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The transverse susceptibility in the linear XY model

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Abstract. The transverse susceptibility χ_z of a linear isotropic XY magnetic chain with spin $S = \frac{1}{2}$ has been calculated exactly in linear response theory.

1. Introduction

The transverse susceptibility χ_z along the z direction of the linear spin-$\frac{1}{2}$ XY model has been calculated by Katsura as early as 1962. In this calculation (Katsura 1962), there is a lowering of the susceptibility χ_z curve as $T \rightarrow 0$ which is not correct. This arises because of a numerical error in the calculations. Katsura (1963) published an erratum in which he pointed out this error and showed that $\chi_z|J|/Nm^2$ should tend to a constant value $2/\pi$ as $T \rightarrow 0$ and the results of $\chi_z|J|/Nm^2$ ($m = \frac{1}{2}g\mu_B$) are wrong for the part $0 < 2kT/|J| < 0.25$. The correct values are obtained in the present calculation where an exact calculation of the zero-field transverse susceptibility is performed using linear response theory. The results are the same as obtained by Katsura and Inawashiro (1964) in later calculations.

In this later paper, Katsura and Inawashiro solved the anisotropic linear Heisenberg model

$$\mathcal{H} = -\tfrac{1}{2}\sum_l [J_\perp(\sigma_l^x\sigma_{l+1}^x + \sigma_l^y\sigma_{l+1}^y) + J_\parallel\sigma_l^z\sigma_{l+1}^z] - mH\sum_l \sigma_l^z$$

by the linked-cluster expansion method and obtained results up to second order in the anisotropy parameter $J_\parallel/J_\perp$. The zeroth-order result of this Hamiltonian corresponds to spin-$\frac{1}{2}$ XY model calculations and gives correct values of χ_z. We have, however, approached this in a different way to solve for χ_z in the 1D XY model and obtained the same results as those of Katsura and Inawashiro (1964).

In the present calculation, we considered the Hamiltonian without the magnetic field and solved it in the same way as Lieb *et al* (1961). Using the eigenvalues and eigenfunctions of this Hamiltonian, the zero-field transverse susceptibility χ_z in the 1D XY model was calculated exactly in the linear response theory and it was found to agree with the results obtained by Katsura and Inawashiro (1964).

2. Theory

The Hamiltonian for the 1D XY model is given by

$$\mathcal{H} = \mathcal{H}_0 + V \tag{1}$$

where

$$\mathcal{H}_0 = -2J \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)$$

and

$$V = -g\mu_B H \sum_{i=1}^{N} S_i^z$$

with $S_{N+1} = S_1$ for a chain satisfying the periodic boundary condition. The Hamiltonian $\mathcal{H}_0$ has been diagonalised as suggested by Lieb *et al* (1961) and one obtains

$$\mathcal{H}_0 = -2J \sum_k \lambda_k \eta_k^+ \eta_k + \text{constant} \tag{2}$$

where η_k and η_k^+ are Fermi operators and λ_k is given by

$$\lambda_k^2 = \cos^2 k. \tag{3}$$

The zero-field finite-temperature susceptibility is calculated using the linear response theory. In this theory, V is treated as a perturbation over $\mathcal{H}_0$ and only the terms linear in H in the expression for the magnetisation are retained.

The magnetisation per spin is given by

$$M_z = \frac{g\mu_B}{N} \sum_i \mathrm{Tr}[\exp(-\beta\mathcal{H})\, S_i^z]/\mathrm{Tr}[\exp(-\beta\mathcal{H})]. \tag{4}$$

To the first order in V, one obtains

$$\exp(-\beta\mathcal{H}) = \exp(-\beta\mathcal{H}_0)\left(1 - \int_0^\beta \exp(t\mathcal{H}_0)\, V \exp(-t\mathcal{H}_0)\,\mathrm{d}t\right)$$

and

$$\mathrm{Tr}[\exp(-\beta\mathcal{H})] = \mathrm{Tr}[\exp(-\beta\mathcal{H}_0)] - \mathrm{Tr}\left(\exp(-\beta\mathcal{H}_0)\int_0^\beta \exp(t\mathcal{H}_0)\, V \exp(-t\mathcal{H}_0)\,\mathrm{d}t\right). \tag{5}$$

Therefore,

$$\mathrm{Tr}[\exp(-\beta\mathcal{H})\, S_i^z]/\mathrm{Tr}[\exp(-\beta\mathcal{H})] = \langle\langle S_i^z\rangle\rangle + \int_0^\beta \mathrm{d}t\,(\langle\langle S_i^z\rangle\rangle\,\langle\langle \exp(t\mathcal{H}_0)\, V \exp(-t\mathcal{H}_0)\rangle\rangle$$
$$- \langle\langle \exp(t\mathcal{H}_0)\, V \exp(-t\mathcal{H}_0)\, S_i^z\rangle\rangle) \tag{6}$$

where $\langle\!\langle A\rangle\!\rangle = \mathrm{Tr}[\exp(-\beta\mathcal{H}_0)A]/\mathrm{Tr}[\exp(-\beta\mathcal{H}_0)]$ is the canonical average for any operator A with respect to $\mathcal{H}_0$. So we get

$$M_z = \frac{g\mu_B}{N}\left(\sum_{i=1}^{N}\langle\!\langle S_i^z(0)\rangle\!\rangle - g\mu_B H\int_0^\beta \mathrm{d}t\sum_{i,j=1}^{N}[\langle\!\langle S_i^z(0)\rangle\!\rangle\langle\!\langle S_j^z(t)\rangle\!\rangle - \langle\!\langle S_j^z(t)S_i^z(0)\rangle\!\rangle]\right) \quad (7)$$

where $S_j^z(t) = \exp(t\mathcal{H}_0)\,S_j^z(0)\exp(-t\mathcal{H}_0)$. The zero-field susceptibility

$$\chi_z = \frac{\partial M_z}{\partial H}\bigg|_{H\to 0} = \frac{g^2\mu_B^2}{N}\sum_{i,j=1}^{N}\int_0^\beta \mathrm{d}t\,[\langle\!\langle S_j^z(t)S_i^z(0)\rangle\!\rangle - \langle\!\langle S_i^z(0)\rangle\!\rangle\langle\!\langle S_j^z(t)\rangle\!\rangle]. \quad (8)$$

Now the z component of the correlation function between lth and mth spins at a finite temperature T has been given by Lieb *et al* (1961):

$$\rho_{lm}^z = \tfrac{1}{4}(G_{ll}G_{mm} - G_{ml}G_{lm}) \quad (9)$$

where $G_{ij} = G_{i-j} = G_r$. For $N\to\infty$ with $i - j = r$ fixed

$$G_r = \begin{cases} -\tfrac{1}{2}[L_{r+1} + L_{r-1}] & \\ 0 & \end{cases} \quad \text{when} \begin{cases} r \text{ is odd} \\ r \text{ is even.}\end{cases}$$

Here L_r is given by

$$L_r = \frac{2}{\pi}\int_0^{\pi/2}\mathrm{d}k\,\frac{\cos(kr)}{\cos k}\tanh(-J\beta\cos k) \quad (10)$$

and

$$\rho_r^z = -\tfrac{1}{4}G_rG_{-r}. \quad (11)$$

Now,

$$S_i^z = a_i^+a_i - \tfrac{1}{2} = -\tfrac{1}{2}A_iB_i$$

(Lieb *et al* 1961) and, therefore,

$$\langle\!\langle S_i^z(0)\rangle\!\rangle = -\tfrac{1}{2}\langle\!\langle A_iB_i\rangle\!\rangle_\beta = -\tfrac{1}{2}G_0 = 0. \quad (12)$$

Again, as $\Sigma_{i=1}^N S_i^z$ commutes with $\mathcal{H}_0$,

$$\left\langle\!\!\left\langle\sum_i S_i^z(t)\right\rangle\!\!\right\rangle = \left\langle\!\!\left\langle\exp(t\mathcal{H}_0)\sum_i S_i^z(0)\exp(-t\mathcal{H}_0)\right\rangle\!\!\right\rangle = \left\langle\!\!\left\langle\sum_i S_i^z(0)\right\rangle\!\!\right\rangle = 0. \quad (13)$$

Hence equation (8) reduces to

$$\chi_z = \frac{g^2\mu_B^2}{N}\sum_{i,j=1}^{N}\int_0^\beta \mathrm{d}t\,\langle\!\langle S_j^z(t)S_i^z(0)\rangle\!\rangle. \quad (14)$$

Since $\Sigma_{i=1}^N S_i^z$ commutes with $\mathcal{H}_0$

$$\sum_j S_j^z(t) = \exp(t\mathcal{H}_0)\sum_j S_j^z(0)\exp(-t\mathcal{H}_0) = \sum_j S_j^z(0). \quad (15)$$

Using equations (14) and (15),

$$\chi_z = \frac{g^2\mu_B^2}{N}\sum_{i,j=1}^{N}\int_0^\beta \mathrm{d}t\,\langle\!\langle S_i^zS_j^z\rangle\!\rangle \qquad S_i^z \equiv S_i^z(0)$$

$$= \frac{g^2\mu_B^2}{NkT}\sum_{i,j=1}^{N}\langle\!\langle S_i^zS_j^z\rangle\!\rangle$$

Table 1. Variation in the number of terms in the summation with temperature.

N	$2kT/\|J\|$	$\chi_M\|J\|/Nm^2$
11	1.0	0.7125
14	0.8	0.6924
17	0.6	0.6678
23	0.4	0.6486
45	0.2	0.6392
75	0.1	0.6372
95	0.08	0.6370
139	0.06	0.6368
165	0.04	0.6367

$$= \frac{g^2\mu_B^2}{kT}\sum_{i=1}^{N}\rho_{ij}^z \qquad \text{for a cyclic chain}$$

$$= \frac{g^2\mu_B^2}{kT}\sum_{r=-\infty}^{+\infty}\rho_r^z.$$

Since $\rho_r = \rho_{-r}$,

$$\chi_z = \frac{g^2\mu_B^2}{kT}\left(\rho_0 + 2\sum_{r=1}^{\infty}\rho_r^z\right)$$

and the molar susceptibility is given by

$$\chi_M = \frac{Ng^2\mu_B^2}{kT}\left(\rho_0 + 2\sum_{r=1}^{\infty}\rho_r^z\right) \qquad (16)$$

where N is Avogadro's number.

3. Results and discussion

At any temperature T, ρ_r^z is calculated according to equation (11) with an increasing value of r. As r increases, ρ_r^z decreases and $\Sigma_r\rho_r^z$ converges to a limiting value after a certain number of r-values have been included in the summation. In order to compare our results with the existing results, we computed $\chi_M|J|/Nm^2$ and, therefore, we are interested in the sum

$$S(N) = \frac{4|J|}{kT}\left(2\sum_{r=1}^{N}\rho_r^z + \rho_0\right)$$

as evident from equation (16). The convergence in this sum is obtained when $S(N+1) - S(N) \sim 10^{-6}$. In table 1 we show how the number N of appreciable terms in the summation varies with temperature. As we go to lower and lower temperatures, we have to include an increasing number of terms in the series. In this way we are able to reproduce the results at low temperatures in the region $0 < 2kT/|J| < 0.25$ in which Katsura (1962) obtained the wrong results. The value of $\chi_M|J|/Nm^2$ at $T = 0$ is equal to

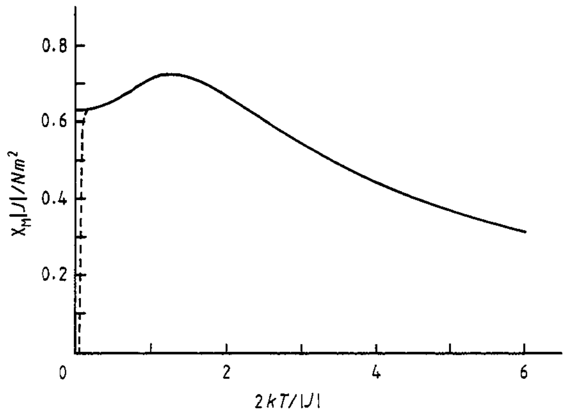

Figure 1. Transverse susceptibility of spin-$\frac{1}{2}$ *XY* model in 1D.

$2/\pi$ as calculated by Niemeijer (1967). It is evident from our calculation also (figure 1) that $\chi_M|J|/Nm^2$ approaches $2/\pi$ as $T \rightarrow 0$. In figure 1 our results are shown by a full curve and the results of Katsura (1962) are shown by a broken curve. Our results agree with the later calculation of Katsura and Inawashiro (1964). Since no experimental results for the 1D *XY* magnetic chain are available, we have no experimental data to compare our theoretical results with.

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