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Excitation Spectrum and Thermodynamic Properties of the Ising-Heisenberg Linear Ferromagnet

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New analytic results are presented for the low-T thermodynamics of the Ising-Heisenberg linear ferromagnetic in a magnetic field H_0. For small H_0 the thermodynamic functions show unexpected and interesting structure as a function of H_0 and the anisotropy Δ. The thermal and magnetic energy gaps have singularities, not necessarily at the same Δ-H_0 location, as changes occur in the type of excitation dominating the low-T behavior. The results may relate to quantum solitons in the linear ferromagnet.

There has been a renewed interest in exact solutions of nontrivial, quantum-mechanical, one-dimensional models.[1] For example, exact and fairly complete solutions are now available for the one-dimensional (1D), δ-function potential, Fermi- and Bose-gas models,[2] the linear Hubbard model of a metal-insulator transition,[3] and the linear, spin-$\frac{1}{2}$, Ising-Heisenberg XY continuum model.[4] Exact solutions for a continuum electron gas[5] and an electron gas on a lattice[6] are known. These are relevant to the important field of 1D organic conductors.[7] Models for organic charge-transfer salts can be mapped into a quantum magnetic chain[8] which in the antiferromagnetic limit corresponds to the Hubbard dimer gas.[9] The exact solutions of the 1D quantum-mechanical sine-Gordon and related equations (solitons) have been extensively applied to charge-density waves in 1D conductors.[6,10] Very recently the Bethe's *Ansatz* techniques have been used to solve the massive Thirring model.[11,12] Fadeev's review presents a unified approach to all the models discussed above.[12] Sutherland gives an overview of the quantum soliton concept and its connections to Bethe's *Ansatz*.[13]

In this Letter we present new, unanticipated, and interesting exact results for the 1D, spin-$\frac{1}{2}$, ferromagnetic, Ising-Heisenberg model. The Hamiltonian[14] is

$$H=-\sum_{i=1}^{N}[S_i{}^xS_{i+1}{}^x+S_i{}^yS_{i+1}{}^y+\Delta(S_i{}^zS_{i+1}{}^z-\tfrac{1}{4})]-H_0\sum_{i=1}^{N}S_i{}^z. \tag{1}$$

The S's are $\frac{1}{2}$ the respective Pauli matrices, and there are periodic boundary conditions on the system. $\Delta \geq 1$ except, if H_0 is in a small, order T^0, neighborhood of zero, we restrict $\Delta > 1$. (T is temperature.) We set Boltzmann's constant to 1 throughout the body of this paper.

This system was first studied[15] in the 1930's; a formalism for the thermodynamics was derived by Gaudin much later.[16] In Gaudin's work assumptions were made which are difficult to verify directly. In this and previous work[17] we have made comparisons of the predictions of Gaudin's formalism to numerical results on finite systems.[18] All comparisons are favorable thus enhancing our faith in the assumptions contained in the thermodynamic formalism.

We have performed low-temperature expansions of Gaudin's formalism to derive *all* of our results. We will not present this approach in this paper, however, since it is a fairly long and detailed derivation. We will give a "physical" argument for the results which shows the connection between the low-temperature thermodynamics and the excitations of the system.

It is known that the zero-temperature dispersion curves for this system[17] are given by

$$E_n(P)=nH_0+\sinh\Phi(\cosh n\Phi-\cos P)/\sinh n\Phi, \tag{2}$$

where $\Delta=\cosh\Phi$, $0\leq P\leq 2\pi$, and $n=1, 2, \ldots$. The $n=1$ excitations and linear combination of the $n=1$ excitations are spin waves, and the higher-n excitations are bound states of spin waves. The P's are distributed uniformly between 0 and 2π and, for a given n, obey a Fermi-like exclusion principle.

The energies of the first excited states are $E(q)=H_0+\Delta-\cos q$. There are N such states with $q=2\pi m/N$, $0\leq q\leq 2\pi$. The states we first sum to derive the partition function are these N states, the $\frac{1}{2}N(N-1)$ states with energies $E(q_1)+E(q_2),\ldots$, the $N!/[l!(N-l)]$ states with energies $E(q_1)+E(q_2)+\ldots+E(q_l)$, etc. These are all the spin-wave excitations, and they provide a contribution[17] to $F(T,\sigma)$ of

$$F(T,\sigma)=\sigma H_0-(T/2\pi)\int_0^{2\pi}dq\exp[-(\Delta+H_0-\cos q)/T], \tag{3}$$

where σ is the magnetization per spin.

For H_0 far enough away from zero, this is all we need to obtain the low-temperature thermoydnamics to exponential accuracy in T. However, for small H_0 other excitations, the high-lying bound states, can dominate. For large n $E_n(P)\sim nH_0+\sinh\Phi$; note that the $E_n(P)$ are independent of P and, accordingly, are effectively just the energies of a 1D Ising model with exchange constant $J=\sinh\Phi$. Therefore, we add to Eq. (3) the Ising free energy for this J.[19] We obtain, after some simplification for low T of the Ising-model result,

$$F(T,\sigma)-\sigma H_0=-\{H_0^2/4+T^2\exp[-(\Delta^2-1)^{1/2}/T]\}^{1/2}-(T/2\pi)\int_0^{2\pi}dq\exp[-(\Delta+H_0-\cos q)/T]+E. \tag{4}$$

This is our basic result and is the same result as obtained by the low-T expansion of the Gaudin formalism. It is valid for low T, $O(T)>H_0\geq 0$ and $\Delta>1$. The correction, E, is exponentially higher order in T than the larger of the two terms on the right-hand side of Eq. (4) *even after* taking an arbitrary number of T derivatives or up to and including two H_0 derivatives. {Note that this means, in particular, that if one expands the square root for H_0 exponentially larger or smaller than $\exp[-(\Delta^2-1)^{1/2}/2T]$, one should retain *two terms* in the expansion. Both terms are significant, and E is exponentially higher order than the integral or the second term of the square-root expansion, whichever is larger.}[20]

We now discuss the detailed behavior of Eq. (4) in terms of the susceptibility $\chi\equiv-[\partial^2(F-\sigma H_0)/\partial H_0^2]_T$ and specific heat $C_H\equiv-T[\partial^2(F-\sigma H_0)/\partial T^2]_{H_0}$. We find from Eq. (4)

$$\chi=T^2\exp[-(\Delta^2-1)^{1/2}/T]\left(4\{H_0^2/4+T^2\exp[-(\Delta^2-1)^{1/2}/T]\}^{3/2}\right)^{-1}+(2\pi T)^{-1}\int_0^{2\pi}dq\exp[-(\Delta+H_0-\cos q)/T]+E_\chi. \tag{5}$$

E_χ is exponentially higher order in T than the larger of the first two terms. If we asymptotically expand the integral,

$$\chi=T^2\exp[-(\Delta^2-1)^{1/2}/T]\left(4\{H_0^2/4+T^2\exp[-(\Delta^2-1)^{1/2}/T]\}^{3/2}\right)^{-1}+(2\pi T)^{-1/2}\exp[-(\Delta+H_0-1)/T]+E_\chi'. \tag{6a}$$

E_χ' is exponentially higher order than the first term of Eq. (6a) or $O(T)$ higher order than the second term, whichever is larger. Similarly, for C_H, we obtain

$$C_H=(\Delta^2-1)\exp[-(\Delta^2-1)^{1/2}/T]\{H_0^2/2+T^2\exp[-(\Delta^2-1)^{1/2}/T]\}\times\left(4T\{H_0^2/4+T^2\exp[-(\Delta^2-1)^{1/2}/T]\}^{3/2}\right)^{-1}+(2\pi T^3)^{-1/2}(\Delta+H_0-1)^2\exp[-(\Delta+H_0-1)/T]+E_c. \tag{6b}$$

E_c is $O(T)$ higher order than the larger of the first two terms. The first terms of both χ and C_H are bound-state contributions and the second terms are spin-wave contributions.

For χ we redefine variables to $H_0=e^{\alpha/T}$; Fig. 1 illustrates the following discussion. For $\alpha>\alpha_b=\frac{1}{3}[\Delta-1-(\Delta^2-1)^{1/2}]$ the spin-wave term dominates the bound-state term. For $\alpha<\alpha_b$ the bound-state term dominates. Obvious simplifications can be made to either Eq. (5) or (6a) by dropping appropriate terms in these cases. The bound-state region subdivides into $\alpha<\alpha_c=-(\Delta^2-1)^{1/2}/2$ and $\alpha>\alpha_c$. For $\alpha<\alpha_c$, Eq. (5) simplifies to

$$\chi=(4T)^{-1}\exp[(\Delta^2-1)^{1/2}/(2T)]. \tag{7a}$$

For $\alpha_b>\alpha>\alpha_c$,

$$\chi=2T^2H_0^{-3}\exp[-(\Delta^2-1)^{1/2}/T]. \tag{7b}$$

Corrections to both these equations are exponentially higher order in T. We thus have three separate regions for χ with different exponential behavior in each.

C_H is somewhat different from χ and is illustrat-

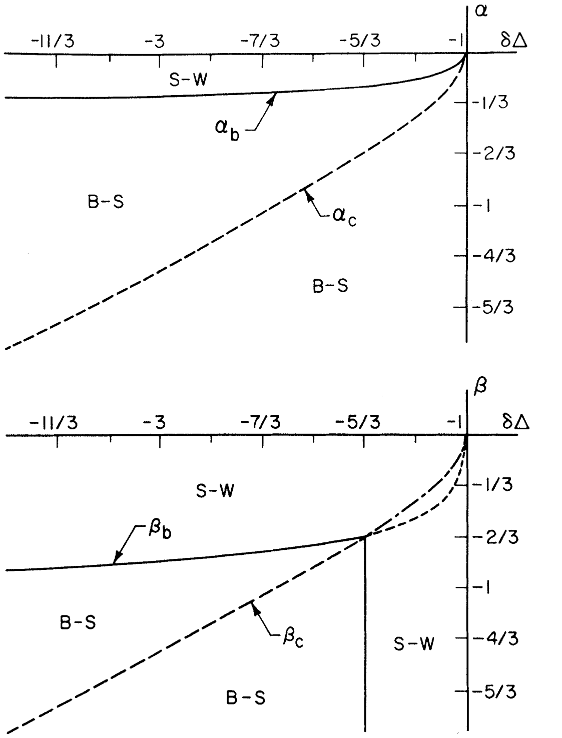

FIG. 1. The top portion presents the various regions for χ, the susceptibility. The bottom portion illustrates the character of C_H, the specific heat. In both cases S-W labels the spin-wave regions, B-S labels the bound-state regions, and $\delta = -1$.

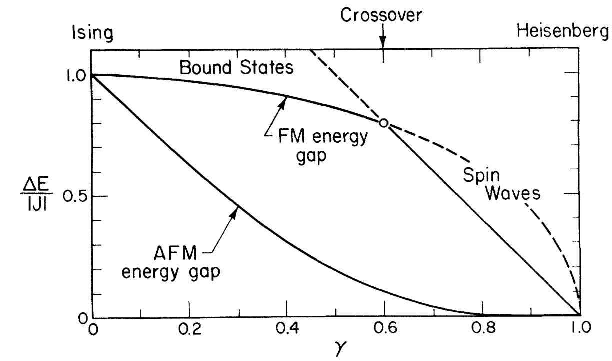

FIG. 2. We plot the effective energy gap for C_H. Shown are the gaps for the ferromagnet and antiferromagnet. The ferromagnet curve illustrates the singularity (kink) described in the text. The antiferromagnet gap is given by a single expression over the whole anisotropy range.

ed in Fig. 1. We define $H_0 = e^{\beta/T}$. Then for $\beta > \beta_b = \Delta - 1 - (\Delta^2 - 1)^{1/2} = 3\alpha_b$ and *also* for $\frac{5}{3} > \Delta > 1$, all β, the spin waves dominate. One can then drop the first term in Eq. (6b). For $\beta < \beta_b$, $\Delta > \frac{5}{3}$, the bound states dominate and one can drop the second term. The bound-state region again subdivides into $\beta < \beta_c = -(\Delta^2 - 1)^{1/2}/2 = \alpha_c$ and $\beta > \beta_c$. For $\beta > \beta_c$ with $\Delta > \frac{5}{3}$,

$$C_H = (TH_0)^{-1}(\Delta^2 - 1)\exp[-(\Delta^2 - 1)^{1/2}/T] \qquad (8a)$$

and, for $\beta < \beta_c$ with $\Delta > \frac{5}{3}$,

$$C_H = (4T^2)^{-1}(\Delta^2 - 1)\exp[-(\Delta^2 - 1)^{1/2}/(2T)]. \qquad (8b)$$

The corrections are $O(T)$ and exponentially higher order for Eqs. (8a) and (8b), respectively. Again one has three separate regions with different exponential behavior in each (as for χ), but the details are different from χ.

To emphasize this difference between χ and C_H, look at $H_0 = 0$. For $H_0 = 0$ χ is given by Eq. (7a) to exponential accuracy for all $\Delta > 1$. C_H, however, is given by Eq. (8b) for $\Delta > \frac{5}{3}$ and by

$$C_H = (2\pi T^3)^{-1/2}(\Delta - 1)^2 e^{-(\Delta - 1)/T} \qquad (9)$$

for $\frac{5}{3} > \Delta > 1$. Corrections to Eq. (9) are $O(T)$ higher order. Thus χ has a single effective gap for all Δ at $H_0 = 0$ while C_H has two effective gaps with a crossover between the two at $\Delta = \frac{5}{3}$.[21] The bound states dominate for large Δ while the spin waves dominate for small Δ. This is shown in Fig. 2, where the notation is that of Ref. 14.

It would be of considerable interest to investigate these crossover effects experimentally. Far-infrared studies like those of Torrance and Tinkham[22] on $CoCl_2 \cdot 2H_2O$ might be performed on the Ising-like linear ferromagnet cobalt chloride dipyridine ($CoCl_2 \cdot 2NC_5H_5$). The very recent discovery of a family of good Heisenberg-like ferromagnets[23] offers the possibility of studies by neutrons or other means of the more isotropic region. Finally, we note that an understanding of the excitations of the linear ferromagnet may be important for the quantum soliton problem.[24]

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[20]For larger H_0 and $\Delta \geqslant 1$, except for an $O(T^0)$ neighborhood of $H_0=0$, $\Delta=1$, our answer is Eq. (4) with the square-root term replaced by $-H_0/2$. E in this case is exponentially higher order than the integral. All results for $H_0 > O(T^2)$ have no structure and merge smoothly onto the $H_0 < O(T)$ results. Therefore, in all that follows we restrict $H_0 < O(T)$.

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NEW APPROACH TO PERTURBATION THEORY. Y. Aharonov and C. K. Au [Phys. Rev. Lett. 42, 1582 (1979), and 43, 176(E) (1979)].

Equations (12) and (40) in this paper should read as follows:

$$-\tfrac{1}{2}(g^2-g')e^{-G} = (E - V_0 - \lambda V_1)e^{-G}; \tag{12}$$

$$F_i(x) \equiv 2\alpha_{i-1}[g_1 + g_0\alpha_1/(x-\alpha_0)]\exp(-2G_0) + \sum_{m=2}^{i-1}\alpha_{i-m}\Big[\sum_{j=0}^{m} g_j g_{m-j} - g_m' + 2E_m\Big](x-\alpha_0)\exp(-2G_0) - \sum_{j=1}^{i=1} g_j g_{i-j}(x-\alpha_0)^2\exp(-2G_0). \tag{40}$$