Low-temperature behavior of the $S=\frac{1}{2}$ ferromagnetic Heisenberg chain

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A detailed account of the results of the numerical solution of the thermodynamic Bethe-ansatz equations for the isotropic ferromagnetic $S=\frac{1}{2}$ Heisenberg chain is presented. The extrapolation procedure used in approximating the infinite set of coupled nonlinear integral equations is discussed. The data for the truncated integral equations are analyzed in terms of a finite-string-size scaling. Analytic expressions for the free energy and susceptibility for $T\to 0$ are obtained. All the results are consistent with entropy $S\sim(T/|J|)^{1/2}$ and

$$\chi\sim\frac{|J|}{T^2}[\mathscr{L}^{-1}+(\ln\mathscr{L})/\mathscr{L}^2+\cdots]+O(T^{-3/2}),$$

where $\mathscr{L}=\ln(|J|/T)$, suggesting the existence of a marginal variable. The logarithmic corrections reflect the analogy to the Kondo problem.

I. INTRODUCTION

The critical behavior of the isotropic, ferromagnetic $S=\frac{1}{2}$ Heisenberg chain has been investigated previously by several methods, which gave quite different results for the critical exponents γ of the susceptibility and α of the specific heat. Bonner and Fisher[1] studied the thermodynamic properties of rings of size up to $N=11$ and obtained $-\alpha\simeq0.45$–0.5 and $\gamma\simeq1.8$ by extrapolation to rings of infinite size. Baker, Rushbrooke, and Gilbert[2] computed the high-temperature-series expansion up to tenth order and analyzed the energy and magnetic susceptibility by means of Padé approximants, obtaining $\gamma=1.66\pm0.07$. Kondo and Yamaji[3] used a Green's-function decoupling procedure taking one magnon self-consistently into account, and obtained $\gamma=2$ and $-\alpha=\frac{1}{2}$, as expected from spin-wave theory. Monte Carlo simulations for the Heisenberg chain were performed by Cullen and Landau[4] ($\gamma\simeq1.32$). More accurate Monte Carlo results were provided by Lyklema,[5,6] who obtained $-\alpha=0.3\pm0.1$, $\gamma=1.75\pm0.02$, and, via finite-size scaling, $(\gamma-1)/\nu=1.01\pm0.01$.

The above values for γ, except that from Kondo and Yamaji,[3] differ from the classical analog $\gamma_{cl}=2$. Moreover, Lyklema's Monte Carlo data exclude $\alpha=-0.5$, the value expected from spin waves. In Ref. 3 Nagaoka's Green's-function decoupling procedure was employed, such that classical behavior at low T is expected. These interesting results lead us to reanalyze the critical behavior of the ferromagnetic chain by a different method, namely the numerical solution of the thermodynamic Bethe-ansatz equations.[7,8] In contrast to other methods, the Bethe ansatz provides the exact solution of the problem. The main conclusions have been presented in a recent paper.[9] We obtained $\alpha=-0.49\pm0.02$ and $\gamma=2.00\pm0.02$. The purpose of this paper is to present more details of the calculation, as well as some analytical expressions extracted from the thermodynamic Bethe-ansatz equations.

The rest of the paper is organized as follows. In Sec. II we restate the thermodynamic Bethe-ansatz equations for the isotropic Heisenberg chain,[7,8] as well as Takahashi's[7] solutions of these equations for $T=0$ and ∞. Using the crossover between the strong- and weak-coupling regimes, we define a correlation length. In Sec. III the numerical procedure for obtaining the solution of the integral equations is discussed. The infinite set of integral equations is truncated and actually only n_0 (with $n_0\leq280$) coupled nonlinear integral equations are solved. The results are discussed in terms of a finite-string-size scaling in Sec. IV. The data are consistent only if logarithmic corrections that already appear in the correlation length are taken seriously. This finding is supported by analytic expressions extracted from the thermodynamic Bethe-ansatz equations in Sec. V. A summary and discussion follows in Sec. VI.

Our main results are that at low temperatures the entropy and susceptibility depend on T as

$$S=a(T/|J|)^{1/2}+O(T), \tag{1.1}$$

$$\chi=b\frac{|J|}{T^2}[\mathscr{L}^{-1}+(\ln\mathscr{L})/\mathscr{L}^2+\cdots]+O(T^{-3/2}), \tag{1.2}$$

where $\mathscr{L}=\ln(|J|/T)$, a is close to $\frac{3}{2}\times1.042$, and b is of order of 1.

Recently Takahashi and Yamada[10] calculated the free energy and susceptibility of the isotropic model by numerically solving the thermodynamic Bethe-ansatz equations of the planar XXZ model and extrapolating the anisotropy to zero. They also concluded that $\alpha=-\frac{1}{2}$ and $\gamma=2$, and the data are in excellent agreement with ours throughout the whole temperature range (see Sec. III).

II. THERMODYNAMIC BETHE-ANSATZ EQUATIONS

We consider the isotropic quantum Heisenberg chain for $S=\frac{1}{2}$,

$$\mathcal{H}=J\sum_{i=1}^{N}\mathbf{S}_i\cdot\mathbf{S}_{i+1}-\tfrac{1}{4}JN+2H\sum_{i=1}^{N}S_i^z \qquad (2.1)$$

with N sites and periodic boundary conditions in the limit $N\rightarrow\infty$. Here J is the (ferromagnetic) coupling constant and the magnetic field H is along the z direction.

On the basis of Bethe's famous work,[11] Takahashi[7] and Gaudin[8] derived the thermodynamic Bethe-ansatz equations for the model (2.1). They consist of an infinite set of nonlinearly coupled integral equations for functions $\eta_n(\Lambda)$. The function $\eta_n(\Lambda)$ characterizes a string excitation of order n with real rapidity Λ. A string excitation of order n represents a bound-magnon state of n magnons. It is usual to define an energy function for the string excitation, which is given by

$$\varepsilon_n(\Lambda)=T\ln\eta_n(\Lambda)\ . \qquad (2.2)$$

There are several equivalent sets of integral equations yielding the $\eta_n(\Lambda)$. The most convenient representation for a numerical solution is the recursion sequence

$$\ln\eta_n=G*\ln[(1+\eta_{n-1})(1+\eta_{n+1})]-2\pi(J/T)\delta_{n,1}G\ ,\qquad n=1,2,3,\ldots,\quad \eta_0\equiv0 \qquad (2.3)$$

where the center star denotes a convolution and

$$G(\Lambda)=[4\cosh(\tfrac{1}{2}\pi\Lambda)]^{-1}\ . \qquad (2.4)$$

These equations are completed by the asymptotic condition

$$\lim_{n\rightarrow\infty}\left[\frac{1}{n}\ln\eta_n(\Lambda)\right]=\frac{2H}{T}=2X_0\ , \qquad (2.5)$$

and the free energy of the model is given by

$$F=-J\ln2-T\int d\Lambda\,G(\Lambda)\ln[1+\eta_1(\Lambda)]\ . \qquad (2.6)$$

We consider $J=-1$ throughout the rest of the paper.

The zero-temperature (strong-coupling) and high-temperature (free-spin) solutions of the integral equations have been explicitly obtained by Takahashi.[7] In the critical region the solution is an interpolation between these free-spin and zero-temperature limits. It is then useful to restate the results known for these limits.

(a) In the high-temperature limit the driving term in (2.3) can be neglected. It is the only explicit temperature dependence the integral equations have. The solutions for the η_n are then constants fixed by the asymptotic condition (2.5) to be

$$\eta_n=\{\sinh[(n+1)X_0]/\sinh X_0\}^2-1\ . \qquad (2.7)$$

(b) As $T\rightarrow0$ the driving term dominates, such that necessarily

$$\ln(1+\eta_n)\sim\ln\eta_n\sim\varepsilon_n/T\ ,$$

and (2.3) reduces to a set of linear integral equations for the potentials ε_n. The solution can be obtained by Fourier transformation:

$$\varepsilon_n(\Lambda)=2nH+\frac{2n\,|J|}{\Lambda^2+n^2}\ . \qquad (2.8)$$

Then we have $\eta_n=\infty$ for all n, i.e., no magnons, $S_z/N=\frac{1}{2}$, and $E/N=-H$. This is the ferromagnetic ground state.

At low but finite temperatures the functions $\varepsilon_n(\Lambda)$ as a function of Λ and n show crossovers between the asymptotic behaviors (2.7) and (2.8). For sufficiently large Λ the driving term in (2.3) becomes negligible and we obtain (2.7) for all n. If the string index is sufficiently large, the effect of the driving term is again negligible, and the solution will be close to (2.7). For small Λ and n, on the other hand, the driving term dominates and $\eta_n(\Lambda)$ is given by (2.2) equated to (2.8). For intermediate Λ and n we have a crossover regime.

For small Λ and H and as a function of n, we define a crossover index $n_c(T)$ by equating (2.8) with (2.7) inserted into (2.2),

$$|J|/n_c=\tfrac{1}{2}T\ln[n_c(n_c+2)]\simeq T\ln(n_c+1)\ . \qquad (2.9)$$

Here we used that, at low T, $n_c^2\gg1$. For $n>n_c$ the solution is then closer to the one of a free spin, while for $n<n_c$ the strong-coupling solution dominates. This means that in thermal equilibrium the average number of correlated spins is $n_c(T)$. In other words, $n_c(T)$ is the correlation length of the system. Solving (2.9) iteratively we obtain, for $T\ll|J|$,

$$\xi\simeq\frac{|J|}{T}\left[\frac{1}{\ln(|J|/T)}+\frac{\ln\ln(|J|/T)}{\ln^2(|J|/T)}+\cdots\right]\ , \qquad (2.10)$$

corresponding to $\nu=1$, with logarithmic corrections.

The logarithmic corrections in (2.10) resemble very much the high-temperature results for the Kondo problem. Andrei, Furuya, and Lowenstein[12] have pointed out that the thermodynamic Bethe-ansatz equations for the Kondo problem are also given by (2.3), if the driving term is replaced by

$$-\frac{2T_0}{T}e^{\Lambda}\ , \qquad (2.11)$$

where T_0 is the Kondo temperature and $\Lambda\ll-1$. Note that for large Λ the driving term of the Heisenberg chain asymptotically reduces to (2.11). In Sec. V we show that $|\Lambda|$ values smaller than a $\Lambda_0\gg1$ do not contribute to the temperature dependence of F at low T.

III. NUMERICAL PROCEDURE

In principle, an infinite number of integral equations should be solved for every temperature with the asymptotic field boundary condition (2.5). However, we have argued in Sec. II that for a sufficiently large string index the solution for η_n asymptotically approaches the free-spin value (2.7). A good estimate of the free energy can then be obtained by choosing an index n_0 and replacing η_n for

$n > n_0$ by the asymptotical free-spin value, and then numerically solving the system of n_0 integral equations. The procedure is repeated for several n_0 and the result extrapolated to $n_0 \to \infty$.

In order to get a reasonable estimate of the free energy and its derivatives, the number of integral equations solved, n_0, should be much larger than $n_c(T)$. This means that we have to consider system sizes much larger than the correlation length. The number of integral equations grows then when the temperature is lowered. For the lowest temperatures, we consider n_0 up to 280.

The integration interval for the convolution is the entire real axis. As a result of the exponential decrease of both the kernel and the driving force, the integration simplifies for large Λ values. At finite temperature the functions $\eta_n(\Lambda)$ asymptotically approach the free-spin solution for $|\Lambda| \to \infty$, as discussed in Sec. II. Hence, we can find a Λ_0 such that we can replace η_n by (2.7) for $|\Lambda| > \Lambda_0$. Λ_0 depends on temperature and it must be chosen such that a considerable enlargement of Λ_0 does not affect the significant figures of the derivatives of the free energy. In some cases we considered several Λ_0 values and extrapolated to $\Lambda_0 \to \infty$. The results depend much stronger on n_0 than on Λ_0.

The set of integral equations has been solved iteratively. Several iteration procedures have been employed, with different stability and convergence properties. The convergence becomes very slow for large n_0, such that up to 10^4 iterations were needed for the lowest-temperature points. The speed of convergence can be improved by choosing an adequate initial set of functions. An interpolation between the strong-coupling solution for small Λ and n and the free-spin solution for Λ and/or n large was found to be the most appropriate starting point. The temperature and field derivatives of the free energy were obtained numerically.

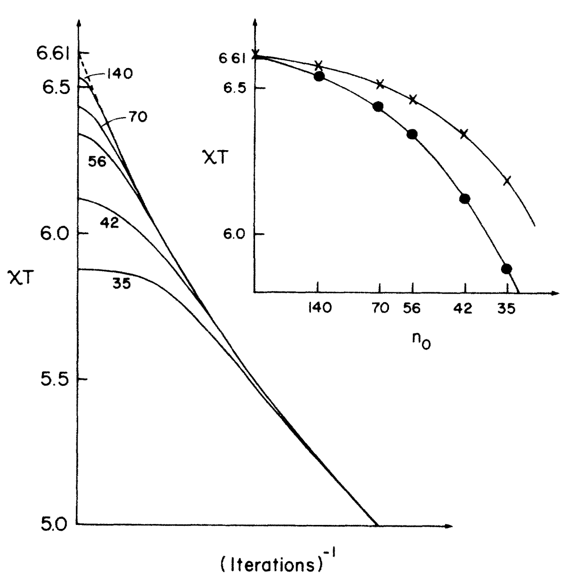

FIG. 1. χT as a function of inverse iterations for various n_0, the number of solved integral equations. Iterations are in arbitrary units, since convergence depends on the employed procedure (we used 10^2 up to 10^4 iterations). The saturation values (dots) and intersections with the χT axis of the tangent through the inflection point of each curve (crosses) are shown in the inset as function of $1/n_0$. Envelop curve (dashed) intersects the χT axis at the same point as the curves in the inset extrapolated to $n_0 \to \infty$. The data are for $T=0.05$.

In Fig. 1 we show a typical extrapolation to $n_0 \to \infty$ for the susceptibility for $T=0.05$. χT, calculated after each iteration, is plotted as a function of the inverse of the iteration number for several values of n_0. The iteration has an arbitrary scale, since it depends on the initial set of functions and the iteration procedure employed. For the following discussion it is important to always use the same procedure and initial conditions for a given temperature. The susceptibility eventually saturates at a value which depends on n_0. These are plotted in the inset as a function of $1/n_0$. It is easy to see that the curves of χT versus inverse iterations have an inflection point. The tangential line to the curve at the inflection point intersects the χT axis. We have also plotted these intersection values in the inset. Both extrapolations to $1/n_0 \to 0$ agree usually within 0.3%. A third criterion serves as a check: The family of χT versus inverse iteration curves has an envelope which when extrapolated cuts the χT axis (dotted line).

The error bar attributed to the final χT value is chosen to be larger than the scattering of the values obtained by the three criteria. In most of the cases we added a (subjective) confidence error in order to account for possible systematic errors.

The dependence on n_0 is much weaker for nondiverging quantities like the free energy and entropy. In the case of the entropy a plot similar to the inset of Fig. 1 has a dependence of S on n_0 of only 2–3 %. The values of χT and S are given in Tables I and II with their respective errors, which include the estimate for a systematic error. Note that when derivatives are calculated as in Ref. 9 the systematic errors cancel and smaller errors can be considered.

In Fig. 2 the temperature-dependent part of the free energy is plotted against $T^{3/2}$. It is seen that for $T \to 0$ it asymptotically approaches a straight line. The same data are shown in Fig. 3 together with the entropy data as a

TABLE I. Values of χT for various temperatures as obtained by extrapolating $n_0 \to \infty$ with their respective errors.

T	χT
0.100	4.21±0.02
0.070	5.26±0.02
0.0625	5.69±0.01
0.050	6.61±0.03
0.0375	8.15±0.04
0.030	9.57±0.06
0.025	11.00±0.07
0.020	12.98±0.08
0.016	15.55±0.15
0.0125	19.15±0.20
0.008 75	26.25±0.20
0.006 25	35.3±0.4
0.0045	47.0±0.4

TABLE II. Values of S for various temperatures as obtained by extrapolating $n_0 \to \infty$. The error is 10^{-4} unless indicated. A systematic confidence error (the same for all T) of 4×10^{-4} should be added.

T	S
0.100	0.3485
0.070	0.3069
0.050	0.2704
0.030	0.2209
0.020	0.1867
0.015	0.1651±0.0002
0.010	0.1380±0.0002
0.007	0.1175±0.0003
0.005	0.1010±0.0010

function $T^{1/2}$. Again, both curves asymptotically approach straight lines. The solid and dashed lines correspond to the fit given by Takahashi and Yamada[10] to their data when analyzed in powers of $T^{1/2}$. The agreement is remarkably good. While our entropy data are slightly below theirs, our values of $-F/T^{3/2}$ have a tendency to be larger than those of Takahashi and Yamada. The differences, although systematic, are within the error bars.

It may be surprising that the data for F are more scattered than the data for S. The computer program was designed to calculate S with high precision. The integral in (2.6) giving the free energy yields ln2 plus the small temperature dependence shown in Fig. 2. The scattering is due to errors in the fifth digit in the evaluation of ln2. These errors cancel when we look for differences in the free energy, as for the entropy, calculated in exactly the same way.

The temperature range and the number of equations considered by Takahashi and Yamada[10] are essentially the same as ours. They also do not *prove* conclusively that $\alpha=-\frac{1}{2}$ and $\gamma=2$. Their data, as well as ours, are still compatible with $\gamma=1.98$ or $\gamma=2.02$, and also $\alpha=-0.48$ cannot be ruled out.

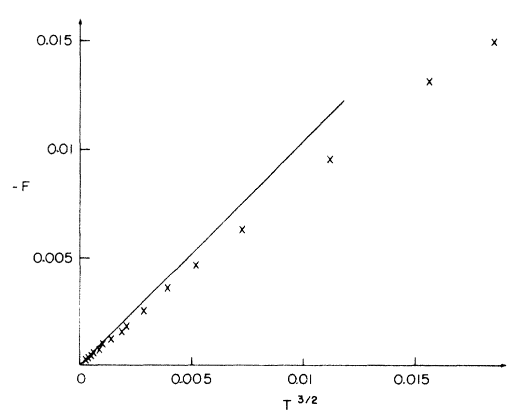

FIG. 2. Low-temperature free energy as a function of $T^{3/2}$. The solid line is $F=-1.042T^{3/2}$, which is approached asymptotically as $T\to0$.

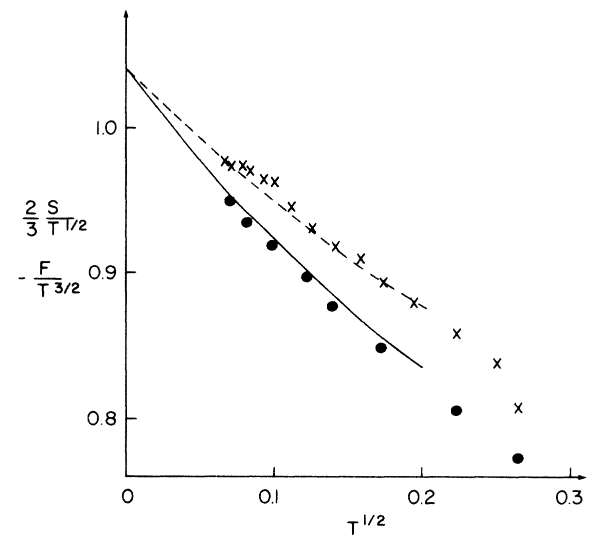

FIG. 3. $-F/T^{3/2}$ (crosses) and $\frac{2}{3}S/T^{1/2}$ (dots) as a function of $T^{1/2}$. Dashed and solid lines correspond to the fit given by Takahashi and Yamada (Ref. 10) to their data. Differences are within the error bars. For the scattering of the free-energy data see text.

IV. FINITE-"STRING-SIZE" SCALING

In Sec. II we defined the correlation length n_c as the average number of bound spins in thermal equilibrium and in Sec. III we showed the results of the numerical solution of a system of n_0 integral equations, where n_0 is larger than n_c. In this way at most n_0 spins can be correlated. This is similar to considering a system of finite size n_0 larger than the correlation length. The variation of χT as a function of n_0^{-1} also resembles a dependence on finite size. In view of this analogy Lyklema suggested analyzing the data for finite n_0 under the assumption of finite-size scaling.

The finite-size scaling hypothesis for an ordinary critical quantity X yields[13]

$$X_n \simeq n^{x/\nu} Q(n^{1/\nu}(T-T_c)) , \tag{4.1}$$

where n is the size of the system and x is the critical exponent associated with the intensive property X as $T\to T_c$ in the finite system. Here Q is a scaling function. In our case $T_c=0$. This causes an ambiguity when defining the critical quantity, e.g., we may choose the susceptibility χ or as well any power of T times χ, $T^k\chi$. Following Lyklema[5] we choose X to be the "Curie constant" χT, which is a dimensionless quantity. The second difficulty arises due to the logarithmic corrections we found in the correlation length, (2.10). In the absence of a well-founded theory we neglect the logarithms in a first approximation.

Assuming then that $\nu=1$, $x=\gamma-1=1$, we have that $T\chi n(T)/n$ should be a universal function of nT. If the finite-n_0 data for χT obey this universal relation, then our choice of γ and ν is consistent. However, for each temperature the finite-n_0 values for χT lie on different curves. It is a family of almost parallel curves with a spacing that is roughly logarithmic.

In view of (2.9), which defines ξ given by $n_c T \ln(n_c+1)$ equated to 1, we have plotted $T\chi_n(T)/n$ against $nT\ln(n+1)$ in Fig. 4. All the points are close to one curve. There is some scattering, which is not at random, but systematic. The lower-T points lie below the curve, while the high-temperature data are above. Other attempts to impose logarithmic corrections on (4.1) that we tried were less successful.

If we accept the result that $T\chi_n(T)/n$ is a universal function of $z=Tn\ln(n+1)$, then for any fixed value of z we have

$$\chi_n(T)=\frac{A}{T^2}\left[\frac{1}{\ln(1/T)}+\frac{\ln\ln(1/T)}{\ln^2(1/T)}+\cdots\right]. \quad (4.2)$$

We will get a similar dependence analytically in Sec. V.

We did not analyze the entropy data with finite-string-size scaling, since its dependence on n_0 is much smaller than it is for χ. Also, the leading term of the entropy does not have logarithmic corrections.

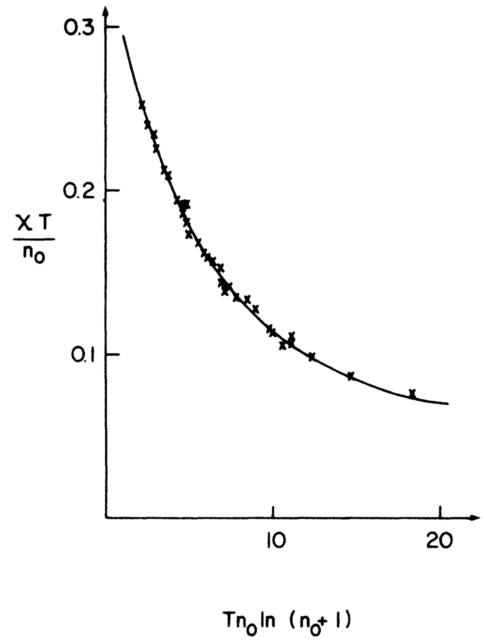

FIG. 4. Finite-string-size scaling analysis of the susceptibility. n_0 is the number of integral equations actually solved at each T. For the scattering of the data, see text.

V. ANALYTIC RESULTS

In this section we derive analytic expressions for χ and F valid asymptotically as $T\to 0$. We first determine the asymptotic behavior of $\ln[1+\eta_1(\Lambda)]$ and then calculate the free energy via (2.6). At low temperatures it is convenient to use the expression[7]

$$\ln[1+\eta_1(\Lambda)]=2\frac{|J|}{T}\frac{1}{\Lambda^2+1}+\frac{1}{\pi}\sum_{m=1}^{\infty}\int d\Lambda'\ln[1+\eta_m^{-1}(\Lambda')]\times\left[\frac{m+1}{(\Lambda-\Lambda')^2+(m+1)^2}+\frac{m-1}{(\Lambda-\Lambda')^2+(m-1)^2}\right], \quad (5.1)$$

which is equivalent to (2.3). The second Lorentzian for $m=1$ is to be interpreted as a delta function. The magnetic field has been incorporated into the boundary conditions for the $\eta_m(\Lambda)$.

We noted in Sec. II that in the strong-coupling regime $\eta_m\to\infty$. Hence the strong-coupling regime does not contribute to the integrals in (5.1). The leading contribution is due to the free-spin solution for large n and/or Λ. We make the following simplifying assumption, which does not affect the leading temperature dependence but only the amplitudes. We assume that $\eta_n(\Lambda)=\infty$ for $|\Lambda|<\Lambda_c(n)$ and $n<n_c$ and elsewhere is given by (2.7). This is equivalent to an abrupt crossover. The n-dependent crossover rapidity is obtained via similar arguments as for the correlation length,

$$\Lambda_c(n)\simeq\left[\frac{n}{\ln(n+1)}\frac{|J|}{T}\right]^{1/2}. \quad (5.2)$$

We divide the contributions to (5.1) into two parts: (a) $|\Lambda|>\Lambda_c(n)$, $n<n_c$ and (b) $n\geq n_c$.

(a) We expand for small fields, $X_0=H/T$,

$$\ln(1+\eta_m^{-1})=\ln\left[1+\frac{1}{m(m+2)}\right]-\tfrac{2}{3}X_0^2+\cdots, \quad (5.3)$$

and inserting this expression into (5.1) we get

$$\frac{1}{\pi}\sum_{m=1}^{n_0}\left[\ln\left[1+\frac{1}{m(m+2)}\right]-\tfrac{2}{3}X_0^2\right]\times\left[\arctan\left[\frac{m+1}{\Lambda_c-\Lambda}\right]+\arctan\left[\frac{m-1}{\Lambda_c-\Lambda}\right]+(\Lambda\leftrightarrow-\Lambda)\right]. \quad (5.4)$$

In order to obtain the free energy this expression times $[\cosh(\pi/2)\Lambda]^{-1}$ is integrated over Λ. Since $\Lambda_c\gg 1$ only small Λ, i.e., $|\Lambda|\ll\Lambda_c$, are relevant. Since $\Lambda_c\sim 1/\sqrt{T}$, a Taylor expansion in Λ/Λ_c generates a power series $\sqrt{T}$. We keep only the leading term, which corresponds to $\Lambda=0$ in (5.4).

In zero field the convergence of the sum (5.4) is fast, such that the arctan functions can be expanded in powers of $(m\pm 1)/\Lambda_c$. The linear term contributes as $T^{1/2}$ and all other terms contribute with a higher power of the temperature. The result is

$$T^{1/2}\frac{4}{\pi}\sum_{m=1}^{n_0}\ln\left[1+\frac{1}{m(m+2)}\right][m\ln(m+1)]^{1/2}\simeq 2.2T^{1/2}\,, \tag{5.5}$$

where the sum can be extended to ∞ and its numerical value is approximately 2.2.

The finite-field contribution is mainly determined by the larger m indices. We can then approximate $m\pm 1$ in the argument of the arctan by m and convert the sum into an integral. The leading-order contribution is given by

$$-\frac{8}{3\pi}X_0^2\frac{2}{T\ln(n_c)}\int_0^1 dx\, x\arctan(x)$$
$$=-\frac{8}{3\pi}X_0^2\frac{0.57}{T}\left[\frac{1}{\ln(1/T)}+\frac{\ln\ln(1/T)}{\ln^2(1/T)}+\cdots\right]. \tag{5.6}$$

(b) Since η_m in the integrand is independent of Λ, the integrals are straightforward and we obtain

$$2\sum_{m=n_c}^{\infty}\ln(1+\eta_m^{-1})=2\ln\frac{\sinh[(n_c+1)X_0]}{\sinh(n_cX_0)}\,. \tag{5.7}$$

Expanding for small X_0 the expression reduces to

$$2\left[\ln\left[\frac{n_c+1}{n_c}\right]+\frac{2n_c+1}{3}X_0^2\right]\simeq\frac{2}{n_c}+\tfrac{4}{3}n_cX_0^2\,. \tag{5.8}$$

Note that the field-independent term is of order T and hence of higher order than (5.5). The field-dependent term is of the same type as (5.6) and hence of leading order.

Collecting (5.5), (5.6), and (5.8), and using (5.1) inserted into (2.6), we have, for the leading order of the free energy,

$$F=-1.1T^{3/2}|J|^{-1/2}$$
$$-0.42|J|\frac{H^2}{T^2}\left[\frac{1}{\ln(1/T)}+\frac{\ln\ln(1/T)}{\ln^2(1/T)}+\cdots\right]. \tag{5.9}$$

This has the same functional dependence on T as our numerical results discussed in Secs. III and IV. Even the amplitudes agree remarkably well with those obtained numerically.

The above results were obtained by integrating over the free-spin regime on the right-hand side of (5.1). If we assume that the free-spin solution in part (a) is valid only for $|\Lambda|>a\Lambda_c$, $n<an_c$, and the one in part (b) for $n\geq an_c$, where $a\geq 1$, the temperature dependence of our results remains unchanged, and only the amplitudes are rescaled. We have assumed in our calculation that the crossover from strong coupling to free spin is abrupt. Since all terms on the right-hand side of (5.1) are positive, a smooth crossover region cannot modify our conclusions.

VI. CONCLUSIONS

In this paper we gave a detailed description of our numerical procedure for the solution of the thermodynamic Bethe-ansatz equations for the Heisenberg chain. The data were presented in a previous paper[9] and are in good agreement with later results by Takahashi and Yamada[10] for the same temperature range. We discussed the truncation of the infinite set of nonlinear integral equations and the extrapolation procedure for $n_0\to\infty$. In our previous paper we assumed a power-law dependence on T for the entropy and the susceptibility and obtained $\alpha=-0.49\pm0.02$ and $\eta=2.00\pm0.02$.

In Sec. II we obtained the correlation length by equating the strong-coupling and free-spin solutions of the system of equations. We obtained $\nu=1$ with logarithmic corrections given by (2.10). From our finite-string-size analysis of the susceptibility data we found that this logarithmic dependence cannot be ignored. The results for the susceptibility are consistent with $\gamma=2$ and logarithmic corrections. These logarithmic corrections indicate the existence of a marginal variable, which is not present in the classical solution. The logarithmic corrections are also very suggestive in view of the analogy between the thermodynamic Bethe-ansatz equations of the Heisenberg chain and the Kondo problem.[12] For the exchange model with $S=\frac{1}{2}$ the Kondo logarithms appear in the high-T expansion and for $S>\frac{1}{2}$ in both the high- and low-T series.[12]

In Sec. V we obtained analytic expressions for the zero-field free energy and the susceptibility. The calculation is based on the strong-coupling and free-spin solutions of the integral equations. The leading term for the free energy is $T^{3/2}$, i.e., $\alpha=-\frac{1}{2}$, while for χ we obtain again $\gamma=2$ with logarithmic corrections. The leading zero-field dependence of the free energy is a rigorous result; it depends neither on the logarithms in the correlation length nor on the cutoff of the sum. The absence of logarithms is confirmed by the relatively weak finite-string-size dependence of S. Note that the $T^{3/2}$ arises from the large $|\Lambda|$ values on the right-hand side of (5.1). Large $|\Lambda|$ corresponds to small momenta, such that the result is indeed due to long-wavelength magnons. The amplitude of the $T^{3/2}$ term is the same as for spin waves.[10]

The situation is more complicated for the susceptibility, since strings of all orders contribute. The logarithmic corrections in χ arise from those in the correlation length and depend, hence, on the temperature dependence of the cutoff in the sums (5.5) and (5.7). The result, however, strongly suggests the existence of logarithmic corrections, in agreement with the numerical data and the analogy with the Kondo problem.

Note added in proof. In a recent paper M. Marcu, J. Müller, and F. K. Schmatzer [J. Phys. A 18, 3189 (1985)] obtained $\alpha=-0.261\pm0.013$ and $\gamma=1.552\pm0.008$ by Monte Carlo simulations. Their data are restricted to temperatures higher than $0.06|J|$.

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