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1996 J. Phys. A: Math. Gen. 29 6395

(http://iopscience.iop.org/0305-4470/29/19/023)

J. Phys. A: Math. Gen. **29** (1996) 6395–6405. Printed in the UK

The zero-field susceptibility of the transverse Ising chain with arbitrary spin

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Received 20 May 1996, in final form 15 July 1996

Abstract. The zero-field susceptibility of the transverse Ising chain with arbitrary spin-S is expressed in terms of the eigenvector for the maximum eigenvalue of its transfer matrix. As a result, the exact susceptibility is explicitly obtained for $S = \frac{1}{2}$, 1, $\frac{3}{2}$ and can be obtained at least for $S \leqslant \frac{7}{2}$. The numerical calculations of the susceptibility for arbitrary spin are possible and those for $S = 6$, 12 and 24 are given. It is also derived that the zero-temperature limit of the susceptibility is independent on spin-S.

1. Introduction

The transverse Ising chain is one of the most fundamental spin systems with non-trivial quantum effects. The Hamiltonian of this system is

$$\mathcal{H} = -J \sum_{i=1}^{N} s_i^z s_{i+1}^z - g\mu_{\rm B} H \sum_{i=1}^{N} s_i^x \tag{1.1}$$

where $s_{N+i}^l = s_i^l (l = x, y, z)$ and s_i^l is the l-component of spin operator on site i.

This model has been studied as a model of a one-dimensional magnetic system and also in connection with tunnelling effects [1, 2]. The model with spin $\frac{1}{2}$ is equivalent [3] to the two-dimensional Ising model with spin $\frac{1}{2}$ on a rectangular lattice. The zero-field transverse susceptibility for (1.1) with spin $\frac{1}{2}$ was obtained exactly by Fisher [4, 5]. The complete free energy for (1.1) with spin $\frac{1}{2}$ was obtained by Katsura [6] and later by Pfeuty [7].

Ising models with higher spin values have been investigated mainly for the case without transverse magnetic field. Ising models with small spin S have been exactly treated [8–10] in one-dimension, and also studied [11–13] from the viewpoint of the theorem of Lee and Yang. Spin-one cases of the Ising model with quadratic terms have been investigated [14–19] originally in connection with first-order phase transitions in a UO_2 magnet and in mixtures of liquid He^3–He^4. A continuous version of the spin chain, which is regarded as the infinite S limit of the Ising chain, can be treated exactly [20–22].

The transverse Ising chain with arbitrary spin has also been of interest to several authors [23–26].

The purpose of this paper is to calculate the zero-field susceptibility of transverse Ising chain with arbitrary spin, i.e. the magnetic fluctuation in the transverse direction of the Ising model (1.1) at $H = 0$. In section 2.1 the susceptibility is expressed in terms of the eigenvector for the maximum eigenvalue of the transfer matrix for the Ising chain. The exact susceptibility is in section 2.2 explicitly obtained for $S \leqslant \frac{3}{2}$ and can trivially be

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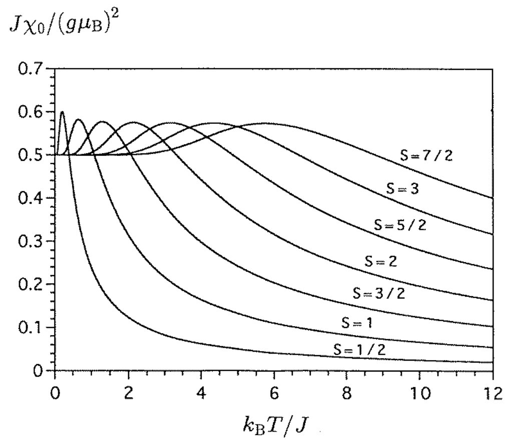

Figure 1. The zero-field susceptibility of transverse Ising chain (1.1) with spin $S \leqslant \frac{7}{2}$.

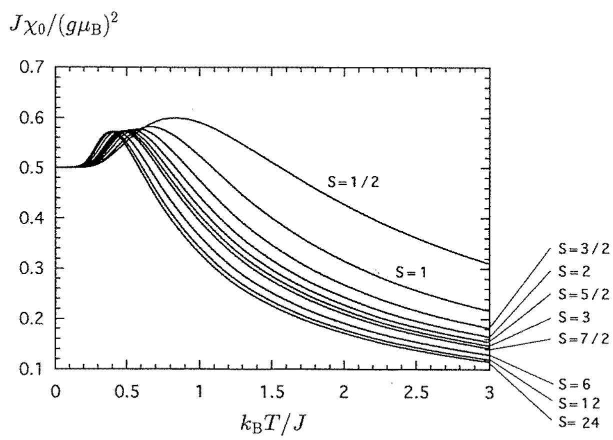

Figure 2. The zero-field susceptibility of transverse Ising chain with spin $S \leqslant \frac{7}{2}$, $S = 6$, 12 and 24, where s_i^l $(l = x, y, z)$ in (1.1) are replaced by s_i^l/S $(l = x, y, z)$ so that the model is described by the Hamiltonian (2.28).

obtained for $S = 2$ and $\frac{5}{2}$, from the eigenvector and the maximum eigenvalue listed in the appendix. Analytic expression is possible at least up to $S = \frac{7}{2}$. It is also possible to calculate the exact value of the susceptibility for arbitrary spin-S numerically. The results for $S \leqslant \frac{7}{2}$ are shown in figure 1. The equivalent results for $S \leqslant \frac{7}{2}$ are shown in figure 2 for different normalization of the spin operator $s_i^l \mapsto s_i^l/S$ $(l = x, y, z)$ together with the results for $S = 6$, 12 and 24. High- and low-temperature expansions are given in section 2.3 for arbitrary spin-S with the result that the zero temperature limit of the susceptibility is a finite constant independent on spin values.

In the present paper, the susceptibility is calculated by a perturbative expansion and each term in the expansion is expressed by some correlation functions. The terms in the expansion are correctly summerized. This is possible because, in the present method for this model, only short-ranged correlations appear and they can be calculated explicitly.

2. The transverse susceptibility at zero-field

2.1. Formulation in terms of the eigenvector

Let us introduce new notations as

$$\mathcal{H} = \mathcal{H}_0 - H\mathcal{Q} \tag{2.1}$$

where

$$\mathcal{H}_0 = -J\sum_{i=1}^{N} s_i^z s_{i+1}^z \qquad \mathcal{Q} = g\mu_{\mathrm{B}}\sum_{i=1}^{N} s_i^x. \tag{2.2}$$

We assume $J > 0$ but our results are not affected by the sign of J. The susceptibility χ at zero-field of the transverse Ising model described by the Hamiltonian (2.1) is by definition

$$\begin{aligned}\chi &= \frac{\partial}{\partial H}\langle\mathcal{Q}\rangle|_{H=0} \\ &= \frac{\partial}{\partial H}\frac{\mathrm{Tr}\,\mathcal{Q}\exp(-\beta\mathcal{H})}{\mathrm{Tr}\exp(-\beta\mathcal{H})}|_{H=0}\end{aligned} \tag{2.3}$$

where $\langle\rangle$ is the expectation taken by $\mathcal{H}$, $\beta = 1/k_B T$, k_B is the Boltzmann constant and T is the temperature. We have to note the uncommutability $[\mathcal{H}_0, \mathcal{Q}] \neq 0$ in (2.3).

Here let us introduce the following formula

$$\frac{\mathrm{d}}{\mathrm{d}H}\exp(-\beta\mathcal{H}) = \exp(-\beta\mathcal{H})\int_0^\beta \exp(\lambda\mathcal{H})\mathcal{Q}\exp(-\lambda\mathcal{H})\,\mathrm{d}\lambda. \tag{2.4}$$

To derive (2.4) one should multiply $\exp(\beta\mathcal{H})$ from the left-hand side to (2.4) and consider the derivative in terms of β. With the use of (2.4) the expectation $\langle\mathcal{Q}\rangle$ is expanded in terms of H and we obtain

$$\begin{aligned}\chi &= \frac{\partial}{\partial H}\left[\frac{\langle\mathcal{Q}\rangle_0 + H\int_0^\beta\langle\exp(\lambda\mathcal{H}_0)\mathcal{Q}\exp(-\lambda\mathcal{H}_0)\mathcal{Q}\rangle_0\,\mathrm{d}\lambda}{1 + H\int_0^\beta\langle\mathcal{Q}\rangle_0\,\mathrm{d}\lambda} + \mathrm{O}(H^2)\right]\Bigg|_{H=0} \\ &= \int_0^\beta\langle\exp(\lambda\mathcal{H}_0)\mathcal{Q}\exp(-\lambda\mathcal{H}_0)\mathcal{Q}\rangle_0\,\mathrm{d}\lambda\end{aligned} \tag{2.5}$$

where $\langle\rangle_0$ is the expectation taken at $H = 0$. Next let us introduce the operation δ by the relation

$$\delta^0\mathcal{Q} = \mathcal{Q} \qquad \delta^{n+1}\mathcal{Q} = [\mathcal{H}_0, \delta^n\mathcal{Q}]. \tag{2.6}$$

With the use of the following expansion

$$\exp(\lambda\mathcal{H}_0)\mathcal{Q}\exp(-\lambda\mathcal{H}_0) = \sum_{p=0}^{\infty}\frac{\lambda^p}{p!}\delta^p\mathcal{Q} \tag{2.7}$$

(2.5) is expressed as

$$\chi = \int_0^\beta\left\langle\sum_{p=0}^{\infty}\frac{\lambda^p}{p!}\delta^p\mathcal{Q}\mathcal{Q}\right\rangle_0\mathrm{d}\lambda. \tag{2.8}$$

This equals to

$$\begin{aligned}\chi &= \sum_{p=0}^{\infty}\frac{1}{p!}\int_0^\beta\lambda^p\,\mathrm{d}\lambda\,\langle\delta^p\mathcal{Q}\mathcal{Q}\rangle_0 \\ &= \sum_{p=0}^{\infty}\frac{\beta^{p+1}}{(p+1)!}\langle\delta^p\mathcal{Q}\mathcal{Q}\rangle_0.\end{aligned} \tag{2.9}$$

Then our subject is to evaluate the correlation function $\langle \delta^p \mathcal{Q}\mathcal{Q}\rangle_0$ and to perform the infinite sum in (2.9).

It is straightforward to show inductively for integer $p \geqslant 0$ that

$$\delta^p \mathcal{Q} = (-J)^p \tau_p g\mu_{\mathrm{B}} \sum_{i=1}^{N} \sum_{l=0}^{p} \binom{p}{l} (s_i^z)^{p-l} s_{i+1}^k (s_{i+2}^z)^l$$

where $\tau_p = 1$ for even p, $\tau_p = i$ for odd p, $k = x$ for even p, $k = y$ for odd p and

$$\binom{p}{l} = \frac{p!}{(p-l)!l!}.$$

Next let $|m\rangle$ be the eigenstate of $\mathcal{H}_0$ with eigenvalue $E_m : \mathcal{H}_0|m\rangle = E_m|m\rangle$. The state $|m\rangle$ is a direct product of eigenstate of each s_i^z. Obviously $\langle m|(s_i^z)^l s_i^x|m\rangle = 0$ $(l = 0, 1, 2, \ldots)$ for all $|m\rangle$ and therefore $\langle (s_i^z)^{p-l} s_{i+1}^k (s_{i+2}^z)^l s_j^x\rangle_0 = 0$ for $j \neq i+1$. As a result $\langle \delta^p \mathcal{Q}\mathcal{Q}\rangle_0$ is expressed as

$$\langle \delta^p \mathcal{Q}\mathcal{Q}\rangle_0 = (-J)^p \tau_p (g\mu_{\mathrm{B}})^2 N \sum_{l=0}^{p} \binom{p}{l} \langle (s_1^z)^{p-l} (s_2^k s_2^x)(s_3^z)^l\rangle_0. \tag{2.10}$$

The correlation inside the sum in (2.10) is obtained by the transfer matrix method. Let V (which is written as V_S in the appendix) be the transfer matrix for the Hamiltonian (1.1) as

$$V_{ij} \equiv (V)_{ij} = \exp[\beta J(S-i+1)(S-j+1)] \tag{2.11}$$

where $i, j = 1, 2, \ldots, n$ with $n = 2S+1$, and let U be the matrix whose element $(U)_{ij} = u_{ij}$ is the ith element of the orthonormalized eigenvector corresponding to the jth eigenvalue λ_j: they satisfy the relation $V = U\Lambda U^{-1}$, $(\Lambda)_{ij} = \lambda_j \delta_{ij}$. Here λ_1 denotes the maximum eigenvalue, which is non-degenerate. The operator $s^k s^x (k = x, y)$ is non-diagonal in the standard representation where s^2 and s^z are diagonalized simultaneously. Its diagonal elements are quantum expectations for each corresponding basic state. The expectation $\langle s_i^k s_i^x\rangle_0$, for example, can be calculated with the use of the transfer matrix as

$$\begin{aligned}\langle s_i^k s_i^x\rangle_0 &= \frac{\mathrm{Tr}\, s_i^k s_i^x \exp(-\beta\mathcal{H}_0)}{\mathrm{Tr} \exp(-\beta\mathcal{H}_0)} = \frac{\sum_m \langle m|s_i^k s_i^x|m\rangle \exp(-\beta E_m)}{\sum_m \exp(-\beta E_m)} \\ &= \frac{\mathrm{Tr}\, D^{(p)} V^N}{\mathrm{Tr}\, V^N}\end{aligned} \tag{2.12}$$

where $D^{(p)}$ is the matrix with the element

$$\begin{aligned}(D^{(p)})_{ll'} &= D_l^{(p)} \delta_{ll'} \\ D_l^{(p)} &= \begin{cases} (s^y s^x)_{ll} = (S-l+1)/2i & (\text{odd } p) \\ (s^x s^x)_{ll} = (S(S+1) - (S-l+1)^2)/2 & (\text{even } p).\end{cases}\end{aligned} \tag{2.13}$$

Similarly our expectation is obtained by

$$\langle (s_1^z)^{p-l} (s_2^k s_2^x)(s_3^z)^l\rangle_0 = \frac{\mathrm{Tr} (s^z)^{p-l} V D^{(p)} V (s^z)^l V^{N-2}}{\mathrm{Tr}\, V^N}$$

$$= \frac{\mathrm{Tr}(s^z)^{p-l} V D^{(p)} V (s^z)^l U \begin{pmatrix} 1 & & & \\ & (\lambda_2/\lambda_1)^{N-2} & & \\ & & \ddots & \\ & & & (\lambda_n/\lambda_1)^{N-2} \end{pmatrix} U^{-1}}{\mathrm{Tr}\, V^2 U \begin{pmatrix} 1 & & & \\ & (\lambda_2/\lambda_1)^{N-2} & & \\ & & \ddots & \\ & & & (\lambda_n/\lambda_1)^{N-2} \end{pmatrix} U^{-1}}. \tag{2.14}$$

In the thermodynamic limit $N \to \infty$, the correlation is obtained as

$$\langle (s_1^z)^{p-l} (s_2^k s_2^x)(s_3^z)^l \rangle_0 = \sum_{ij=1}^{n} d_i^{p-l} d_j^l c_{ij}^{(p)}/c \tag{2.15}$$

where

$$\begin{aligned} c_{ij}^{(p)} &= \sum_{l=1}^{n} V_{il} D_l^{(p)} V_{lj} u_{j1} u_{i1} \\ c &= \sum_{ij=1}^{n} \sum_{l=1}^{n} V_{il} V_{lj} u_{j1} u_{i1} \end{aligned} \tag{2.16}$$

and

$$d_i = (s^z)_{ii} = S - i + 1. \tag{2.17}$$

Here we note that $u_{j1}u_{i1}$ can be regarded as the exactly renormalized Boltzmann weight. The susceptibility in the thermodynamic limit

$$\chi_0 = \lim_{N\to\infty} \frac{\chi}{N} \tag{2.18}$$

is obtained as

$$\begin{aligned} \chi_0 &= \sum_{p=0}^{\infty} \frac{\beta^{p+1}}{(p+1)!} \lim_{N\to\infty} \langle \delta^p \mathcal{Q}\mathcal{Q} \rangle_0 / N \\ &= \sum_{p=0}^{\infty} \frac{\beta^{p+1}}{(p+1)!} (-J)^p \tau_p (g\mu_{\mathrm{B}})^2 \sum_{l=0}^{p} \binom{p}{l} \sum_{ij=1}^{n} d_i^{p-l} d_j^l c_{ij}^{(p)}/c \\ &= \frac{(g\mu_{\mathrm{B}})^2}{-J} \sum_{p=0}^{\infty} \frac{(-\beta J)^{p+1}}{(p+1)!} \sum_{ij=1}^{n} \frac{\tau_p c_{ij}^{(p)}}{c} (d_i + d_j)^p. \end{aligned} \tag{2.19}$$

This should be classified according to $d_i + d_j$ and p. We note that $(d_i + d_j)^0 = 1$ and obtain

$$\begin{aligned} \frac{J\chi_0}{(g\mu_{\mathrm{B}})^2} &= \beta J \sum_{ij=1}^{n} \frac{c_{ij}^{(0)}}{c} - \sum_{ij=1}^{n} \Bigg[\sum_{p=1(p=\mathrm{odd})}^{\infty} \frac{(-\beta J)^{p+1}}{(p+1)!} \frac{\tau_p c_{ij}^{(p)}}{c} (d_i + d_j)^p \\ &\quad + \sum_{p=2(p=\mathrm{even})}^{\infty} \frac{(-\beta J)^{p+1}}{(p+1)!} \frac{\tau_p c_{ij}^{(p)}}{c} (d_i + d_j)^p \Bigg] \\ &= \frac{1}{c} \beta J \sum_{ij=1}^{n} u_{j1} u_{i1} \sum_{l=1}^{n} D_l^{(0)} \mathrm{e}^{(S-l+1)(d_i+d_j)\beta J} \end{aligned}$$

$$-\frac{1}{c}\sum_{ij=1 d_i+d_j\neq 0}^{n}\left[\frac{u_{j1}u_{i1}}{d_i+d_j}\sum_{l=1}^{n} i D_l^{(1)} \mathrm{e}^{(S-l+1)(d_i+d_j)\beta J}[\cosh((d_i+d_j)\beta J)-1] + \frac{u_{j1}u_{i1}}{d_i+d_j}\sum_{l=1}^{n} D_l^{(2)} \mathrm{e}^{(S-l+1)(d_i+d_j)\beta J}[(d_i+d_j)\beta J-\sinh((d_i+d_j)\beta J)]\right]. \tag{2.20}$$

After all, from (2.20), the susceptibility is exactly obtained as

$$\frac{J\chi_0}{(g\mu_{\mathrm{B}})^2} = \frac{1}{c}\sum_{ij=1 d_i+d_j\neq 0}^{n}\frac{u_{j1}u_{i1}}{d_i+d_j}\sum_{m=-S}^{S} m\mathrm{e}^{m(d_i+d_j)K} + S(S+1)(2S+1)K/3c \tag{2.21}$$

where $K=\beta J$. We use the fact $\sum_{i=1}^{n} u_{i1}u_{n+1-i1}=1$ derived in the appendix. The constant c in (2.21) is rewritten from (2.16) as

$$c=\sum_{ij=1}^{n} u_{j1}u_{i1}\sum_{m=-S}^{S}\mathrm{e}^{m(d_i+d_j)K}. \tag{2.22}$$

The only unknown quantity in (2.21) and (2.22) is the eigenvector u_{i1} for the maximum eigenvalue λ_1 of V. To obtain u_{i1} for general spin S is one of the unsolved problems but is possible for small S by direct calculations. The eigenvalue λ_1 and the eigenvector u_{i1} for $S\leqslant\frac{3}{2}$, and the eigenvalue λ_1 for $S=\frac{5}{2}$ are shown in the appendix. It is possible to write down the exact susceptibility explicitly at least up to $S=\frac{7}{2}$ as easily seen in the appendix. Numerical calculations are easy for arbitrary spin-S.

2.2. *The transverse susceptibility*

The exact transverse susceptibility for $S=\frac{1}{2}$ is immediately obtained when u_{11} and u_{21} in the appendix are substituted to (2.21) and (2.22) as

$$\frac{J\chi_0}{(g\mu_{\mathrm{B}})^2}=\frac{1}{2}\left[\frac{K/4}{\cosh^2(K/4)}+\tanh(K/4)\right]. \tag{2.23}$$

This result was already obtained by Fisher [4, 5] and Katsura [6]. The exact susceptibility for $S\geqslant 1$ are also obtained from u_{i1} listed in the appendix as

$$\frac{J\chi_0}{(g\mu_{\mathrm{B}})^2}=\frac{1}{c}[2K+4\sqrt{2}\sin\theta_1\cos\theta_1\sinh K+\cos^2\theta_1\sinh 2K] \tag{2.24}$$

where

$$c=3+2\sqrt{2}\sin\theta_1\cos\theta_1(1+2\cosh K)+\cos^2\theta_1(1+2\cosh 2K)$$
$$\tan 2\theta_1=\frac{\sqrt{2}}{\cosh K-1/2} \tag{2.25}$$

for $S=1$ and

$$\frac{J\chi_0}{(g\mu_{\mathrm{B}})^2}=\frac{1}{c}[5K+\sin^2\theta_{\frac{3}{2}}(\sinh(K/2)+3\sinh(3K/2))+\sin\theta_{\frac{3}{2}}\cos\theta_{\frac{3}{2}}(2\sinh(K/2) +6\sinh(3K/2)+\sinh K+3\sinh 3K) +\cos^2\theta_{\frac{3}{2}}(\sinh(3K/2)+3\sinh(9K/2))/3] \tag{2.26}$$

where

$$c = 4 + 2\sin^2\theta_{\frac{3}{2}}(\cosh(K/2) + \cosh(3K/2)) + 4\sin\theta_{\frac{3}{2}}\cos\theta_{\frac{3}{2}}(\cosh(K/2) + \cosh(3K/2) + \cosh K + \cosh 3K) + 2\cos^2\theta_{\frac{3}{2}}(\cosh(3K/2) + \cosh(9K/2))]$$
$$\tan 2\theta_{\frac{3}{2}} = \frac{2\cosh(3K/4)}{\cosh(9K/4) - \cosh(K/4)} \tag{2.27}$$

for $S = \frac{3}{2}$. The analytic expression for spin at least up to $S = \frac{7}{2}$ and numerical calculations for arbitrary spin are possible, as mentioned at the end of section 2.1. The results for $S \leqslant \frac{7}{2}$ are shown in figure 1. The equivalent results are also shown in figure 2 where s_i^l $(l = x, y, z)$ in (1.1) are replaced by s_i^l/S $(l = x, y, z)$, i.e. the susceptibility for the Hamiltonian

$$\mathcal{H} = -\frac{J}{S^2}\sum_{i=1}^{N} s_i^z s_{i+1}^z - g\mu_{\rm B}\frac{H}{S}\sum_{i=1}^{N} s_i^x. \tag{2.28}$$

The results of numerical calculations for (2.28) with $S = 6$, 12 and 24 are shown together in figure 2.

2.3. Low- and high-temperature expansions

Although the maximum eigenvalue λ_1 and the eigenvector u_{i1} have been obtained only for small S, the low- and high-temperature expansions of λ_1 and u_{i1} are exactly possible for arbitrary spin-S. The eigenvalue λ_1 and the eigenvector u_{i1} are

$$\begin{aligned} \lambda_1 &= {\rm e}^{K/4} + {\rm e}^{-K/4} \\ u_{11} &= u_{21} = 1/\sqrt{2} \end{aligned} \tag{2.29}$$

for $S = \frac{1}{2}$. At low temperatures, it is easy to show that

$$\begin{aligned} \lambda_1 &= {\rm e}^{K}(1 + 3{\rm e}^{-2K} + 2{\rm e}^{-3K} - 4{\rm e}^{-4K} + {\rm O}({\rm e}^{-5K})) \\ u_{11} &= u_{31} = (1 - {\rm e}^{-2K} - 2{\rm e}^{-3K} + 9{\rm e}^{-4K}/2)/\sqrt{2} + {\rm O}({\rm e}^{-5K}) \\ u_{21} &= \sqrt{2}({\rm e}^{-K} + {\rm e}^{-2K} - 3{\rm e}^{-3K} - 10{\rm e}^{-4K}) + {\rm O}({\rm e}^{-5K}) \end{aligned} \tag{2.30}$$

for $S = 1$ and

$$\begin{aligned} \lambda_1 &= {\rm e}^{9K/4}(1 + {\rm e}^{-3K} + 3{\rm e}^{-9K/2} + {\rm O}({\rm e}^{-5K})) \\ u_{11} &= u_{41} = (1 - {\rm e}^{-3K}/2 - {\rm e}^{-9K/2})/\sqrt{2} + {\rm O}({\rm e}^{-5K}) \\ u_{21} &= u_{31} = ({\rm e}^{-3K/2} + {\rm e}^{-3K} + {\rm e}^{-7K/2} + {\rm e}^{-4K} - 3{\rm e}^{-9K/2}/2)/\sqrt{2} + {\rm O}({\rm e}^{-5K}) \end{aligned} \tag{2.31}$$

for $S = \frac{3}{2}$. One can obtain the low-temperature expansion of λ_1 for $S \geqslant 2$ as

$$\lambda_1 = {\rm e}^{S^2K}(1 + {\rm e}^{-2SK} + {\rm o}({\rm e}^{-2SK})). \tag{2.32}$$

Then it is straightforward to show

$$\begin{aligned} u_{11} &= u_{51} = (1 - {\rm e}^{-4K})/\sqrt{2} + {\rm O}({\rm e}^{-6K}) \\ u_{21} &= u_{41} = {\rm e}^{-2K}/\sqrt{2} + {\rm O}({\rm e}^{-6K}) \\ u_{31} &= \sqrt{2}{\rm e}^{-4K} + {\rm O}({\rm e}^{-6K}) \end{aligned} \tag{2.33}$$

for $S = 2$ and

$$\begin{aligned} u_{11} &= u_{n1} = (1 - \mathrm{e}^{-2SK})/\sqrt{2} + \mathrm{o}(\mathrm{e}^{-2SK}) \\ u_{21} &= u_{n-11} = \mathrm{e}^{-SK}/\sqrt{2} + \mathrm{o}(\mathrm{e}^{-2SK}) \\ u_{31} &= u_{n-21} = \mathrm{e}^{-2SK}/\sqrt{2} + \mathrm{o}(\mathrm{e}^{-2SK}) \\ u_{i1} &= \mathrm{o}(\mathrm{e}^{-2SK}) \qquad (4 \leqslant i \leqslant n-3) \end{aligned} \tag{2.34}$$

for $S \geqslant \frac{5}{2}$.

From (2.21), (2.22) and (2.29)–(2.34), the low-temperature expansions of the susceptibility are obtained as

$$\frac{J\chi_0}{(g\mu_B)^2} = \frac{1}{2} - \left(1 - \frac{K}{2}\right)\mathrm{e}^{-K/2} + (1-K)\mathrm{e}^{-K} + \mathrm{O}(K\mathrm{e}^{-3K/2}) \tag{2.35}$$

for $S = \frac{1}{2}$,

$$\frac{J\chi_0}{(g\mu_B)^2} = \tfrac{1}{2} + 2K\mathrm{e}^{-2K} - 4(4+3K)\mathrm{e}^{-4K} + \mathrm{O}(K\mathrm{e}^{-5K}) \tag{2.36}$$

for $S = 1$,

$$\frac{J\chi_0}{(g\mu_B)^2} = \tfrac{1}{2} + \tfrac{1}{6}\mathrm{e}^{-3K} + (\tfrac{1}{2} + 5K)\mathrm{e}^{-9K/2} + \mathrm{O}(K\mathrm{e}^{-5K}) \tag{2.37}$$

for $S = \frac{3}{2}$ and

$$\frac{J\chi_0}{(g\mu_B)^2} = \frac{1}{2} + \frac{1}{2S(2S-1)}\mathrm{e}^{-2SK} + \mathrm{o}(K\mathrm{e}^{-3SK}) \tag{2.38}$$

for $S \geqslant 2$. The coefficient of the term e^{-2SK} can be expressed as $[2S(2S-1)]^{-1}$ for $S \geqslant \frac{3}{2}$, although the eigenvector u_{i1} show such uniform structure only for $S \geqslant \frac{5}{2}$. From (2.35)–(2.38) we have derived for arbitrary spin that the $T \to 0$ limit is a finite constant and independent on spin-S.

At high temperatures the eigenvector is given by

$$u_{i1} = 1/\sqrt{n} + \mathrm{O}(K^2) \tag{2.39}$$

where the term proportional to K vanishes as seen in the appendix. From (2.19) and (2.39) the high-temperature expansion of the susceptibility is obtained as

$$\begin{aligned} \frac{J\chi_0}{(g\mu_B)^2} &= K\sum_{ij=1}^{n}\frac{c_{ij}^{(0)}}{c} - \frac{1}{2}K^2\sum_{ij=1}^{n}\frac{ic_{ij}^{(1)}}{c}(d_i + d_j) + \mathrm{O}(K^3) \\ &= \frac{J}{k_BT}\frac{1}{3}S(S+1) + \mathrm{O}\left(\left(\frac{1}{T}\right)^3\right). \end{aligned} \tag{2.40}$$

The first term in (2.40) denotes the Curie's law as is expected. The term proportional to T^{-p} always vanish for even p. This is consistent with the following fact that χ_0 is invariant under the sign reversal of interaction $J \mapsto -J$, and $J\chi_0/(g\mu_B)^2$ depends on J and T only through $K = J/k_BT$, so that $J\chi_0/(g\mu_B)^2$ is an odd function of K and hence an odd function of T.

3. Conclusions

The main result of this paper is (2.21) and (2.22) which is the zero-field susceptibility of the transverse Ising chain (1.1) with arbitrary spin. The parameter d_i in (2.21) and (2.22) is defined in (2.17) and the parameters $u_{i1} (i = 1, \ldots, n)$ are elements of the eigenvector corresponding to the maximum eigenvalue of the transfer matrix (2.11). The eigenvector u_{i1} and the eigenvalue λ_1 for $S \leqslant \frac{3}{2}$, and the eigenvalue λ_1 for $S = 2$ and $\frac{5}{2}$ are obtained in the appendix and hence the susceptibility is obtained for $S \leqslant \frac{5}{2}$. Analytic expression is obviously possible at least up to $S = \frac{7}{2}$. Numerical calculations are easy for arbitrary spin. Low- and high-temperature expansions are performed for arbitrary spin as (2.35)–(2.38) and (2.40) and it is derived that the $T \to 0$ limit of the susceptibility is a constant independent on spin values.

Acknowledgment

The author would like to thank Dr H Ohta for discussions.

Appendix

The transfer matrix V_S for $S = \frac{1}{2}$ Ising chain is diagonalized by a unitary matrix $R_{\frac{1}{2}}$ as

$$R_{\frac{1}{2}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$
$$R_{\frac{1}{2}}^{-1} V_{\frac{1}{2}} R_{\frac{1}{2}} = \begin{pmatrix} 2\cosh(K/4) & 0 \\ 0 & 2\sinh(K/4) \end{pmatrix}. \tag{A.1}$$

Our subject to diagonalize the transfer matrix V_S for arbitrary spin S is simplified by the following unitary matrix

$$R_S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & & & & & & 1 \\ & \ddots & & & & \cdot^{\cdot^{\cdot}} & \\ & & 1 & & 1 & & \\ & & & \sqrt{2} & & & \\ & & 1 & & -1 & & \\ & \cdot^{\cdot^{\cdot}} & & & & \ddots & \\ 1 & & & & & & -1 \end{pmatrix}$$

and

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & & & & & 1 \\ & \ddots & & & \cdot^{\cdot^{\cdot}} & \\ & & 1 & 1 & & \\ & & 1 & -1 & & \\ & \cdot^{\cdot^{\cdot}} & & & \ddots & \\ 1 & & & & & -1 \end{pmatrix} \tag{A.2}$$

for integer and half-integer spin, respectively. The elements $(R_S)_{ij}$ except for $j = i$ or $j = n - i + 1$ are zero in (A.2). With the use of this R_S, the transfer matrix V_S is block-diagonalized as

$$R_S^{-1} V_S R_S = \begin{pmatrix} A_S & O_S \\ O_S & B_S \end{pmatrix} \tag{A.3}$$

where O_S is the matrix and all the elements are zero and

$$A_S = \begin{pmatrix} 2c_{S\times S} & \dots & 2c_{S\times 1} & \sqrt{2} \\ \vdots & & \vdots & \vdots \\ 2c_{1\times S} & \dots & 2c_{1\times 1} & \sqrt{2} \\ \sqrt{2} & \dots & \sqrt{2} & 1 \end{pmatrix} \qquad B_S = \begin{pmatrix} 2s_{1\times 1} & \dots & 2s_{1\times S} \\ \vdots & & \vdots \\ 2s_{S\times 1} & \dots & 2s_{S\times S} \end{pmatrix} \tag{A.4}$$

for integer spin and

$$A_S = \begin{pmatrix} 2c_{S\times S} & \dots & 2c_{S\times \frac{1}{2}} \\ \vdots & & \vdots \\ 2c_{\frac{1}{2}\times S} & \dots & 2c_{\frac{1}{2}\times \frac{1}{2}} \end{pmatrix} \qquad B_S = \begin{pmatrix} 2s_{\frac{1}{2}\times \frac{1}{2}} & \dots & 2s_{\frac{1}{2}\times S} \\ \vdots & & \vdots \\ 2s_{S\times \frac{1}{2}} & \dots & 2s_{S\times S} \end{pmatrix} \tag{A.5}$$

for half-integer spin. In (A.4) and (A.5) we use the notation $c_m \equiv \cosh mK$ and $s_m \equiv \sinh mK$. The maximum eigenvalue λ_1 of V_S and the eigenvector u_{i1} for λ_1 are obtained from the maximum eigenvalue of A_S and the eigenvector for it. As a result all the elements $u_{i1} (i = 1, \dots, n)$ are even functions of K and satisfy the relation $u_{n+1-i1} = u_{i1}$. So the normalization condition yields $\sum_{i=1}^{n} u_{i1}u_{n+1-i1} = 1$. From the theorem of Frobenius all the elements u_{i1} should be positive. The degree of the characteristic equation of A_S is $[(n+1)/2]$, where [] is the Gauss symbol, and the equation can be solved at least for $S \leqslant \frac{7}{2}$ i.e. for $[(n+1)/2] \leqslant 4$.

Here we would like to list the maximum eigenvalue λ_1, the eigenvector u_{i1} of V_S for $S \leqslant \frac{3}{2}$, and λ_1 for $S = 2$ and $\frac{5}{2}$. It is easy to obtain

$$\begin{aligned} &\lambda_1 = 2c_1 \\ &u_{11} = u_{21} = 2^{-1/2} \end{aligned} \tag{A.6}$$

for $S = \frac{1}{2}$,

$$\begin{aligned} &\lambda_1 = ((2c_1 + 1) + ((2c_1 - 1)^2 + 8)^{1/2})/2 \\ &u_{11} = u_{31} = 2^{-1/2}\cos\theta_1 \\ &u_{21} = \sin\theta_1 \\ &\tan 2\theta_1 = 2^{1/2}/(c_1 - 1/2) \end{aligned} \tag{A.7}$$

for $S = 1$ and

$$\begin{aligned} &\lambda_1 = (c_{\frac{9}{4}} + c_{\frac{1}{4}}) + ((c_{\frac{9}{4}} - c_{\frac{1}{4}})^2 + (2c_{\frac{3}{4}})^2)^{1/2} \\ &u_{11} = u_{41} = 2^{-1/2}\cos\theta_{\frac{3}{2}} \\ &u_{21} = u_{31} = 2^{-1/2}\sin\theta_{\frac{3}{2}} \\ &\tan 2\theta_{\frac{3}{2}} = 2c_{\frac{3}{4}}/(c_{\frac{9}{4}} - c_{\frac{1}{4}}) \end{aligned} \tag{A.8}$$

for $S = \frac{3}{2}$.

The maximum eigenvalue λ_1 for $S = 2$ and $\frac{5}{2}$ are obtained as the maximum root of the characteristic equation for A_S as

$$\lambda_1 = 2\Lambda_0^{1/2}\cos\frac{\phi}{3} \tag{A.9}$$

where $\tan\phi = (4\Lambda_0^3/\Lambda_1^2 - 1)^{1/2}$, $\Lambda_0 = (\xi_1 + \xi_2^2/3)/3$, $\Lambda_1 = \xi_0 + \xi_1\xi_2/3 + 2\xi_2^3/27$, $\xi_0 = \det A_S$, $\xi_1 = -(\Delta_S^{(1)} + \Delta_S^{(2)} + \Delta_S^{(3)})$ and $\xi_2 = \operatorname{tr} A_S$. The new notation $\Delta_S^{(l)} = (A_S^{-1})_{ll} \times \det A_S$ is the cofactor of the matrix A_S.

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