}+O(T^{1/2})] \ , \quad (4.15c)$$

and

$$C_H=B^2A^{1/2}e^{-B/T}[T^{-3/2}+O(T^{-1/2})] \ , \quad (4.15d)$$

where

$$A=k'/[2\sinh(\Phi)Kk^2] \quad (4.15e)$$

and

$$B=\sinh(\Phi)Kk'/\pi-\tfrac{1}{2}H_0 \ . \quad (4.15f)$$

Note that B is equal to one-half the gap between the ground state and first excited states. Also, $\epsilon_1^{(1)} \lesssim -\rho_1$ translates to $\tfrac{1}{2}H_0-\sinh(\Phi)Kk'/\pi \lesssim -\rho_1$.

D. Region D; $\epsilon_1^{(1)}$ Both Negative and Positive, not $O(T)$ near Lines b or c

Expand $\epsilon_n=\epsilon_n^{(1)}+\epsilon_n^{(2)}+\cdots$ and define $\alpha>0$ by $\epsilon_1^{(1)}(\alpha)=0$. ($\epsilon_1^{(1)}$ has only two zeros α and $-\alpha$.) The $\epsilon_n^{(1)}$ for $n\geq 2$ are again positive which allows the 1's in the logarithms of Eqs. (2.7) to be disregarded. The integral of $\ln(1+e^{\epsilon_1^{(1)}/T})$ can be split into two parts with the $[-\alpha,\alpha]$ range exponentially small in T since $\epsilon_1^{(1)}$ is negative there, and the remaining range can be treated the same as the other $\epsilon_n^{(1)}$. This gives coupled equations of the form

$$\epsilon_n^{(1)}=dn(\phi)*(\epsilon_{n+1}^{(1)}+\epsilon_{n-1}^{(1)}), \quad n\geq 3 \quad (4.16a)$$

$$\epsilon_2^{(1)}=dn(\phi)*\epsilon_3^{(1)}+dn(\phi)*_0^\alpha\epsilon_1^{(1)} \quad (4.16b)$$

and

$$\epsilon_1^{(1)}=dn(\phi)*\epsilon_2^{(1)}-\sinh(\Phi)dn(\phi) \quad (4.16c)$$

with $\lim_{n\to\infty}\epsilon_n^{(1)}/n=H_0$ and $*_0^\alpha$ denoting

$$f(\phi)*_0^\alpha g\equiv(2\pi)^{-1}\left(\int_{-\pi}^{-\alpha}+\int_\alpha^\pi\right)f(\phi-\phi')g(\phi')d\phi' \ .$$

For later convenience take $*_i^\alpha$ to mean

$$f(\phi)*_i^\alpha g\equiv(2\pi)^{-1}\int_{-\alpha}^{\alpha}f(\phi-\phi')g(\phi')d\phi' \ .$$

By procedure A the solution to Eqs. (4.16) is

$$\epsilon_n^{(1)}=H_0(n-1)+j_n(\phi)*_0^\alpha\epsilon_1^{(1)}, \quad n\geq 2 \quad (4.17a)$$

with $\epsilon_1^{(1)}$ given by the integral equation

$$\epsilon_1^{(1)}=\tfrac{1}{2}H_0-\sinh(\Phi)dn(\phi)+h(\phi)*_0^\alpha\epsilon_1^{(1)} \ . \quad (4.17b)$$

h and j_n are given by Eqs. (4.13c) and (4.2b). For cases in which α is small another form of the equations is more suitable. By adding and subtracting $h(\phi)*_i^\alpha\epsilon_1^{(1)}$ to Eq. (4.17b) and $j_n(\phi)*_i^\alpha\epsilon_1^{(1)}$ to Eq. (4.17a), and by applying procedure A to Eqs. (4.17), one obtains

$$\epsilon_n^{(1)}=H_0n-\sinh(\Phi)j_{n+1}(\phi)-h_n(\phi)*_i^\alpha\epsilon_1^{(1)}, \quad n\geq 1 \ . \quad (4.18)$$

Note that α as a function of H_0 and Δ is obtained, after solving either Eq. (4.17b) or (4.18) for $n=1$, by setting $\epsilon_1^{(1)}(\alpha)=0$.

$\epsilon_1^{(1)}$ in the neighborhood of α and $-\alpha$ provides the driving term to the $\epsilon_n^{(2)}$ equations. This implies that the parameter that enters into the asymptotic expansion is the slope of $\epsilon_1^{(1)}$ at α, and that the coefficient of the driving term is given by $\int_0^\infty\ln(1+e^{-x})dx$. Therefore, let $\epsilon_1^{(1)}=t(\phi-\alpha)$ in the neighborhood of α and set $\epsilon_n^{(2)}=T^2\pi f_n/(12t)$. The coupled equations for the f_n are

$$f_n=dn(\phi)*(f_{n+1}+f_{n-1}), \quad n\geq 3 \quad (4.19a)$$

$$f_2=dn(\phi)*f_3+dn(\phi)*_0^\alpha f_1+dn(\phi+\alpha)+dn(\phi-\alpha) \ , \quad (4.19b)$$

and

$$f_1=dn(\phi)*f_2 \ . \quad (4.19c)$$

By applying procedure A it follows that

$$f_n=j_n(\phi+\alpha)+j_n(\phi-\alpha)+j_n(\phi)*_0^\alpha f_1, \quad n\geq 2 \quad (4.20a)$$

and

$$f_1=h(\phi+\alpha)+h(\phi-\alpha)+h(\phi)*_0^\alpha f_1 \ . \quad (4.20b)$$

For α small, a set of relations similar to Eq. (4.18) is desired. They are

$$f_n=h_n(\phi+\alpha)+h_n(\phi-\alpha)-h_n(\phi)*_i^\alpha f_1, \quad n\geq 1 \ . \quad (4.21)$$

The next-order term $\epsilon_n^{(3)}$ in ϵ_n is of order T^3.

The free energy can be treated with the same methods used to obtain Eqs. (4.17b), (4.18), (4.20b), and (4.21). One obtains two equivalent expressions for F and C_H. They are

$$F(T,\sigma)=E_0/N+\sigma H_0-dn(0)*_0^\alpha\epsilon_1^{(1)}-T^2(24t)^{-1}dn(0)*_0^\alpha f_1-T^2dn(\alpha)\pi(6t)^{-1}+O(T^3), \quad (4.22a)$$

with

$$C_H=T(12t)^{-1}dn(0)*_0^\alpha f_1+T\,dn(\alpha)\pi(3t)^{-1}+O(T^2) \quad (4.22b)$$

and

$$F(T,\sigma)=\sigma H_0-\tfrac{1}{2}H_0+j_2(0)*_i^\alpha\epsilon_1^{(1)}+T^2(24t)^{-1}j_2(0)*_i^\alpha f_1-T^2\pi j_2(\alpha)(6t)^{-1}+O(T^3) \ , \quad (4.23a)$$

with

$$C_H = T\pi j_2(\alpha)(3t)^{-1} - T(12t)^{-1} j_2(0) *_i^{\alpha} f_1 + O(T^2) . \quad (4.23b)$$

σ cannot be obtained in a compact form.

The limit $\Phi \to 0$ is allowed on all expressions in this subsection if it is remembered to scale all variables. Because we need the equations later, we include here one of the two equivalent sets of equations for $\Phi = 0$. We denote all scaled variables and functions by a prime with the exception of ϵ_1 and $\epsilon_1^{(1)}$ where primes would cause some confusion. If one defines $\text{ch}(x) = \pi 2^{-1} \text{sech}(\frac{1}{2}\pi x)$, we have

$$\epsilon_1 = \epsilon_1^{(1)} + T^2 \pi f_1'(x)(12t')^{-1} + O(T^3) , \quad (4.24a)$$

$$\epsilon_1^{(1)}(x) = t'(x - \alpha'), \quad x \text{ near } \alpha' \quad (4.24b)$$

$$h'(x) = \int_{-\infty}^{\infty} dy\, e^{-ixy - |y|} (2\cosh y)^{-1} , \quad (4.24c)$$

$$\epsilon_1^{(1)} = \tfrac{1}{2}H_0 - \text{ch}(x) + (2\pi)^{-1} \times \left(\int_{-\infty}^{-\alpha'} + \int_{\alpha'}^{\infty}\right) h'(x - x') \epsilon_1^{(1)}(x') dx' , \quad (4.24d)$$

$$f_1' = h'(x + \alpha') + h'(x - \alpha') + (2\pi)^{-1} \times \left(\int_{-\infty}^{-\alpha'} + \int_{\alpha'}^{\infty}\right) h'(x - x') f_1'(x') dx' , \quad (4.24e)$$

$$F(T, \sigma) = E_0/N + \sigma H_0 - (2\pi)^{-1}\left(\int_{-\infty}^{-\alpha'} + \int_{\alpha'}^{\infty}\right) \text{ch}(x) \epsilon_1^{(1)}(x) dx - T^2(24t')^{-1}\left(\int_{-\infty}^{-\alpha'} + \int_{\alpha'}^{\infty}\right) \text{ch}(x) f_1'(x) dx - T^2\pi(6t')^{-1}\text{ch}(\alpha) + O(T^3) , \quad (4.24f)$$

and

$$C_H = T(12t')^{-1}\left(\int_{-\infty}^{-\alpha'} + \int_{\alpha'}^{\infty}\right) \text{ch}(x) f_1'(x) dx + T\pi(3t')^{-1}\text{ch}(\alpha) + O(T^2) . \quad (4.24g)$$

E. Existence of $\epsilon_1^{(1)}$ and f_1 in Region D

By writing Eqs. (4.17b) and (4.20b) in operator notation and examining the eigenvalue spectrum of the operator corresponding to $h(\phi)$, one can show by arguments identical to those of Yang and Yang[14] that unique solutions exist for the two equations.

F. Approximate Solutions $O(1)$ near Boundaries of Region D

For H_0 such that one is near either line b or c and in D, approximate expressions can be found for $\epsilon_1^{(1)}$ and f_1. [It must be understood that in this subsection when we speak of "near" a boundary, it is not meant that the boundary is approached as $T \to 0$, but rather that one is first expanding in T, then in the distance from the boundary along a constant $\delta\Delta$ line. At times we refer to this as "$O(1)$ near."] Let us first look near line b, and let

$$G = (\sinh\Phi) j_2(0) - H_0 = \Delta + 1 - H_0 . \quad (4.25)$$

Since α is small, Eqs. (4.18) and (4.21) can be solved by iterating the equations and expanding the resulting solutions around $\alpha = 0$. This gives

$$\epsilon_1^{(1)} = H_0 - (\sinh\Phi) j_2(\phi) + (2G)^{3/2} j_3(\phi)[3\pi j_2(0)]^{-1} + O(G^2) \quad (4.26a)$$

and

$$f_1 = 2 j_3(\phi) + O(G^{1/2}) . \quad (4.26b)$$

Therefore, we have

$$\alpha = (2G)^{1/2}/j_2(0) + O(G) \quad (4.26c)$$

and

$$t = \alpha[j_2(0)]^2 + O(G^{3/2}) . \quad (4.26d)$$

Upon insertion into the free-energy expression,

$$F(T, \sigma) = \sigma H_0 - \tfrac{1}{2}H_0 - (2G)^{3/2}(3\pi)^{-1} + O(G^2) - T^2\pi[6(2G)^{1/2}]^{-1} + O(T^2 G^0) + O(T^3) . \quad (4.27a)$$

The G dependence of the $O(T^3)$ term is not known. It follows that

$$\sigma = \tfrac{1}{2} - (2G)^{1/2}\pi^{-1} + O(G) + T^2\pi[6(2G)^{3/2}]^{-1} + O(T^2 G^{-1/2}) + O(T^3) , \quad (4.27b)$$

$$\chi = \pi^{-1}(2G)^{-1/2} + O(G^0) + T^2\pi(8G^{5/2} 2^{1/2})^{-1} + O(T^2 G^{-3/2}) + O(T^3) , \quad (4.27c)$$

and

$$C_H = T\pi[3(2G)^{1/2}]^{-1} + O(T^1 G^0) + O(T^2). \quad (4.27d)$$

There is no problem in allowing $\Delta \to 1$; for $\Delta \to 1$, $G \to 2 - H_0$.

In the neighborhood of line c, α is near π. Therefore, let $\beta = \pi - \alpha$ and $\gamma = -B$. For α near π, Eqs. (4.17b) and (4.20b) are the appropriate equations to iterate. After expanding the resulting solutions one obtains

$$\epsilon_1^{(1)} = \tfrac{1}{2}H_0 - \sinh(\Phi) dn(\phi) + O(\gamma^{3/2}) , \quad (4.28a)$$

$$f_1 = 2h(\phi \pm \pi) + O(\gamma^{1/2}) , \quad (4.28b)$$

$$\beta = \{2\gamma[\sinh(\Phi) k' k^2]^{-1}\}^{1/2}(\pi/K)^{3/2} + O(\gamma) , \quad (4.28c)$$

and

$$t = (\sinh\Phi) K^3 k^2 k' \beta \pi^{-3} + O(\gamma^{3/2}) . \quad (4.28d)$$

The free energy is

$$F(T, \sigma) = E_0/N + \sigma H_0 - 4(3\pi^{1/2})^{-1}\gamma^{3/2} A^{1/2} + O(\gamma^2) - T^2 A^{1/2}\pi^{3/2}(6\gamma^{1/2})^{-1} + O(T^2\gamma^0) + O(T^3) , \quad (4.29a)$$

with

$$\sigma = (\gamma A/\pi)^{1/2} + O(\gamma) - T^2 A^{1/2}\pi^{3/2}(24\gamma^{3/2})^{-1}$$

$$+O(T^2\gamma^{-1/2})+O(T^3)\,, \qquad (4.29b)$$

$$\chi=\tfrac{1}{4}A^{1/2}(\pi\gamma)^{-1/2}+O(\gamma^0)+T^2A^{1/2}\pi^{3/2}(32\gamma^{5/2})^{-1}+O(T^2\gamma^{-3/2})+O(T^3)\,, \qquad (4.29c)$$

and

$$C_H=T(A/\gamma)^{1/2}\pi^{3/2}3^{-1}+O(T\gamma^0)+O(T^2)\,. \qquad (4.29d)$$

A is given by Eq. (4.15e), and the γ dependence of the last temperature order in Eqs. (4.29) is not known.

Since $A\to 0$ as $\Delta\to 1$, the work for near line c is not valid at $\Delta=1$. For $\Delta=1$ and H_0 near zero, a separate treatment, similar to the Wiener-Hopf calculation that Yang and Yang[14] performed, must be done.

We define

$$S(u)=\epsilon_1^{(1)}(u+\alpha')\,e^{\pi\alpha'/2} \quad \text{and} \quad T(u)=f_1'(u+\alpha')$$

and use the evenness of $\epsilon_1^{(1)}$ and f_1' to derive from Eqs. (4.24):

$$S(u)=\tfrac{1}{2}H_0e^{\pi\alpha'/2}-\operatorname{ch}(u+\alpha')\,e^{\pi\alpha'/2}+(2\pi)^{-1}\int_0^\infty h'(u-u')\,S(u')du'+(2\pi)^{-1}\int_0^\infty h'(u+u'+2\alpha')S(u')du' \qquad (4.30a)$$

and

$$T(u)=h'(u)+h'(u+2\alpha')+(2\pi)^{-1}\int_0^\infty h'(u-u')T(u')du'+(2\pi)^{-1}\int_0^\infty h'(u+u'+2\alpha')T(u')du'\,. \qquad (4.30b)$$

For H_0 near zero α' is large, and since it can be shown by an integration by parts that $h'(u)\sim u^{-2}$ for large u, an expansion of both S and T can be made. Let $S=S_0+S_1+\cdots$ and $T=T_0+T_1+\cdots$. To have the proper H_0 dependence in each of the first two orders, α' must be given by

$$\alpha'=-2\pi^{-1}\ln(H_0\eta)+2\eta\xi\,[\pi(\ln H_0)^2]^{-1}+O[(\ln H_0)^{-4}]\,, \qquad (4.31)$$

where η and ξ are constants independent of H_0. The resulting equations are

$$S_0=(2\eta)^{-1}-\pi e^{-\pi u/2}+(2\pi)^{-1}\int_0^\infty h'(u-u')S_0(u')du'\,, \qquad (4.32a)$$

$$S_1=\xi[2(\ln H_0)^2]^{-1}+(2\pi)^{-1}\int_0^\infty h'(u-u')S_1(u')du'+(2\pi)^{-1}\int_0^\infty h'(u+u'+2\alpha')S_0(u')du'\,, \qquad (4.32b)$$

$$T_0=h'(u)+(2\pi)^{-1}\int_0^\infty h'(u-u')T_0(u')du'\,, \qquad (4.32c)$$

and

$$T_1=h'(u+2\alpha')+(2\pi)^{-1}\int_0^\infty h'(u-u')T_1(u')du'+(2\pi)^{-1}\times\int_0^\infty h'(u+u'+2\alpha')T_0(u')du'\,. \qquad (4.32d)$$

The constants η and ξ are found by solving for S_0 and S_1 and requiring that $S_0(0)=S_1(0)=0$. S_2 and T_2 are of order $(\ln H_0)^{-4}$. To the order we wish to calculate, from Eq. (4.24f), the free energy is

$$F(T,\sigma)=E_0/N+\sigma H_0-(H_0\eta)^2\int_0^\infty e^{-\pi u/2}S_0(u)\,du+O[H_0^2(\ln H_0)^{-2}]-T^2\pi\{12[S_0'(0)+S_1'(0)]\}^{-1}\int_0^\infty e^{-\pi u/2}(T_0+T_1)\,du-T^2\pi^2\{6\,[S_0'(0)+S_1'(0)]\}^{-1}+O[T^2(\ln H_0)^{-4}]+O(T^3). \qquad (4.33)$$

The primes on S_0 and S_1 indicate differentiation with with respect to u.

Equations (4.32) are solved by a standard Wiener-Hopf technique.[15] As in many cases it is not difficult to write the resulting solutions as functions in the Fourier-transformed space, but it is very difficult to obtain closed forms in u space. The trick is to observe that one can work completely in the Fourier space; for example, the condition $S_0(0)=0$ is equivalent to requiring $\lim_{y\to\infty}y\,\hat{S}_0(y)=0$ and $S_0'(0)$ is obtained from

$$S_0'(0)=-(2\pi)^{1/2}\lim_{y\to\infty}y^2\hat{S}_0(y)\,,$$

where the "caret" indicates the Fourier-transformed function. These relations are derived by expressing S_0 in terms of $\hat{S}_0$ and doing two integrations by parts. Likewise, once $\hat{S}_0$, $\hat{T}_0$, and $\hat{T}_1$ are known, the integrals in Eq. (4.33) can be converted into integrals over Fourier space and evaluated. This procedure yields

$$F(T,\sigma)=E_0/N+\sigma H_0-H_0^2(2\pi^2)^{-1}+O[H_0^2(\ln H_0)^{-2}]-\tfrac{1}{3}T^2-T^2[6(\ln H_0)^2]^{-1}+O[T^2(\ln H_0)^{-3}]+O(T^3)\,, \qquad (4.34a)$$

with

$$\sigma=H_0\pi^{-2}+O[H_0(\ln H_0)^{-2}]-T^2[3H_0(\ln H_0)^3]^{-1}+O\{T^2[H_0(\ln H_0)^4]^{-1}\}+O(T^3)\,, \qquad (4.34b)$$

$$\chi=\pi^{-2}+O[(\ln H_0)^{-2}]+T^2[3H_0^2(\ln H_0)^3]^{-1}+O\{T^2[H_0^2(\ln H_0)^4]^{-1}\}+O(T^3)\,, \qquad (4.34c)$$

and

$$C_H=\tfrac{2}{3}T+T[3(\ln H_0)^2]^{-1}+O[T(\ln H_0)^{-3}]+O(T^2)\,. \qquad (4.34d)$$

The H_0 dependence of the last temperature order is not known.

G. $O(T)$ near Line b; $\delta=1$ (Antiferromagnetic), $\epsilon_1^{(1)}\geq-\tau T$ and $\epsilon_1^{(1)}=O(T)$ at $\phi=0$

Equations (4.7) and (4.8) are correct for $\epsilon_1^{(1)}\geq-\tau T$. To satisfy $\epsilon_1^{(1)}\geq-\tau T$ and have $\epsilon_1^{(1)}=O(T)$ at some points, it is possible to have $\epsilon_1^{(1)}=O(T)$ only in the neighborhood of $\phi=0$. Therefore, the equation for line b is $\epsilon_1^{(1)}(0)=0$ or $H_0=\Delta+1$.

To find the free energy, a suitably modified form of Eq. (4.9) is needed. The asymptotic analysis of

Eq. (4.8) for $\epsilon_1^{(1)}(0)=O(T)$ is performed by Taylor expanding $\epsilon_1^{(1)}$ around $\phi=0$. The integral that is evaluated is of the integrand $\ln(1+Ce^{-x^2})$, not e^{-x^2}. This gives us an $\epsilon_1^{(2)}$ of the form

$$\epsilon_1^{(2)}=-(2\pi)^{-1/2}(\Delta-1)\,j_3(\phi)\,(\sinh\Phi)^{-1} \times F_0(-e^{G/T},\tfrac{3}{2})[T^{3/2}+O(T^2)]\,, \quad (4.35)$$

where $F_0(z,s)=\sum_{n=1}^{\infty}z^n/n^s$, and $G=\Delta+1-H_0$ is an $O(T)$ quantity that is either positive or negative. Also,

$$F_0(z,\tfrac{3}{2})=-\pi^{-1/2}\int_{-\infty}^{\infty}dx\ln(1-ze^{-x^2})\,.$$

(Note that F_0 arises in the study of the free quantum gases.)

The analysis of the free energy has to be modified in the same manner as the preceding. One finds

$$F(T,\sigma)=\sigma H_0-\tfrac{1}{2}H_0+(2\pi)^{-1/2}F_0(-e^{G/T},\tfrac{3}{2}) \times[T^{3/2}+O(T^2)]\,, \quad (4.36a)$$

$$\sigma=\tfrac{1}{2}+T^{1/2}(2\pi)^{-1/2}F_0(-e^{G/T},\tfrac{1}{2})+O(T)\,, \quad (4.36b)$$

$$\chi=-(2\pi T)^{-1/2}F_0(-e^{G/T},-\tfrac{1}{2})+O(T^0)\,, \quad (4.36c)$$

and

$$C_H=(2\pi)^{-1/2}[-\tfrac{3}{4}T^{1/2}F_0(-e^{G/T},\tfrac{3}{2}) +T^{-1/2}GF_0(-e^{G/T},\tfrac{1}{2}) -T^{-3/2}G^2F_0(-e^{G/T},-\tfrac{1}{2})]+O(T)\,. \quad (4.36d)$$

F is equal to the limiting form from region B multiplied by $-F_0(-e^{G/T},\tfrac{3}{2})$. The $\Delta\to1$ limit is again allowed if ϕ is rescaled. By taking G/T large and negative, F_0 can be approximated to recover Eq. (4.10a) and for G/T large and positive to recover the T-independent terms of Eq. (4.27a).

H. $O(T)$ near Line c; $\delta=1$ (Antiferromagnetic), $\epsilon_1^{(1)}\leqslant\tau T$, $\epsilon_1^{(1)}=O(T)$ at $\phi=\pi$, $\Delta\neq1$

The analysis of line c parallels that described in Sec. IV G. Equations (4.12) and (4.13) are correct for $\epsilon_1^{(1)}\leqslant\tau T$. This implies that $\epsilon_1^{(1)}=O(T)$ in the neighborhood of $\phi=\pm\pi$, and allows one to describe line c by

$$H_0=2\sinh(\Phi)dn(\pi)\quad\text{or}\quad H_0=2\sinh(\Phi)Kk'\pi^{-1}\,.$$

After substituting $\epsilon_1^{(1)}$ into the free energy the logarithm cannot be expanded, but the method described in Sec. IV G must be applied. This results in

$$F(T,\sigma)=E_0/N+\sigma H_0+A^{1/2}F_0(-e^{-B/T},\tfrac{3}{2}) \times[T^{3/2}+O(T^2)]\,, \quad (4.37a)$$

$$\sigma=-2^{-1}(TA)^{1/2}F_0(-e^{-B/T},\tfrac{1}{2})+O(T)\,, \quad (4.37b)$$

$$\chi=-4^{-1}(A/T)^{1/2}F_0(-e^{-B/T},-\tfrac{1}{2})+O(T^0)\,, \quad (4.37c)$$

and

$$C_H=-A^{1/2}[\tfrac{3}{4}T^{1/2}F_0(-e^{-B/T},\tfrac{3}{2}) +BT^{-1/2}F_0(-e^{-B/T},\tfrac{1}{2}) +B^2T^{-3/2}F_0(-e^{-B/T},-\tfrac{1}{2})]+O(T)\,. \quad (4.37d)$$

B, given by Eq. (4.15f), is $O(T)$ and is either positive or negative. Equation (4.15a) is recovered from $F(T,\sigma)$ by taking B large and positive, and the temperature-independent terms of Eq. (4.29a) result from B large and negative.

I. $O(T)$ near Line d; $\delta=1$ (Antiferromagnetic), $H_0=O(T)$, $\Delta\neq1$

It is observed from Eqs. (4.12) and (4.14) that for $H_0=O(T)$ the $\epsilon_n^{(1)}$, $n\geqslant2$, are $O(T)$ and the $\epsilon_n^{(2)}$ are linear in T. Therefore, $\epsilon_1^{(2)}$ now contributes to the free energy, and since $e^{-\epsilon_n^{(1)}/T}$ is not small, the previous solution for the $\epsilon_n^{(2)}$ in region C is not valid at line d. To obtain the correct $\epsilon_n^{(2)}$ solution, let $\epsilon_n^{(1)}=H_0(n-1)$, $n\geqslant2$, and $\epsilon_1^{(1)}=\tfrac{1}{2}H_0-\sinh(\Phi)\times dn(\phi)$. If $\epsilon_n^{(2)}=Tg_n$, the g_n are given by

$$g_n=dn(\phi)*\ln[(e^{-H_0n/T}+e^{g_{n+1}}) \times(e^{-H_0(n-2)/T}+e^{g_{n-1}})]\,,\quad n\geqslant3 \quad (4.38a)$$

$$g_n=dn(\phi)*\ln(e^{-H_0n/T}+e^{g_{n+1}})\,,\quad n=1,2 \quad (4.38b)$$

with $\lim_{n\to\infty}g_n/n=0$. These equations are found by dropping the exponentially small ϵ_1 term in the $n=2$ equation. We observe that the g_n are constants and, therefore, the ϵ_n are

$$\epsilon_n=T\ln\left[\left(\frac{\sinh(\tfrac{1}{2}nH_0/T)}{\sinh(\tfrac{1}{2}H_0/T)}\right)^2-1\right]+\cdots,\quad n\geqslant2 \quad (4.39a)$$

and

$$\epsilon_1=-(\sinh\Phi)dn(\phi)+T\ln[2\cosh(\tfrac{1}{2}H_0/T)]+\cdots\,. \quad (4.39b)$$

The next term in the ϵ_n expansion is exponentially small in T. Upon substituting ϵ_1 into the free energy the results are

$$F(T,\sigma)=E_0/N+\sigma H_0-A^{1/2}(1+e^{-H_0/T})e^{-B/T} \times[T^{3/2}+O(T^{5/2})]\,, \quad (4.40a)$$

$$\sigma=A^{1/2}\sinh(\tfrac{1}{2}H_0/T)e^{-B'/T}[T^{1/2}+O(T^{3/2})]\,, \quad (4.40b)$$

$$\chi=\tfrac{1}{2}A^{1/2}\cosh(\tfrac{1}{2}H_0/T)e^{-B'/T}[T^{-1/2}+O(T^{1/2})]\,, \quad (4.40c)$$

and

$$C_H=(B')^2A^{1/2}2\cosh(\tfrac{1}{2}H_0/T)e^{-B'/T} \times[T^{-3/2}+O(T^{-1/2})]\,, \quad (4.40d)$$

where $B'=\sinh(\Phi)Kk'/\pi$. For H_0/T large $F(T,\sigma)$ in region C is recovered.

J. $O(T)$ near Point P; $\delta = 1$ (Antiferromagnetic), $H_0 = O(T)$, $\Delta = 1$

In the expressions for the free energy in region C and near lines c and d, the coefficient A goes to zero as point P is approached. This indicates that the limit is not valid. Furthermore, for the free energy in region D there are coefficients that go to infinity near P. Therefore, a separate treatment of point P is necessary. As previously mentioned, ϕ is scaled to $x = \phi/\Phi$, when $\Phi \to 0$. If one remembers that $\mathrm{ch}(x) = \frac{1}{2}\pi\,\mathrm{sech}(\frac{1}{2}\pi x)$ and defines a $*^\infty$ operation such that

$$f(x) *^\infty g \equiv (2\pi)^{-1} \int_{-\infty}^{\infty} f(x - x')\, g(x')\, dx' ,$$

the coupled equations for the ϵ_n are

$$\epsilon_n/T = \mathrm{ch}(x) *^\infty \ln[(1 + e^{\epsilon_{n+1}/T})(1 + e^{\epsilon_{n-1}/T})], \quad n \geqslant 2 \qquad (4.41a)$$

and

$$\epsilon_1/T = \mathrm{ch}(x) *^\infty \ln(1 + e^{\epsilon_2/T}) - \mathrm{ch}(x)/T , \qquad (4.41b)$$

with $\lim_{n\to\infty} \epsilon_n/n = H_0$ and

$$F(T, \sigma) = E_0/N + \sigma H_0 - T(2\pi)^{-1} \times \int_{-\infty}^{\infty} \mathrm{ch}(x) \ln(1 + e^{\epsilon_1/T}) dx . \qquad (4.41c)$$

One sets

$$\epsilon_n = H_0(n-1) + T g_n(x) + \cdots \quad \text{for } n \geqslant 2$$

and

$$\epsilon_1 = \tfrac{1}{2}H_0 - \mathrm{ch}(x) + T g_1(x) + \cdots \; ;$$

the next term will be of order T^2. The g_n satisfy

$$g_n = \mathrm{ch}(x) *^\infty \ln[(e^{-H_0 n/T} + e^{g_{n+1}})(e^{-H_0(n-2)/T} + e^{g_{n-1}})], \quad n \geqslant 3 \qquad (4.42a)$$

$$g_2 = \mathrm{ch}(x) *^\infty \ln[(e^{-2H_0/T} + e^{g_3})(1 + e^{[H_0/2 + g_1 T - \mathrm{ch}(x')]/T})] , \qquad (4.42b)$$

and

$$g_1 = \mathrm{ch}(x) *^\infty \ln(e^{-H_0/T} + e^{g_2}) , \qquad (4.42c)$$

with $\lim_{n\to\infty} g_n/n = 0$. The driving term in Eq. (4.42b) is exponentially small for $\ln T < x < -\ln T$, while the $\mathrm{sech}(\frac{1}{2}\pi x)$ in the free-energy integral eliminates the contribution of $x < \ln T$ and $x > -\ln T$. Therefore, the principal contribution to the free energy comes from the ranges $x = y \pm 2\pi^{-1} \ln T$, where $y = O(1)$ in T. Since all functions are even in x, we need only multiply by two in the appropriate places and look at the range $x = y + 2\pi^{-1}\ln T$. After defining $e_n(y) = g_n(y + 2\pi^{-1}\ln T)$ the relevant equations are

$$e_n = \mathrm{ch}(y) *^\infty \ln[(e^{-H_0 n/T} + e^{e_{n+1}})(e^{-H_0(n-2)/T} + e^{e_{n-1}})], \quad n \geqslant 3 \qquad (4.43a)$$

$$e_2 = \mathrm{ch}(y) *^\infty \ln\{(e^{-2H_0/T} + e^{e_3}) \times [1 + \exp(\tfrac{1}{2}H_0/T + e_1 - \pi e^{\pi y'/2})]\} , \qquad (4.43b)$$

and

$$e_1 = \mathrm{ch}(y) *^\infty \ln(e^{-H_0/T} + e^{e_2}) , \qquad (4.43c)$$

with $\lim_{n\to\infty} e_n/n = 0$. The free energy is

$$F(T, \sigma) = E_0/N + \sigma H_0 - T^2 C(H_0/T) + O(T^3) , \qquad (4.44a)$$

with

$$\sigma = TC'(H_0/T) + O(T^2) , \qquad (4.44b)$$

$$\chi = C''(H_0/T) + O(T) , \qquad (4.44c)$$

and

$$C_H = 2TC(H_0/T) - 2H_0 C'(H_0/T) + H_0^2 T^{-1} C''(H_0/T) + O(T^2) , \qquad (4.44d)$$

where

$$C(x) = \int_{-\infty}^{\infty} dy\, e^{\pi y/2} \ln[1 + \exp(\tfrac{1}{2}x + e_1 - \pi e^{\pi y/2})] . \qquad (4.44e)$$

We have been unable to solve Eqs. (4.43) and evaluate $C(x)$ in a closed form. For H_0/T large and positive, $F(T, \sigma)$ in region D is recovered.

V. DISCUSSION

The low-temperature results for regions A, B, and C and $O(T)$ near lines b, c, and d can be obtained by using the dispersion curves for the first excited states and spin-wave arguments. (As we have said before, this technique is not extendable to higher orders in T.) Region D might also be explained by such reasoning, but we do not have the dispersion curves as a function of momentum in D. In an $O(T)$ neighborhood of point P it seems that one cannot use spin-wave theory to derive the results since the function $C(H_0/T)$ comes from the solution of an infinite set of nonlinear integral equations.

We divide the discussion similar to the order of the low-temperature thermodynamics presentation. The ground-state energy is set equal to zero, since only the temperature dependent terms of $F(T, \sigma)$ are of interest.

A. Regions A and B and $O(T)$ near Line b

It is easier to do the Ising model first, where the Hamiltonian is that one given in the Introduction. Consider the set of states which has no bound states; i.e., no two overturned spins from the aligned ground state are on adjacent sites. Form the partition function by taking only these states. There will be N excitations with energy $B_0 - \delta J$, $\frac{1}{2}N(N-1)$ states with energy $2(B_0 - \delta J)$, $N!/[l! \times (N-l)!]$ states with $l(B_0 - \delta J)$, etc. The partition function is

$$Q^I = \sum_{l=0}^{N} N!\,[l!\,(N-l)!]^{-1} e^{\beta l(\delta J - B_0)} = (1 + e^{\beta(\delta J - B_0)})^N \qquad (5.1)$$

and

$$F_T^I(T, B_0) = -\beta^{-1} e^{\beta(\delta J - B_0)} + \cdots . \qquad (5.2)$$

(Note that the proper variable is the magnetic field, not magnetization, in this calculation.) The above argument is modified away from the Ising limit. From Eq. (3.4) the energies of the first excited states are $E(q)=H_0-\delta(\Delta-\cos q)$. There are N such states with $q=2\pi n/N$, $0\leqslant q\leqslant 2\pi$. The excitations included in the partition function are the N states with energies $E(q)$, the $\frac{1}{2}N(N-1)$ states with energies $E(q_1)+E(q_2)$, the $N!/[l!(N-l)!]$ states with energies $E(q_1)+E(q_2)+\cdots+E(q_l)$, etc. Then, we have

$$Q=\sum_{l=0}^{N}\sum_{0\leqslant q_1<q_2<\cdots<q_l\leqslant 2\pi}\sum\cdots\sum \exp\Big(-\beta\sum_{i=1}^{l}E(q_i)\Big), \quad (5.3)$$

where the q's are summed over $2\pi n/N$, and

$$\ln Q=\sum_q \ln(1+e^{-\beta E(q)}) . \quad (5.4)$$

For $N\to\infty$, we have

$$F_T(T, H_0)=-T(2\pi)^{-1}\int_0^{2\pi}dq\ln(1+e^{-\beta E(q)}) . \quad (5.5)$$

Therefore, in A and B,

$$F_T(T, H_0)=-T^{3/2}(2\pi)^{-1/2}e^{\beta(\delta\Delta+1-H_0)}+\cdots . \quad (5.6)$$

At $O(T)$ near line b, where $E(q)\geqslant-\tau T$ and $E(q)=O(T)$ for a range of q,

$$F_T(T, H_0)=T^{3/2}(2\pi)^{-1/2}F_0(-e^{G/T}, \tfrac{3}{2})+\cdots . \quad (5.7)$$

The two formulas agree with the previously obtained results.

B. Region C and $O(T)$ near Lines c or d

The first excited states of the antiferromagnetic Ising model consist of turning over all spins in a connected region. Such states are specified by giving the positions of the two boundaries of the region. For $B_0\geqslant\rho>0$ there are $\frac{1}{2}N$ positions for the first boundary and $\frac{1}{2}N-1$ positions for the second. Since the boundaries are indistinguishable and the ground state is doubly degenerate, this implies $\frac{1}{2}2(\frac{1}{2}N)(\frac{1}{2}N-1)$ states with energy $J-B_0$. The reason there are not N positions is that the lowest excited states for $B_0\geqslant\rho>0$ consist of only $S^z=1$ and not $S^z=-1, 0$. The other states which we include in Q^I are, in general, n connected nonoverlapping regions with energy $n(J-B_0)$ and multiplicity $2(\frac{1}{2}N)!/[(2n)!(\frac{1}{2}N-2n)!]$. Q^I can be written as

$$Q^I=\sum_{n=0}^{N/2}[1+(-1)^n](\tfrac{1}{2}N)![n!(\tfrac{1}{2}N-n)!]^{-1}e^{\beta n(B_0-J)/2} . \quad (5.8)$$

Therefore, we have

$$Q^I=(1+e^{\beta(B_0-J)/2})^{N/2}+(1-e^{\beta(B_0-J)/2})^{N/2} . \quad (5.9)$$

In the thermodynamic limit the second term can be dropped to give

$$F_T^I(T, B_0)=-(\tfrac{1}{2}T)e^{(B_0-J)/2T}+\cdots . \quad (5.10)$$

Note the half-gap.

For $B_0=O(T)$ (near line d) the first excited states consist of four types for each of the two ground states; states with $S^z=1$ and energy $J-B_0$, states with $S^z=-1$ and energy $J+B_0$, states with $S^z=0$, energy J, and with the first spin up in the region of overturned spins, and states with $S^z=0$, energy J, and with the first spin down. There are $\frac{1}{2}(\frac{1}{2}N)\times(\frac{1}{2}N-1)$ states of each type. The partition function is formed by using these four classes as elementary excitations. Since only one boundary can occupy a given site, a generalized exclusion principle is in effect; i.e., if a particle (boundary) occupies a given state for one of the classes of states, not only other particles of the same class, but particles of the other classes cannot occupy the state. This results in a partition function

$$Q^I=\sum_{n=0}^{N/4}2(\tfrac{1}{2}N)![(2n)!(\tfrac{1}{2}N-2n)!]^{-1}\times(e^{-(J+B_0)/T}+2e^{-J/T}+e^{-(J-B_0)/T})^n . \quad (5.11)$$

The first factor puts in the degeneracy for the ways of distributing n nonoverlapping connected regions on the lattice with a doubly degenerate ground state. The last factor results from fixing the distribution of connected regions on the lattice and calculating the partition function for distributing the states over the four classes. After noting that the last factor is a perfect square and applying the same procedure used to obtain Eq. (5.9), one derives

$$Q^I=[1+e^{-J/2T}2\cosh(\tfrac{1}{2}B_0/T)]^{N/2}+[1-e^{-J/2T}2\cosh(\tfrac{1}{2}B_0/T)]^{N/2} . \quad (5.12)$$

For $N\to\infty$ this results in

$$F_T^I(T, B_0)=-T\cosh(\tfrac{1}{2}B_0/T)e^{-J/2T}+\cdots . \quad (5.13)$$

The preceding illustrates the origin of both the half-gap and the extra factor of $2\cosh(\frac{1}{2}B_0/T)$ near line d. The half-gap comes from the restriction that only an even number of particles (boundaries) can be excited out of the ground state. The factor of $2\cosh(\frac{1}{2}B_0/T)$ comes from an increase in the degeneracies for B_0 small.

Away from the Ising limit one parallels the discussion in Sec. VA with the dispersion curves of the first excited states given by Eqs. (3.6) and (3.7a). In region C and $O(T)$ near line c only the $S^z=1$ dispersion curve contributes to the low-temperature thermodynamics. Therefore, from the restriction to only even fermion excitations,

$$Q=2+\sum_{l=1}^{N/2}[1+(-1)^l]\sum_{0\leq q_1<q_2\cdots<q_l\leq\pi}\sum\cdots\sum\exp\Big(-\beta\sum_{i=1}^{l}E_{1/2}(q_i)\Big)$$

$$=\prod_q(1+e^{-\beta E_{1/2}(q)})+\prod_q(1-e^{-\beta E_{1/2}(q)}) , \quad (5.14)$$

where $E_{1/2}(q)=(\sinh\Phi)K\pi^{-1}(1-k^2\cos^2q)^{1/2}-\frac{1}{2}H_0$.

In the thermodynamic limit

$$F_T(T, H_0) = -T(2\pi)^{-1}\int_0^\pi dq \ln(1+e^{-\beta E_{1/2}(q)}) \;. \quad (5.15)$$

Expanding for region C gives

$$F_T(T, H_0) = -T^{3/2}A^{1/2}e^{-B/T}+\cdots \quad (5.16)$$

and for $0(T)$ near line c,

$$F_T(T, H_0) = T^{3/2}A^{1/2}F_0(-e^{-B/T}, \tfrac{3}{2})+\cdots \;. \quad (5.17)$$

These are our previous answers with the half-gap.

For $O(T)$ near line d all three $E_2(S^z=\pm 1, 0;\; q_1, q_2)$ must be used with four classes of excitations for each ground state and a modified exclusion principle.

Then

$$Q = 2+\sum_{l=1}^{N/2}[1+(-1)^l]\sum_{0\le q_1<q_2}\sum\cdots\sum_{\cdots<q_l\le\pi}\prod_{i=1}^{l/2}(e^{-\beta E_2(1;q_i,q_{i+1})}+2\,e^{-\beta E_2(0;q_i,q_{i+1})}+e^{-\beta E_2(-1;q_i,q_{i+1})})$$

$$=2+\sum_{l=1}^{N/2}[1+(-1)^l]\,2^l\cosh^l(\tfrac{1}{2}H_0/T)\times\sum\sum\cdots\sum_{0\le q_1<q_2<\cdots<q_l\le\pi}\prod_{i=1}^{l/2}e^{-\beta E_2(0;q_i,q_{i+1})} \;. \quad (5.18)$$

One continues as above to get the result

$$F_T(T, H_0) = -T^{3/2}A^{1/2}2\cosh(\tfrac{1}{2}H_0/T)\,e^{-B'/T}+\cdots \;, \quad (5.19)$$

which exhibits the extra factor of $2\cosh(\frac{1}{2}H_0/T)$ and the half-gap.

In conclusion we reiterate that, while physically illuminating, the simple arguments are not generalizable to higher orders in T as are the expansions in Sec. IV.

Finally, we can make a statement about the region $|\delta\Delta|<1$. One knows from Araki's theorem[4] that the free energy is analytic in $\delta\Delta$ and H_0 for $T>0$. Furthermore, from the work of Yang and Yang[14] one knows that the ground state is analytic across $\delta\Delta=\pm 1$ for $\sigma>0$ and σ fixed. Therefore, it is reasonable to expect that Eqs. (4.6) and (4.10) can be continued into the region $|\delta\Delta|<1$ and give the correct low-temperature thermodynamics for $H_0-\delta\Delta-1\ge\rho>0$ and $|\delta\Delta|<1$. [Note that Eqs. (4.6) and (4.10) are analytic continuations of each other.] Also, for $O(T)$ and $O(1)$ near the line $H_0=\delta\Delta+1$ with $\delta\Delta+1\ge\rho$, the analytic continuation of Eqs. (4.36) and (4.27), respectively, should give the correct low-temperature thermodynamics.

ACKNOWLEDGMENT

The authors wish to thank M. Fisher, M. Gaudin, R. Griffiths, and C. N. Yang for stimulating discussions.

*Work supported in part by NSF Grant No. P2P2847-000.

†NSF Predoctoral Fellow.

‡Work supported in part by NSF Grant No. GP-29500.

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