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LETTER TO THE EDITOR

The longitudinal susceptibility of an XY spin-chain

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Abstract. A previously unsolved problem has been solved numerically using transfer matrix renormalization group analysis, based on a density matrix renormalization group idea. This calculation leads to a high-precision prediction of the value of susceptibility in the x- or y- directions of an XY spin-chain, because in the calculation the transfer matrix idea is incorporated and a thermodynamic limit is ensured. From this calculation the susceptibility at zero temperature is predicted for a spin-$\frac{1}{2}$ antiferromagnetic XY model in one dimension.

The study of quantum spin-chains is of growing interest in condensed matter physics. This is because exact solutions are comparatively easier in one dimension than in higher dimensions and the extensive availability of one dimensional compounds makes it possible to verify the theoretical predictions in real systems. The anisotropic spin-$\frac{1}{2}$ XY chain was solved by Lieb, Schultz and Mattis [1]. With the help of the Jordan–Wigner transformation they solved the Hamiltonian and calculated the ground state correlation functions. They also formulated the finite temperature correlation functions. Katsura [2] solved the anisotropic XY chain in the presence of a magnetic field in the z-direction using the Jordan–Wigner transformation and calculated the thermodynamic properties, e.g., the magnetic susceptibility in the z-direction and the specific heat. McCoy [3] calculated the zero and finite temperature correlation functions for different anisotropies in the large N limit. For finite temperatures, McCoy made high and low temperature expansions. Tonegawa [4] calculated analytically the correlation functions at $T = 0$ for an isotropic XY spin-chain. At finite temperatures, Tonegawa calculated numerically the longitudinal as well as transverse spin-correlation functions and the corresponding inverse correlation lengths.

Later, Basak and Chatterjee [5], following the prescription of Lieb *et al* [1], calculated the spin-correlation functions of an anisotropic XY spin-chain and observed the criticality of an XY spin-chain. From the study of critical exponents the anisotropic XY model was shown to behave like an Ising model. The isotropic XY model, on the other hand, was shown to have a criticality at $T = 0$ without any long range order. The correlation lengths in all directions (x, y, z), of course, diverge at $T = 0$. This is due to quantum fluctuations [6], and no gap appears at $T = 0$. When a magnetic field is applied along z-direction, the Hamiltonian can be solved exactly, and the transverse susceptibility (along the z-direction) of the XY spin-chain was calculated [7] exactly using temperature dependent correlation functions. The energy and specific heat were also calculated [8] from temperature dependent correlation functions. These calculations [5, 8] explain the experimental results for the compound Cs_2CoCl_4, which behaves as a linear spin-$\frac{1}{2}$ XY magnetic system [9–12]. Although the susceptibility along the z-direction of an XY spin-$\frac{1}{2}$ chain can be calculated exactly, the same along the x- or y-directions is not possible. The powerful density matrix renormalization group (DMRG) technique [13] at finite temperature [14], known as the transfer matrix renormalization group (TMRG) method,

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however, enables us to calculate the longitudinal susceptibility (along the x-direction) of the antiferromagnetic XY spin-chain. This is reported in this Letter.

The TMRG method is supposed to be the best numerical method for the study of the thermodynamics of a one dimensional quantum system. It is based on a quantum transfer matrix [15, 16] and use has been made of an asymmetric reduced density matrix which optimizes truncated basis states [13]. This method has been successfully applied [17] to the anisotropic spin-$\frac{1}{2}$ Heisenberg antiferromagnetic model, from which the result of spin-$\frac{1}{2}$ XY chain can be derived, and the results have been found to agree with the exact results [2, 8]. The effect of single ion anisotropy in the susceptibility of an $S = 1$ antiferromagnetic Heisenberg chain and in the Haldane gap has been studied by Coombes *et al* [18] using the TMRG method. They compared their theoretical results with the experimental ones and a good agreement over a wide range of temperatures was obtained. Later, Xiang employed [19] the TMRG method to study the thermodynamics of quantum Heisenberg spin-chains with $S = \frac{1}{2}$, 1 and $\frac{3}{2}$, and reproduced the zero temperature results. Since this method provides further insight into the quantum effects in the antiferromagnetic Heisenberg spin-chains the next step is to attempt to apply this method in a problem which cannot be solved exactly.

In this Letter we are considering the isotropic XY spin-chain in the presence of a magnetic field (B) along the x-direction. The Hamiltonian is

$$H = -2J \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) - B \sum_{i=1}^{N} S_i^x. \tag{1}$$

This Hamiltonian has not been solved exactly [20] for spin-$\frac{1}{2}$ and the susceptibility cannot be calculated in the x-direction exactly. But using TMRG it is possible to calculate this susceptibility numerically for an antiferromagnetic ($J < 0$) spin-chain only. The TMRG method has been discussed in great detail in earlier papers [14, 17]. Here we report that this method is successful in calculating the longitudinal susceptibility of an XY spin-chain for spin-$\frac{1}{2}$ only, and predict the value of this susceptibility when $T \to 0$, as there is no analytical result at this temperature.

Following the TMRG procedure as described in an earlier paper [17] we have calculated the energy and specific heat, and the results have been found to agree with the exact results [2, 8]. In this calculation the largest block size used is 4000, having 1999 on either side, and the number of states included is 80. To minimize the truncation error $\epsilon = 0.05$ is used. The susceptibility down to the low temperature $T = 0.01$ has been calculated using the magnetic field $B = 0.01$. The susceptibility is plotted in figure 1. The energy and specific heat are shown in figures 2 and 3, respectively. The results shown in figures 2 and 3 agree by up to five decimal places with the exact results [8]. So we expect the calculation of susceptibility along the x-direction to be almost exact. As there is no exact result, we can only compare the present results with the existing numerical results obtained by finite chain calculations [12]. In [12], susceptibility at $T = 0$ estimated from extrapolation was reported to be $\chi_\infty(0) = 0.115 \pm 0.01$, which is somewhat less than the value calculated here, $\chi(0) = 0.175$ at temperature $T = 0.01$. Using the magnetic field $B = 0.01$ the numerical error is found to be smaller [21] in the calculation of susceptibility compared to the calculation of energy and specific heat. The calculation of energy $U(T)$, specific heat $C(T)$ and magnetization $M(T)$ as a derivative of free energy involves some numerical error. In order to avoid this error, these physical quantities are calculated directly as described earlier [17]. The spin susceptibility $\chi(T)$ and the specific heat $C(T)$, of course, are calculated as first order derivatives of the magnetization $M(T, B)$ with respect to B and as first order derivatives of the energy $U(T, B)$ with respect to T. The susceptibility results show qualitative agreement with the experimental results [12].

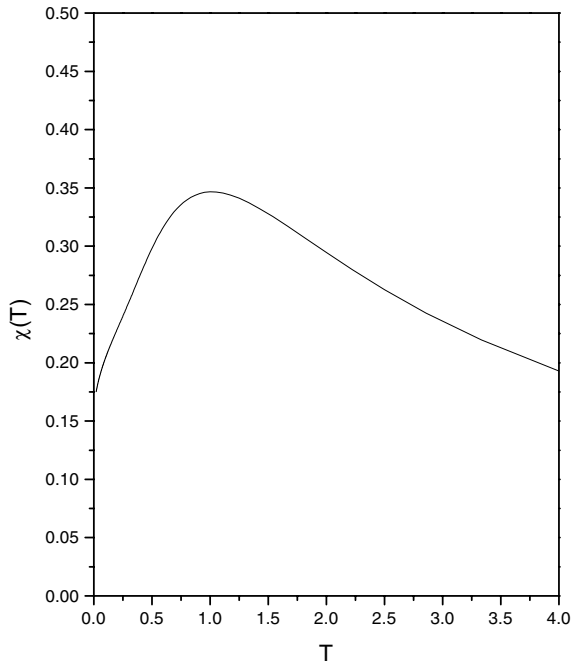

Figure 1. Longitudinal susceptibility along the *x*-direction as a function of temperature.

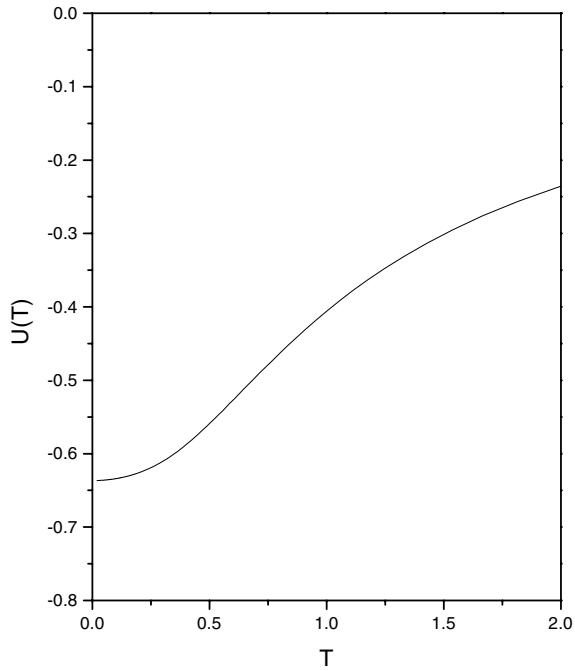

Figure 2. Energy as a function of temperature.

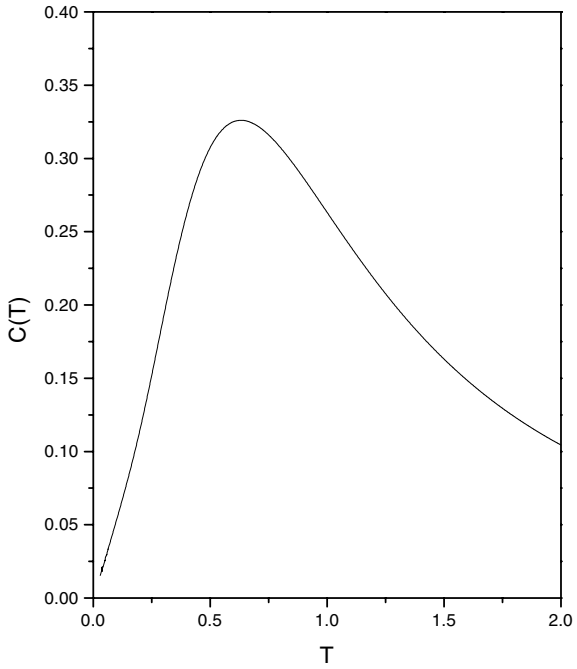

Figure 3. Specific heat as a function of temperature.

The longitudinal susceptibility of the XY spin-chain as shown in figure 1 predicts the susceptibility at $T = 0$ to be very close to 0.175, which is the best numerical value available at present. When the susceptibility data is compared with the numerical results obtained earlier [12, 22] it has been found that the present value is less than the extrapolation value of Bonner [22] and higher than the value reported [12] from finite chain calculations. In the present calculation we have, however, employed the best numerical method and the results thus obtained might be very close to the exact ones if available.

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