Critical Behavior of the Isotropic Ferromagnetic Quantum Heisenberg Chain

P. Schlottmann
Institut für Festkörperforschung, Kernforschungsanlage Jülich, D-5170 Jülich, West Germany
(Received 26 November 1984)

The thermodynamic Bethe-*Ansatz* equations for the isotropic ferromagnetic $S=\frac{1}{2}$ Heisenberg chain have been solved numerically. At low temperatures, I find a power-law dependence on T for the specific heat and the susceptibility with critical exponents $\alpha=-0.49\pm0.02$, $\gamma=2.00\pm0.02$, and $\Delta\simeq\gamma$. The exponent α is compatible with effective spin waves and γ and Δ are the exponents of the classical chain. Amplitudes and corrections to scaling are obtained and differences with previous results are discussed.

PACS numbers: 75.40.Fa, 05.70.Jk, 75.10.Jm

I consider the isotropic quantum Heisenberg chain ($S=\frac{1}{2}$)

$$\mathscr{H}=J\sum_{i=1}^{N}\mathbf{S}_i\cdot\mathbf{S}_{i+1}-\frac{J}{4}N+2H\sum_{i=1}^{N}S_i^z, \qquad (1)$$

with N sites and periodic boundary conditions in the limit $N\to\infty$. For ferromagnetic coupling ($J<0$) the model has a zero-temperature critical point, i.e., the ground state is ferromagnetically ordered, but there is no long-range order at any finite temperature.

The critical behavior of the ferromagnetic $S=\frac{1}{2}$ Heisenberg chain has been investigated previously by several authors: Bonner and Fisher[1] studied the thermodynamic properties of rings of size up to $N=11$ and obtained $-\alpha\simeq0.45$–0.50 and $\gamma\simeq1.8$; Baker, Rushbrooke, and Gilbert[2] computed the high-temperature series expansion and analyzed the energy and magnetic susceptibility by means of Padé approximants ($\gamma=1.66\pm0.07$); and Cullen and Landau[3] ($\gamma\simeq1.32$) and Lyklema[4,5] [$-\alpha=0.3\pm0.1$, $\gamma=1.75\pm0.02$, $(\gamma-1)/\nu=1.01\pm0.01$] performed Monte Carlo simulations for the problem.

The above results indicate that γ differs from the classical analog, $\gamma_{\rm cl}=2$, and Lyklema's Monte Carlo data exclude $\alpha=-0.5$, the value expected from spin waves. These interesting results lead me to reanalyze the critical behavior of the ferromagnetic chain by a different method, namely, the numerical solution of the thermodynamic Bethe-*Ansatz* equations.[6,7] In contrast to other methods, the Bethe-*Ansatz* provides the exact solution of the problem.

On the basis of Bethe's famous work,[8] Takahashi[6] and Gaudin[7] derived the thermodynamic Bethe-*Ansatz* equations. They consist of an infinite set of nonlinearly coupled integral equations for functions $\eta_n(\Lambda)$, which characterize the string excitations of order n with real rapidity Λ. 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

$$\ln\eta_n=G*\ln[(1+\eta_{n-1})(1+\eta_{n+1})]-2\pi\,\delta_{n,1}(J/T)G,\quad n=1,2,\ldots,\quad \eta_0=0, \qquad (2)$$

where the center star denotes a convolution and

$$G(\Lambda)=[4\cosh(\tfrac{1}{2}\pi\Lambda)]^{-1}. \qquad (3)$$

These equations are completed by the asymptotic condition

$$\lim_{n\to\infty}n^{-1}\ln\eta_n(\Lambda)=H/T=x_0>0, \qquad (4)$$

and the free energy of the model is given by

$$F=-J\ln2-T\int d\Lambda\,G(\Lambda)\ln(1+\eta_1). \qquad (5)$$

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.[6] In the critical region the solution is an interpolation between these free-spin and zero-temperature limits. For a very large string index n the free-spin solution

$$\eta_n=\{\sinh[(n+1)x_0]/\sinh x_0\}^2-1 \qquad (6)$$

is reached, as a consequence of the asymptotic condition (4). Expression (6) is also reached for small n and sufficiently large rapidity values, Λ, since the driving term decreases exponentially with Λ. On the other hand, the small-index and small-Λ regime, where the driving term is most effective, is determined by the strong-coupling solution. The index n and the value of Λ at which the crossover between the $T=0$ and the free-spin solutions takes place are a function of T.

The lower the temperature, the more integral equations are needed in order to reach the free-spin solution (6) within a given accuracy. In principle, an infinite number of integral equations should be considered in the critical regime. My procedure to solve the infinite set of integral equations is the following. I chose an index n_0 and replaced η_n for $n>n_0$ by the asymptotical expression (6), and then solved numerically the system of n_0 integral equations. The procedure is repeated for several n_0 and the result extrapolated to $n_0 \to \infty$. For the lowest temperatures, I considered n_0 up to 280.

The integration interval for the convolution is in principle the entire real axis. The integration, however, simplifies as a result of the exponential decrease of the kernel. For large Λ, the function η_n approaches the asymptotic expression (6) such that we can replace η_n by (6) for $|\Lambda| > \Lambda_0$. The range for Λ_0 depends strongly on the temperature and on the n_0 considered. The results are then extrapolated to $\Lambda_0 \to \infty$. At very low T and large n_0 I considered Λ_0 up to 150.

The set of integral equations has been solved iteratively, the convergence being slow for large n_0. The data were analyzed as a function of the number of iterations and extrapolated to obtain the converged solution.

We determine α from the entropy, S, which in the critical region depends on temperature as $T^{-\alpha}$ and is obtained by numerical differentiation of the free energy. It is easily seen that the slope in Fig. 1, which determines α, depends on the temperature. This is explicitly shown in the inset, where the slope is plotted between neighboring points as a function of the mean temperature T. The extrapolation to $T=0$ leads to the value

$$\alpha = -0.49 \pm 0.02,$$

which is in good agreement with the finite-size extrapolation of Bonner and Fisher[1] ($-\alpha \simeq 0.45$–0.50) and with the free-magnon result $\alpha = -0.5$. The Monte Carlo[4] value $\alpha = -0.3 \pm 0.1$ was obtained in the temperature range between 0.025 and 0.1 and not from the asymptotic scaling region.

For the rest of the paper we *assume* that $\alpha = -0.5$. Plotting $ST^{-1/2}$ as a function of T we obtain, extrapolating to $T=0$, that the amplitude of the leading power is 1.50 ± 0.03. The correction to scaling can also be obtained from this plot by consideration of the slope between neighboring points, i.e., $\Delta(ST^{-1/2})/\Delta T$, where Δ denotes increment. This is shown in Fig. 2, where the slope at low temperatures determines the exponent of the first correction to scaling, $\omega = 0.5 \pm 0.1$. The amplitude of this correction to scaling is also obtained from Fig. 2, being 1 if $\omega = 0.5$, 1.75 if $\omega = 0.4$, and 0.56 if $\omega = 0.6$. The most probable expression for the critical behavior of the entropy is then

$$S = \tfrac{3}{2} T^{1/2}(1 - T^{1/2} + \dots), \tag{7}$$

which is displayed by the solid line in Fig. 1. The small discrepancy at low T is attributed to the next scaling correction, which is expected to be linear in T. If we assume a correction of $+2T$ the curve lies on top of the low-T points.

In the critical region the susceptibility diverges with a power law of the temperature, $\chi \sim T^{-\gamma}$. The present data for diverging quantities are less accurate than for the entropy. I calculated χ by numerical differentiation of the free energy with respect to the magnetic field. In Fig. 3, the open triangles represent the Bethe-*Ansatz* data, while the dots correspond to Lyklema's[4,5] Monte Carlo simulation. The agreement between the two methods is excellent (filled triangles).

Again the slope in Fig. 3 is a function of T. This is explicitly shown in the inset, where the slopes between points are plotted against the mean T. There are two regions: For $T < 0.02$ the slope decreases rapidly, but for $T > 0.02$ the slope is approximately $\gamma \simeq 1.7$–1.8. The previous calculations[1-5] refer to the latter temperature range. The extrapolation to $T=0$ depends on the power of the correction to scaling. From previous arguments, as in the paper by Aharony and Fisher,[9] one expects a correction to scaling linear in T. The extrapolated critical exponent is then

$$\gamma = 2.00 \pm 0.02,$$

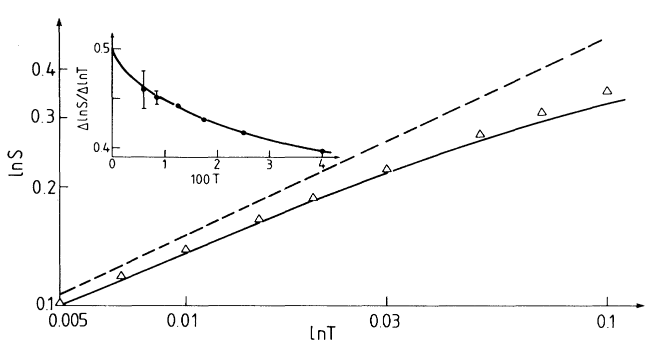

FIG. 1. Data points for the logarithm of the entropy vs $\ln T$. The slope is temperature dependent, as shown in the inset. The full line corresponds to Eq. (7), while the dashed line represents the leading power, $S = 1.5T^{1/2}$. A better fit can be obtained by adjustment of the amplitudes; however, higher-order scaling corrections have been omitted. The curve in the inset is just a guide to the eyes.

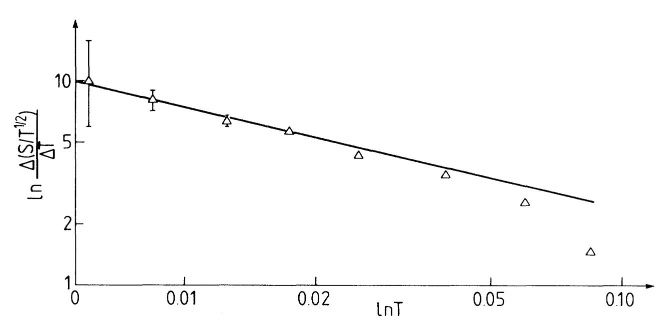

FIG. 2. Logarithm of the variation of $ST^{-1/2}$ with temperature vs $\ln T$. The slope at low T yields the power of the first correction of scaling. The line corresponds to a slope of 0.5.

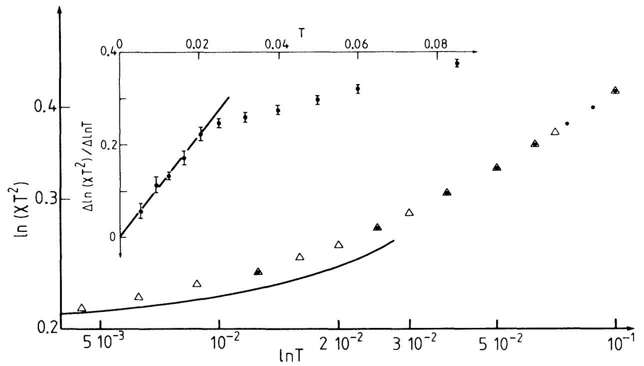

FIG. 3. Logarithm of $T^2\chi$ vs $\ln T$. The open triangles are the solutions of the Bethe-*Ansatz* equations which agree excellently with Lyklema's (Ref. 4) Monte Carlo data represented by the dots (the filled triangles are open triangles plus dot). The curve represents Eq. (8). The slope is a function of T as shown in the inset. The solid line in the inset is only a guide to the eyes.

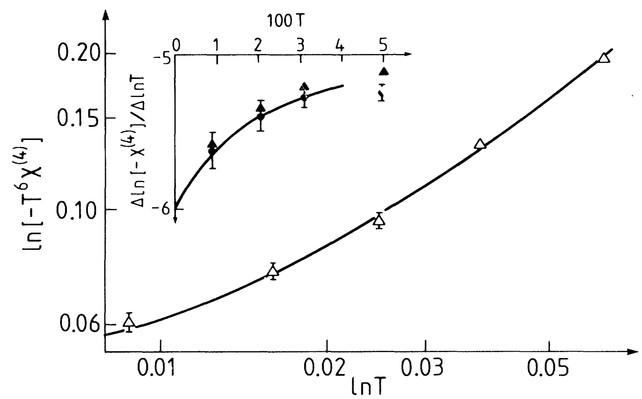

FIG. 4. Logarithm of T^6 times the fourth-order field susceptibility as a function of $\ln T$. The slope between neighboring points is shown in the inset (dots, with error bar). The filled triangles correspond to 3 times the slope in Fig. 3 for the same temperatures. The plot suggests $\Delta \simeq \gamma$. The lines are only guides to the eyes.

i.e., the classical and quantum chains have the same exponent γ. The amplitude of the leading power is 0.202 ± 0.004 and the one of the correction to scaling, 11 ± 2. The curve in Fig. 3 represents

$$\chi T^2 = 0.2 + 2.2T. \tag{8}$$

Sources for the difference with the data points are the error in the amplitude to the correction and neglected higher-order corrections of the type $T^{3/2}$ and T^2.

The exponent Δ characterizes the critical behavior of higher field derivatives. It is substantially more difficult to obtain Δ than γ. The fourth field derivative, $\chi^{(4)} \sim T^{-2\Delta-\gamma}$, is shown in Fig. 4. Again, the slope of the plot is temperature dependent. This is explicitly seen in the inset, where slopes between neighboring points are compared with $3\Delta \ln(T^2\chi)/\Delta \ln T$ for the same temperatures. Within the numerical accuracy the value for Δ reached asymptotically as $T \to 0$ is then $\Delta = \gamma$.

The relations among the critical exponents for a zero-temperature critical point are different from the usual ones where $T_c \neq 0$. Using the scaling and hyperscaling assumptions, Baker and Bonner[10] stated for $T_c = 0$ that (i)

$$\gamma = 1 + (2-\eta)\nu,$$

(ii)

$$\delta = \Delta/(\Delta - \gamma),$$

(iii)

$$\Delta = \tfrac{1}{2}(d\nu + \gamma + 1),$$

(iv)

$$-\alpha_s = d\nu.$$

Since in the ground state of the ferromagnetic Heisenberg chain all spins are aligned, the spin-spin correlation function is independent of the distance, $\eta = 1$, and the magnetization is independent of the field, $\delta = \infty$. Relations (i)–(iii) then yield the exponent of the correlation length $\nu = \gamma - 1 = 1.00 \pm 0.02$ and $\Delta = \gamma$. The latter one confirms our extrapolation to $T = 0$ in Fig. 4. The relation $(\gamma - 1)/\nu = 1$ has been obtained by Lyklema[4] by means of a finite-size scaling analysis of his Monte Carlo data.

The relation (iv), however, is not satisfied. The breakdown of this scaling relation for a zero-temperature critical point has been found previously, e.g., the classical Heisenberg chain.

Hence, the critical exponents of the classical and quantum Heisenberg chains are the same, except for the specific heat. This is then similar (except for α) to systems with $T_c \neq 0$, where quantal effects implied by finite spin values do not seem to affect the critical exponents.[11] This is especially remarkable since for $S = \frac{1}{2}$ and $d = 1$ quantum fluctuations are expected to be the largest. The amplitude of the susceptibility in the quantum case is, however, 7.5 times smaller than that for the classical chain and the ones of the correction to scaling have opposite signs. The specific heat of the classical chain is[12]

$$C_{\text{cl}} = 1 - (\beta J)^2/\sinh^2(\beta J),$$

which yields $\alpha = 0$ and $\alpha_s = -\infty$. Here the behavior of the classical and quantum chains is qualitatively different. Although a naive spin-wave picture is not valid,[13] the exponent $\alpha = -0.5$ of the quantum chain supports the description of the low-T low-energy excitations in terms of effective spin waves.

To my knowledge, this is the first example of critical behavior of a quantum system extracted from the thermodynamic Bethe *Ansatz*. The strength of the method is that it provides exact results in a temperature regime so far not accessible by other methods.

The author is indebted to J. W. Lyklema for innumerable helpful and stimulating discussions, and acknowledges receipt of a Deutsche Forschungsgemeinschaft Heisenberg fellowship.

---

[1]J. C. Bonner and M. E. Fisher, Phys. Rev. **135**, A640 (1964).

[2]G. A. Baker, Jr., G. S. Rushbrooke, and H. E. Gilbert, Phys. Rev. **135**, A1272 (1964).

[3]J. J. Cullen and D. P. Landau, Bull. Am. Phys. Soc. **24**, 361 (1979), and **26**, 576 (1981).

[4]J. W. Lyklema, Phys. Rev. B **27**, 3108 (1983).

[5]J. W. Lyklema, in *Monte Carlo Methods in Quantum Problems,* edited by M. H. Kalos (Reidel, Dordrecht, 1984), p. 145.

[6]M. Takahashi, Prog. Theor. Phys. **46**, 401 (1971).

[7]M. Gaudin, Phys. Rev. Lett. **26**, 1301 (1971).

[8]H. A. Bethe, Z. Phys. **71**, 205 (1931).

[9]A. Aharony and M. Fisher, Phys. Rev. B **27**, 4394 (1983).

[10]G. A. Baker and J. C. Bonner, Phys. Rev. B **12**, 3741 (1975).

[11]M. E. Fisher, Rev. Mod. Phys. **46**, 597 (1974).

[12]H. E. Stanley, Phys. Rev. **179**, 570 (1969).

[13]Note that the functions $\eta_n(\Lambda)$ are associated with the density of bound states of n magnons.