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LETTER TO THE EDITOR

Susceptibility of the spin-S Heisenberg antiferromagnetic chain

P D Sacramento

Centro de Física da Matéria Condensada, Av Professor Gama Pinto, 2, 1699 Lisboa Codex, Portugal

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Abstract. The numerical solution of the low-temperature behaviour of the susceptibility of the spin-S antiferromagnetic chain is presented starting from the exact thermodynamic Bethe *ansatz* equations for the Takhtajan–Babujian model. It is found that the susceptibility for the several values of S tends to its zero-T value with infinite slope, extending previous results obtained by Eggert *et al* for the $S = \frac{1}{2}$ case.

Low-dimensional systems have attracted considerable interest. In particular, many authors have extensively studied the Heisenberg model and in general quantum spin systems. Recently, Eggert *et al* [1] presented results for the low-T dependence of the susceptibility of the $S = \frac{1}{2}$ Heisenberg antiferromagnetic chain. As T is lowered, the susceptibility goes through a maximum [2, 3] and as $T \to 0$ the susceptibility approaches its zero-T finite value with infinite slope. These results were obtained both from conformal field theory and from the numerical solution of the Bethe *ansatz* equations. They predicted that [1]

$$\chi(T) \sim \frac{1}{2\pi v} + \frac{1}{4\pi v \ln(T_0/T)} \tag{1}$$

where v is the spin-wave velocity and T_0 some temperature, perturbing about the scale invariant fixed-point Hamiltonian with the leading irrelevant operator. This equation is expected to hold for arbitrary half-integer spin Heisenberg antiferromagnets. For the ordinary $S = \frac{1}{2}$ Heisenberg model, the spin-wave velocity is $v = (J\pi/2)$, yielding (with $J = 1$)

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

The zero-T term coincides with the exact analytical result, obtained previously from the Bethe *ansatz* [4, 5]. These authors [1] found a very good agreement between equation (2) and the numerical Bethe *ansatz* results for $S = \frac{1}{2}$ (within two percent for $T < 0.1$ and $T > 0.003$, since at very low T the numerical method becomes very difficult).

In this letter we consider the spin-S Takhtajan–Babujian model [6, 7] and show that for higher spin values the susceptibility also appears (within the numerical accuracy) to have an infinite slope as $T \to 0$. This result holds irrespective of the spin value being integer or half-integer. The straightforward extension of the Heisenberg chain to spin values larger than $\frac{1}{2}$ is not integrable. However, an integrable $SU(2)$-invariant generalization of the

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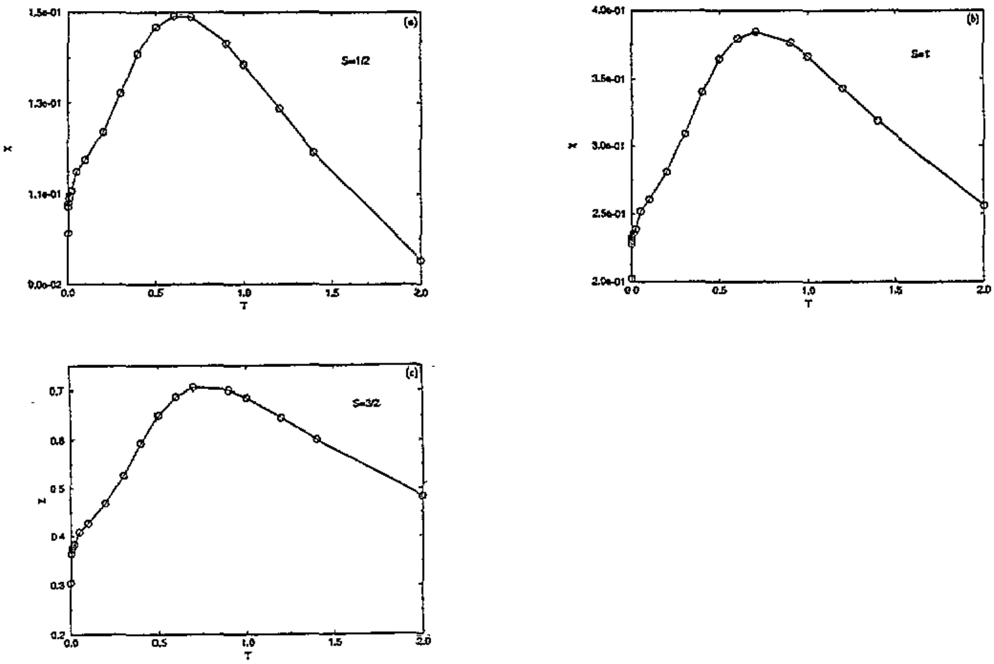

Figure 1. Susceptibility versus T for (a) $S = \frac{1}{2}$ (b) $S = 1$ and (c) $S = \frac{3}{2}$, respectively. The circles are the Bethe *ansatz* results. The zero-T analytical results have been added. The solid lines are just guides to the eye.

Heisenberg chain of arbitrary spin S has been diagonalized. This generalization of the standard Heisenberg model (Takhtajan–Babujian model [6, 7]) is given by

$$H = J\left(\sum_{i=1}^{N} Q_{2S}(S_i \cdot S_{i+1}) - E_{\text{vac}}\right) \tag{3}$$

where E_{vac} is such that the interaction energy is zero for the state with all spins S parallel, N is the number of lattice sites and Q_{2S} is a polynomial of order $2S$ such that the model is integrable [6, 7]. When $S = \frac{1}{2}$ this model reduces to the usual Heisenberg model for the same spin-value. The antiferromagnetic case is obtained taking $J = 1$.

The thermodynamics of model (3) can be obtained from the thermodynamic Bethe *ansatz* equations derived in [7]. They consist of an infinite set of non-linearly coupled integral equations for functions $\eta_k(\Lambda)$, which characterize the string excitations of order k with real rapidity Λ. A string excitation of order k represents a bound-magnon state of k magnons. A convenient representation of these integral equations is the recursion sequence

$$\begin{aligned}
\ln \eta_k(\Lambda) &= G * \ln[(1+\eta_{k-1})(1+\eta_{k+1})] - \frac{2\pi}{T}\delta_{k,2S}G(\lambda) \\
k &= 1, 2, 3, \ldots \\
\eta_0 &= 0
\end{aligned} \tag{4}$$

where the star denotes a convolution and $G^{-1}(\Lambda) = 4\cosh(\pi\Lambda/2)$. These equations are completed by the asymptotic condition $\lim_{k\to\infty}(1/k)\ln\eta_k(\Lambda) = (h/T)$, where h is the magnetic field. The free energy per site of the model is given by

$$F_{2S}(T) = F_{2S}(0) - T \int_{-\infty}^{\infty} \mathrm{d}\Lambda \; G(\Lambda) \ln[1 + \eta_{2S}(\Lambda)]. \tag{5}$$

Solving the set of equations (4) we can obtain the thermodynamics of the model by numerical differentiation of the free energy. The procedure to solve numerically these equations is standard [8, 3]. The infinite sequence is truncated at a finite value. Also, the range of the rapidities is truncated, introducing a cut-off. The accuracy of the method is controlled by varying these two parameters and the errors are estimated to be of the order of one percent. The zero-temperature zero-field susceptibility is finite and given by [7]

$$\chi(T = 0) = \frac{2S}{\pi^2}. \tag{6}$$

For $S = \frac{1}{2}$ this result reproduces equation (2). For $T > 0$ the numerical solution has to be used. The results that we obtain in the case of $S = \frac{1}{2}$ agree well with those of [1] (within one percent, from above). In figure 1 we show the susceptibility for the (a) $S = \frac{1}{2}$, (b) $S = 1$ and (c) $S = \frac{3}{2}$ chains, respectively. The behaviour for higher spin values is similar irrespective of being integer or half-integer (note that in the Takhtajan–Babujian model the spectrum is gapless for all spin values). The case for $S = \frac{1}{2}$ is presented to compare to the results of [1].

For all values of S the susceptibility goes through a maximum as a function of T [3]. In the figures we show the points obtained from the numerical solution of the Bethe *ansatz* equations and we have added the zero-T analytical result of equation (6). Comparing with the $S = \frac{1}{2}$ case ([1] or figure 1(a)) it is clear that the trend towards an infinite slope of the susceptibility as $T \to 0$ is maintained as the spin value increases. The curves for the three values of the spin are very similar in shape but they do not show universal behaviour rescaling by the zero-T value [3] in contrast with the Kondo model [9].

These results further extend the similarity between the various spin values in the Takhtajan–Babujian model [3]. The spin-$\frac{1}{2}$ case is equivalent to the $S = \frac{1}{2}$ Heisenberg model considered in [1].

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