LETTER TO THE EDITOR

Transverse susceptibility in spin S Ising chains†

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Abstract. It is shown that the transverse susceptibility of a one-dimensional spin S Ising system can be calculated by combining linear response theory with the transfer matrix technique. Closed form expressions for infinite chains are obtained for $S = \frac{1}{2}$ and $S = 1$, and numerical results are displayed for $S = \frac{3}{2}$ to $S = \frac{5}{2}$.

The perpendicular susceptibility of a spin $\frac{1}{2}$ Ising chain has been calculated by several methods (e.g. Fisher 1963, Katsura 1962, and Grest and Rajagopal 1974). However, it would appear that these methods have not yet been generalised to higher spin. The free energy and parallel susceptibility have been found for higher spins using transfer matrix techniques (Suzuki et al 1967). In this paper the spin dependence of the perpendicular susceptibility will be studied. We use standard linear response theory (see for example Grest and Rajagopal 1974) and apply it with transfer matrices to obtain exact closed form expressions for the zero field perpendicular susceptibility for spin $\frac{1}{2}$ and spin 1 as well as numerical results for spin $\frac{3}{2}$, 2 and $\frac{5}{2}$.

Our Hamiltonian has the general form

$$H = H_0 + H_1$$

and we wish to find the expectation value of an operator $A$ to first order in $H_1$, where $H_0$, $H_1$ and $A$ do not necessarily commute. It can be shown that if

$$\text{Tr}[\exp(-\beta H_0)A] = 0$$

then

$$\langle A \rangle = \frac{-\text{Tr}\left[ \int_0^\beta \exp[-(\beta - \tau)H_0]H_1 \exp(-\tau H_0) d\tau A \right]}{\text{Tr}[\exp(-\beta H_0)]}$$

(3)

to first order in $H_1$.

In the Ising model for a closed cyclic chain we have

$$H_0 = -J \sum_{i=1}^N S_i S_{i+1}$$

$$H_1 = -\mu h \sum_{i=1}^N S_i$$

(4)

(5)

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where the $S_i$ are quantum spins of magnitude $S$ and site $N + 1$ is equivalent to site 1.

From equation (3) we find

$$
\langle S_i^z \rangle = \text{Tr} \left[ \frac{1}{\sum_{\tau}} \exp[\beta - (\tau - \tau) H_0] \mu h \sum_{\tau = 1}^{N} S_i^z \exp(-\tau H_0) d\tau S_i^z \right] / \text{Tr}[\exp(-\beta H_0)].
$$

(6)

The tracing operation ensures that only the $i = j$ term in the sum contributes. Furthermore, we note that all but two terms of $H_0$ (which are $-JS_{i-1}^z S_j^z - JS_j^z S_{i+1}^z$) commute with $S_i^z$ so that equation (6) can be rewritten as

$$
\langle S_i^z \rangle = \sum_{S_1} \sum_{S_2} \ldots \sum_{S_{i-1}} \sum_{S_{i+2}} \ldots \sum_{S_N} T_{S_1S_2} \ldots T_{S_{i-1},S_i,1} \ldots T_{S_{i+1},S_N} / \text{Tr}[\exp(-\beta H_0)]
$$

(7)

where $\sum_{S_i}$ stands for the sum over the $2S + 1$ possible values of $S_i$. We have defined the standard transfer matrix (Suzuki et al 1967)

$$
T_{S_iS_{i+1}} = \exp(\beta JS_i^z S_{i+1}^z)
$$

(8)

and have defined a new transfer matrix

$$
T_{S_jS_{j+1}} = \mu h \sum_{S_j} \int_0^\beta \exp[J(\beta - \tau)(S_j^z S_{j+1}^z + S_j^z S_{j+1}^z)]
$$

$$
\times S_j^z \exp[J\tau(S_j^z S_{j+1}^z + S_j^z S_{j+1}^z)] d\tau S_j^z.
$$

(9)

Interpreting the sums in equation (7) as a trace and cyclically permuting, we obtain

$$
\langle S_i^z \rangle = \text{Tr}[T^{N-1} T^z] / \text{Tr}[T^N].
$$

(10)

We now define the maximum eigenvalue of $T$ and the corresponding eigenvector to be $\lambda_m$ and $|m\rangle$ respectively, so that in the limit of $N \to \infty$,

$$
\langle S_i^z \rangle = \langle m | T^z | m \rangle / \lambda_m^2.
$$

(11)

Thus the zero field perpendicular susceptibility is

$$
\chi_\perp = N \frac{\mu \langle m | T^z | m \rangle}{\hbar \lambda_m^2}.
$$

(12)

The $(2S + 1)^2$ elements of $T^z$ may be determined analytically from equation (9) by examining the $(2S + 1)^2$ states involved. However, since $T_{S_jS_{j+1}}$ is a function only of $|S_j^z S_{j+1}^z|$, it can be shown that there are just $2S + 1$ independent elements of $T^z$ and hence only $(2S + 1)^2$ states need be examined. A short computer algorithm was developed to evaluate equation (9) analytically for larger spins. For $S = \frac{1}{2}$, we find

$$
T^z = \begin{pmatrix}
\frac{\hbar}{J} \sinh \frac{\beta J}{2} & \frac{\beta h}{2} \\
\frac{\beta h}{2} & \frac{h}{J} \sinh \frac{\beta J}{2}
\end{pmatrix}
$$

(13)
while when $S = 1$

$$T^s = \begin{pmatrix}
\frac{h \sinh 2\beta J}{J} & \frac{2h \sinh \beta J}{J} & 2\beta h \\
\frac{2h \sinh \beta J}{J} & 2\beta h & \frac{2h \sinh \beta J}{J} \\
2\beta h & \frac{2h \sinh \beta J}{J} & \frac{h \sinh 2\beta J}{J}
\end{pmatrix}. \tag{14}$$

Combining well known transfer matrix results with (12) and (13), Fisher's (1963) result for $S = \frac{1}{2}$ is recovered:

$$\frac{X_+}{N\mu^2} = 1\left[\frac{1}{2} \beta \operatorname{sech}^2 \frac{\beta J}{4} + \frac{\tanh (\beta J/4)}{J}\right] \tag{15}$$

while for $S = 1$ we obtain

$$\frac{X_+}{N\mu^2} = \frac{(\cosh \beta J - \frac{1}{3} + \frac{1}{3}q) \sinh 2\beta J + 8 \sinh \beta J + 2\beta Jq}{Jq (\cosh \beta J + \frac{1}{3} + \frac{1}{3}q)^2} \tag{16}$$

where

$$q = [(2 \cosh \beta J - 1)^2 + 8]^{1/2}. \tag{17}$$

With $T$ and $T^s$ both known analytically, equation (11) may be evaluated numerically for larger spins. The results for $S = \frac{1}{2}$ through $S = \frac{5}{2}$ are displayed in figure 1. By evaluating equation (6) considering the two low lying states, all spins pointing up and all spins pointing up with the exception that $S_f = S - 1$, it can be shown that†

$$\frac{JX_+ (T = 0)}{N\mu^2} = \frac{3}{8} \tag{18}$$

independent of $S$, as is shown in figure 1.

![Figure 1](image_url)

Figure 1. The perpendicular susceptibility $(JX_+/N\mu^2)$ plotted against reduced temperature $(k_B T/J)$ for $S = \frac{1}{2}, 1, \frac{3}{2}, 2$ and $\frac{5}{2}$.

† This result can be seen most easily by using ordinary second-order perturbation theory at $T = 0$ to give

$$\Delta E = N(\mu h/2)^2 [(\sqrt{2S})^2/2JS] = h^2 \hbar^2.$$
Figure 2. The perpendicular susceptibility ($\chi_\perp/N\mu^2$) plotted against the reduced temperature ($k_B T/JS(S + 1)$). This is the same as Figure 1 except for the rescaling of the temperature axes. Note that the vertical scale does not begin at zero. Values of $S$ are shown for each curve.

The high-temperature limit

$$\frac{\chi_\perp}{N\mu^2} = \beta \frac{S(S + 1)}{3}$$

suggests rescaling the temperature. The plot in Figure 2 of $\chi_\perp$ against $k_B T/JS(S + 1)$ indicates that in addition the location of the peak scales roughly with $S(S + 1)$ for $S \geq 1$.

The perpendicular susceptibility for an infinite spin $\frac{1}{2}$ chain in the presence of a non-zero parallel field has already been calculated exactly by Grest and Rajagopal (1974). By including parallel field terms in the exponents in equations (8) and (9), similar results may be obtained numerically for larger spins. Finally, we note that some modifications after equation (7) will yield the perpendicular susceptibility for finite open Ising chains and hence for dilute Ising chains (Thomsen and Thorpe 1983).

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References

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