Susceptibility of the Spin 1/2 Heisenberg Antiferromagnetic Chain

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Highly accurate results are presented for the susceptibility $\chi(T)$ of the $s = 1/2$ Heisenberg antiferromagnetic chain for all temperatures, using the Bethe ansatz and field theory methods. After going through a rounded peak, $\chi(T)$ approaches its asympotic zero-temperature value with infinite slope.

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In a pioneering work in 1964, Bonner and Fisher estimated numerically [1] the susceptibility $\chi(T)$ for the $s = 1/2$ Heisenberg antiferromagnetic chain, using chain lengths of up to 11. The exact value at $T = 0$ was obtained using the Bethe ansatz in Ref. [2] and more rigorously in Ref. [3]. Since that time, the Bonner-Fisher curve has frequently been used by experimentalists to determine the value of the exchange coupling J and to determine whether or not a given material has sufficiently small anisotropic exchange and interchain couplings to be approximated by this model. Recently it has become possible to calculate this curve much more accurately, using the Bethe ansatz [4]. This method easily gives very accurate results for T not too small, but becomes increasingly difficult as $T \to 0$. On the other hand, an analytic formula can be derived for $\chi(T)$ at small T, from conformal field theory methods. Perhaps surprisingly, this formula predicts, due to the marginally irrelevant operator, that the susceptibility has infinite slope at $T = 0$. Here we present results for $\chi(T)$ obtained using the Bethe ansatz for $T \geq 0.003J$ and compare them to the conformal field theory prediction, obtaining excellent agreement. The field theory prediction for the general xxz model is also given. Figure 1 shows the susceptibility obtained from the Bethe ansatz and Fig. 2 compares this result to the field theory prediction at low T. Note that, with decreasing T, after passing through the maximum, $\chi \approx 0.147/J$, at $T \approx 0.640\,824J$, the slope of χ starts to *increase* below the inflection point at $T \approx 0.087J$, approaching ∞ as $T \to 0$.

The Heisenberg Hamiltonian is written

$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}. \tag{1}$$

The susceptibility per site is given by

$$\chi(T) \equiv \frac{1}{T} \sum_i \langle S_i^z S_0^z \rangle. \tag{2}$$

The low energy effective field theory description [5] is given by the $k = 1$ Wess-Zumino-Witten (WZW) nonlinear σ model, or equivalently a free, massless boson, with an effective "velocity of light" or spin-wave velocity:

$$v = \pi J/2. \tag{3}$$

This value of v is determined from the slope of the dispersion relation obtained from the Bethe ansatz. The uniform part of the spin density is given by the conserved

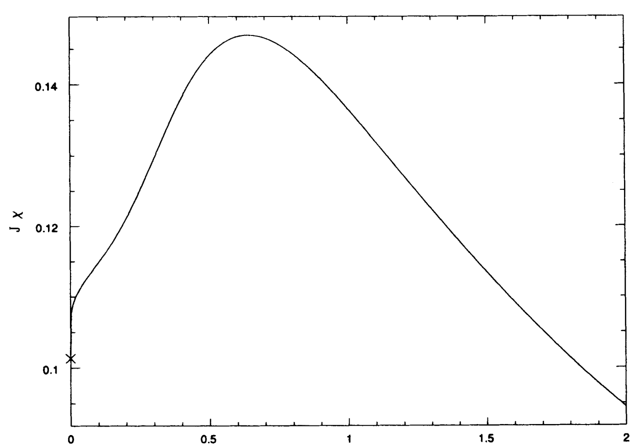

FIG. 1. $\chi(T)$ from the Bethe ansatz. $\chi(0)$ is taken from Ref. [2].

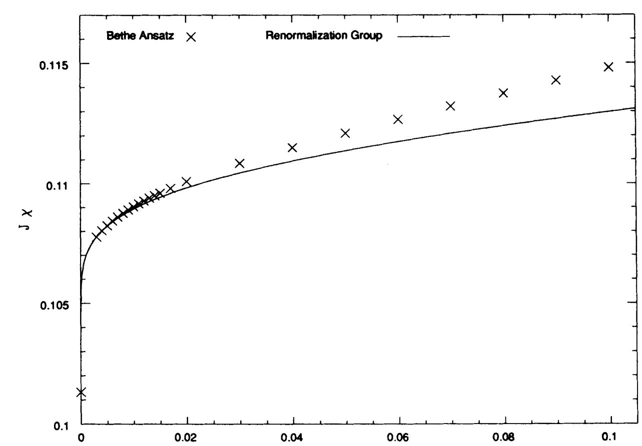

FIG. 2. Field theory [Eq. (14)] versus Bethe ansatz formulas for $\chi(T)$ at low temperature.

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current operators $\vec{J}_L$, $\vec{J}_R$ for left and right movers:

$$\vec{S}_i \approx \vec{J}_L(x_i) + \vec{J}_R(x_i). \tag{4}$$

In the WZW model $\vec{J}_L$ and $\vec{J}_R$ are uncorrelated and their self-correlations are given by

$$\langle J_L^a(\tau,x) J_L^b(0,0)\rangle = \frac{\delta^{ab}}{8\pi^2(v\tau - ix)^2},$$
$$\langle J_R^a(\tau,x) J_R^b(0,0)\rangle = \frac{\delta^{ab}}{8\pi^2(v\tau + ix)^2}. \tag{5}$$

This result can be extended to finite temperature by a conformal transformation. This simply replaces

$$v\tau \mp ix \rightarrow \frac{v\beta}{\pi}\sin\left[\frac{(v\tau \mp ix)\pi}{v\beta}\right], \tag{6}$$

where $\beta \equiv 1/T$.

The susceptibility in the WZW model is thus given by [6]

$$\chi = \frac{\beta}{8\pi^2}\int_{-\infty}^{\infty} dx \left\{\left[\frac{v\beta}{\pi}\sin\left(\frac{(v\tau+ix)\pi}{v\beta}\right)\right]^{-2} + \left[\frac{v\beta}{\pi}\sin\left(\frac{(v\tau-ix)\pi}{v\beta}\right)\right]^{-2}\right\}. \tag{7}$$

The integral can be done by the change of variables: $u = \tan\frac{\tau\pi}{\beta}$ and $w = -i\tan\frac{ix\pi}{v\beta}$, giving

$$\chi = \frac{1}{8\pi^2 v}2\pi(1+u^2)\int_{-1}^{1}\frac{dw}{(u+iw)^2} = \frac{1}{2\pi v}. \tag{8}$$

Note that the integral is independent of τ or u as it should be since the total spin is conserved. Plugging in the spin-wave velocity, $v = J\pi/2$, gives the zero-temperature susceptibility, $\chi(0) = 1/J\pi^2$.

The fact that $\chi(T)$ is independent of T in the WZW model follows from scale invariance. To obtain the leading T dependence, we must perturb about the scale invariant fixed point Hamiltonian with the leading irrelevant operator. This perturbation is written

$$\delta\mathcal{H} = \frac{-8\pi^2 v}{\sqrt{3}} g\vec{J}_L\cdot\vec{J}_R. \tag{9}$$

This term is marginally irrelevant for the coupling constant, $g > 0$. We wish to calculate the correction to $\chi(T)$ to first order in $\delta\mathcal{H}$. Expanding $e^{-\int dx d\tau \delta\mathcal{H}(\tau,x)}$ to first order the correction to χ involves four current operators. Because of the fact that the left and right currents are uncorrelated, this expression factorizes into a product of two two-point Green's functions, one for left movers and one for right movers. Using translational invariance, the spatial integrals factorize into two independent integrals of the form of Eq. (8), giving

$$\chi = \frac{1}{2\pi v} + \frac{g}{v\sqrt{3}}. \tag{10}$$

Again, the correction is naively temperature independent, since g is dimensionless. However, this formula can be improved by replacing g by $g(T)$, the effective renormalized coupling at temperature T. By integrating the lowest order β function, $g(T)$ is given by [7]

$$g(T) \approx \frac{g_1}{1 + 4\pi g_1 \ln(T_1/T)/\sqrt{3}}. \tag{11}$$

Here g_1 is the value of the effective coupling at some temperature T_1. Both g_1 and $g(T)$ must be small for this formula to be valid. We may write this more compactly as

$$g(T) \approx \frac{\sqrt{3}}{4\pi\ln(T_0/T)} \tag{12}$$

for some temperature T_0. Note that the asympotic behavior at small T becomes independent of g_1 or T_0 up to a correction of $O((\ln T)^{-2})$. We expect higher order corrections to $\chi(T)$ of $O(g(T)^2)$, $O(g(T)^3)$, etc. By shifting T_0, we can eliminate the $O((\ln T)^{-2})$ part of the $O(g(T)^2)$ correction. Thus we obtain the leading T dependence of χ:

$$\chi(T) = \frac{1}{2\pi v} + \frac{1}{4\pi v\ln(T_0/T)} + O((\ln T)^{-3}). \tag{13}$$

This formula is universal in the sense that if we add additional interactions to the Heisenberg Hamiltonian that respect the SU(2) and translational symmetry and are not sufficiently large as to drive it into another phase, then this formula applies for some values of v and T_0. In particular, if we add an antiferromagnetic second nearest neighbor interaction, J_2, the value of the bare coupling, g_1, decreases and reaches zero at $J_2 \approx 0.24J$. At this point all logarithmic terms in $\chi(T)$ vanish, corresponding to $T_0 \rightarrow \infty$ and $\chi(T)$ should be analytic near $T = 0$. For larger J_2 the system develops a gap and $\chi(T)$ vanishes exponentially as $T \rightarrow 0$. Equation (13) should be valid for arbitrary half-integer spin Heisenberg antiferromagnets. For the ordinary $s = 1/2$ Heisenberg model, $v = J\pi/2$, giving

$$J\pi^2\chi(T) \approx 1 + \frac{1}{2\ln(T_0/T)}. \tag{14}$$

A good fit to the Bethe ansatz data is obtained with $T_0 \approx 7.7J$, as shown in Fig. 2. Equation (14) is valid to within 2% for $T < 0.1J$. Similar formulas for the finite-size dependent low energy states were obtained in Ref. [7] with T_0/T replaced by L/L_0 where L is the size of the system. The role of infrared cutoff on the renormalization of the coupling constant is played by either the length L or an effective thermal length v/T in the two cases. Note that the field theory calculation of the susceptibility is done in the limit $LT/v \to \infty$ whereas the finite-size spectrum calculations are done in the opposite limit $LT/v \to 0$. In both cases the space–imaginary-time surface is an infinite length cylinder of circumference v/T or L, respectively. (We only expect the susceptibility to be given correctly by a finite-size calculation, such as that of Bonner and Fisher, down to temperatures $T \approx v/L$.) By pushing all calculations to second order in g, predictions could be made relating the various values of the L_0's for different energy levels and T_0. Alternatively, we may use the deviation of $\chi(T)$ and the energy levels from their asymptotic values to define four different estimates of the effective coupling constant versus length. These are shown in Fig. 3. The singlet and triplet excited state estimates of the effective coupling, $g(L)$, only converge very slowly as $g(L)^2$, as we expect since, in general, all these quantities receive corrections at next order in g. Surprisingly, the susceptibility and triplet estimates of g, using the relationship $L \leftrightarrow v/T$, appear to converge much more rapidly as $1/L^2$, suggesting the absence of corrections to any finite order in $g(L)$. (The ground state and triplet estimates appear to converge rapidly to a small nonzero difference. This remains a puzzling discrepancy between conformal field theory and Bethe ansatz calculations. See Ref. [8] for further discussion.)

We now consider the general xxz model:

$$H = J\sum_i \left[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z\right]. \tag{15}$$

For $\Delta > 1$, the Hamiltonian has a Néel ordered ground state and a gap. Hence the susceptibility vanishes exponentially at low T. For $\Delta < 1$, the system remains gapless. It is now convenient to use Abelian bosonization,

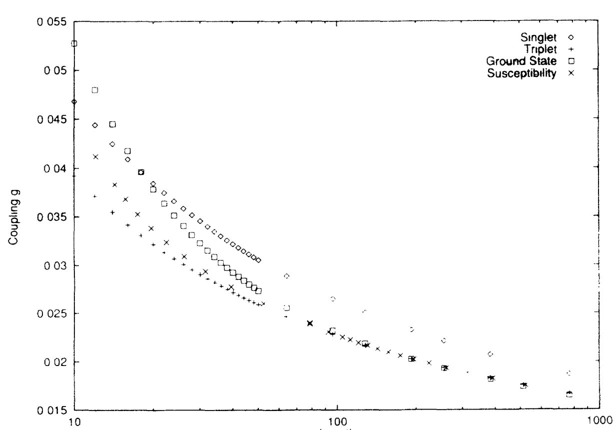

FIG. 3. Estimates of the effective coupling from lowest order perturbation theory correction to finite-size energy of ground state, first excited triplet state, first excited singlet state [7], and to susceptibility, using $L \leftrightarrow v/T$. The renormalization group prediction of Eq. (12) is also shown.

involving a free boson ϕ. The zz component becomes

$$J_L^z J_R^z = \frac{1}{4\pi}\left[\left(\frac{1}{v}\frac{\partial\phi}{\partial t}\right)^2 - \left(\frac{\partial\phi}{\partial x}\right)^2\right]. \tag{16}$$

The other components of the interaction become

$$J_L^x J_R^x + J_L^y J_R^y \propto \cos\sqrt{8\pi}\phi. \tag{17}$$

The zz part is exactly marginal and has the effect of rescaling the boson [5]:

$$\phi \to \frac{\phi}{\sqrt{2\pi}R}, \tag{18}$$

with $R < 1/\sqrt{2\pi}$. The other part then becomes

$$J_L^x J_R^x + J_L^y J_R^y \propto \cos(2\phi/R). \tag{19}$$

This has scaling dimension

$$x = 1/\pi R^2 > 2 \tag{20}$$

and is irrelevant. It is the leading irrelevant operator, provided $x < 4$. A renormalization of the velocity also occurs. The zero-temperature susceptibility gets rescaled to [6]

$$\chi(0) = \frac{1}{v(2\pi R)^2}. \tag{21}$$

The first order contribution to the susceptibility from $\cos(2\phi/R)$ vanishes. The second order contribution is determined by a standard scaling argument, giving

$$\chi(T) \to \frac{1}{v(2\pi R)^2} + \text{const} \times T^{(2/\pi R^2 - 4)}. \tag{22}$$

Again this formula is universal in the sense that the two parameters v and R determine all low energy features of the model for $R < 1/\sqrt{2\pi}$. Increasing anisotropy leads to decreasing R. Equation (22) should apply for arbitrary half-integer spin xxz antiferromagnets in the gapless phase, provided that $1/\pi R^2 < 3$. Otherwise, the exponent is replaced by 2. For the $s = 1/2$ Heisenberg model $R(\Delta)$ and $v(\Delta)$ have been determined from the Bethe ansatz [5,9–11]. Letting

$$\Delta = \cos\theta \tag{23}$$

we find

$$\sqrt{2\pi}R(\Delta) = \sqrt{1 - \frac{\theta}{\pi}},$$
$$v(\Delta) = \frac{J\pi\sin\theta}{2\theta}. \tag{24}$$

Thus

$$\chi(0) = \frac{\theta}{\pi(\pi - \theta)\sin\theta} \tag{25}$$

(in agreement with the explicit Bethe ansatz calculation [3]) and the exponent is given by

$$2/\pi R^2 - 4 = \frac{4\theta}{\pi - \theta}. \tag{26}$$

For small anisotropy,

$$2/\pi R^2 - 4 \approx \frac{4\sqrt{2(1-\Delta)}}{\pi}. \tag{27}$$

$\chi(T)$ has an infinite slope at $T = 0$ for $\Delta > \cos^{-1}(\pi/5) \approx 0.809$. For $\Delta < 0.5$, the exponent $(2\pi/R^2 - 4)$ is replaced by 2.

These results may prove useful in experimental studies of quasi-one-dimensional antiferromagnets. In particular, we may define a "critical region" where the temperature dependence is governed by the leading irrelevant operator so that Eq. (13) or Eq. (22) holds. For the isotropic Heisenberg model, this critical region can be identified approximately as $T < 0.1J$, below the inflection point. Only if the Néel temperature, determined by interchain couplings, is below this value can the one-dimensional critical behavior be observed.

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