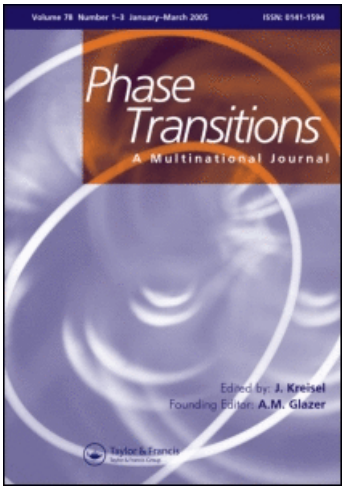

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On the existence of an analytic solution to the 1-D Ising model with nearest and next-nearest neighbor interactions in the presence of a magnetic field

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On the existence of an analytic solution to the 1-D Ising model with nearest and next-nearest neighbor interactions in the presence of a magnetic field

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To solve the controversy, regarding the existence of an analytic solution to the 1-D Ising model with nearest-neighbor (NN) and next-nearest-neighbor (NNN) interactions in the presence of a magnetic field, we apply the transfer matrix method to solve the 1-D Ising model in the presence of a magnetic field, taking both NN and NNN interactions into account. We show that it is possible to write a transfer matrix only if the number of sites is even. Even in such a case, it is impossible to diagonalize the transfer matrix in an analytic form. Therefore, we employ a numerical method to obtain the eigenvalues of the transfer matrix. Moreover, the heat capacity, magnetization, and magnetic susceptibility *versus* temperature for different values of the competition factor (the ratio of NNN to NN interactions) are shown.

Keywords: Ising model; next-nearest interaction; heat capacity; transfer matrix

1. Introduction

1-D Ising models have attracted much interest for a long period of time because they are much easier to be treated theoretically than 2- and 3-D ones [1–7]. Many quasi-1-D magnetic materials have been discovered in recent years, most of them formed by transition metal ions of the 3-D series. Their properties can generally be interpreted in terms of nearest-neighbor (NN) interactions whose sign determines the type of short range order: e.g., ferromagnetic in $CsNiF_3$ and antiferromagnetic in $(CH_3)_4$ $NMnCl_3$ [8]. In recent years, more, complicated 1-D magnetic systems have been synthesized in organic, as well as inorganic, solid state chemistry [9]. In particular, Gatteschi and co-workers investigated a class of quasi-1-D molecular magnetic material [10] $R(hfac)_3$ NITEt ($R = Gd$, Tb, Dy, Ho, Er) [11], whose magnetic properties are determined by rare earth ion with spin $s = 1/2$ and which turned out to be the first example of alternating spin magnetic chains with dominant next-nearest-neighbor (NNN) interactions [12]. The first successful attempt to solve exactly the Ising model with NNN interactions was done by Stephenson

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[13], who obtained the analytical expression for the zero-field static susceptibility in two formal models: NNN interactions and both NN and NNN interactions. Stephenson [13] used an artful contrivance, invented by Dobson [14], in which he reduced the problem under discussion to another one, namely a problem in which the NNN interaction plays the role of the NN interaction and the NN interaction plays the role of a certain "field" [15]. This artful contrivance allowed him to obtain the transfer matrix in the form of 2×2 dimensions and facilitate its solution. Unfortunately, this approach is limited to the zero external magnetic field. The genuine transfer matrix in the presence of a magnetic field should be of 4×4 dimensions, this has been obtained for the first time by Oguchi [16], who also obtained the secular equation, but only in the approximation of zero-temperature.

Deriving the transfer matrix for the model with NN interactions only, both in the presence and in the absence of a magnetic field, is an easy task [17,18]. Pini and Rettori [2] mentioned that it is possible to write the transfer matrix for the model only with even number of sites (N), in the presence of both NN and NNN interactions, but that its analytical solution to find the eigenvalues in the presence of a magnetic field is an impossible task. In a recent study, we have obtained an analytical expression for the partition function of the model when $3 \leq N \leq 14$ by using the Matlab software [19]. The transfer matrix was numerically solved in the thermodynamic limit, to find its maximum eigenvalues. The aim of this study is to write a correct transfer matrix for the model in the thermodynamic limit and then to find its exact solution for non-zero temperature. The results will be used to calculate the dependence of the heat capacity, the magnetization and the magnetic susceptibility on temperature, magnetic field strength, and competition factor (the ratio of NNN to NN interactions).

2. Solving the model *via* transfer matrix method

The Hamiltonian for the Ising model in the presence of a magnetic field, B, taking both NN and NNN interactions into account, is:

$$H = \sum_i J s_i s_{i+1} + \sum_i J_1 s_i s_{i+2} + B \sum_i s_i \tag{1}$$

where J and J_1, are the NN and NNN interactions, respectively, s_i the state of ith spin, and B the magnetic field.

In 2001, Ogly [15] claimed that the transfer matrix can be written as follows:

$$W = \begin{pmatrix} \exp(K+K_1+H/T) & \exp(K-K_1+H/T) & 0 & 0 \\ 0 & 0 & \exp(-K+K_1+H/T) & \exp(-K-K_1+H/T) \\ \exp(-K-K_1-H/T) & \exp(-K+K_1-H/T) & 0 & 0 \\ 0 & 0 & \exp(K-K_1-H/T) & \exp(K-K_1-H/T) \end{pmatrix} \tag{2}$$

where $K \equiv J/k_B T$, $K_1 \equiv J_1/k_B T$, T the absolute temperature, and k_B the Bolzmann factor. On the basis the Equation (2), he suggested that the partition function, Z, can be given as [15]:

$$Z = \mathrm{Tr}[W^N] = \left(\lambda_1^N + \lambda_2^N + \cdots + \lambda_N^N\right) = \lambda_1^N \left(1 + \frac{\lambda_2^N}{\lambda_1^N} + \cdots + \frac{\lambda_N^N}{\lambda_1^N}\right) \approx \lambda_{\max}^N \tag{3}$$

in which,

$$\lambda_{\max} = \frac{\sqrt{a^2 - 4b + 4y}}{4} - a + \sqrt{\left(\frac{\sqrt{a^2 - 4b + 4y} - a}{4}\right)^2 - \frac{y}{2} - \frac{2c - ya}{2\sqrt{a^2 - 4b + 4y}}} \tag{4}$$

where,

$$\begin{aligned} y &= \sqrt[3]{\sqrt{Q} - \frac{q}{2}} + \sqrt[3]{-\sqrt{Q} - \frac{q}{2}} + \frac{b}{3}, \quad Q = \frac{p^3}{27} + \frac{q^2}{4}, \\ p &= -\frac{b^2}{3} + ac - 4\mathrm{d}, \quad q = -\frac{2b^3}{27} + \frac{bac}{3} - \frac{8bd}{3} - a^2 d - c^2, \\ a &= -2e^{J+J'/T}\cosh(H/T), \quad b = 2e^{J'/T}\sinh\left(\frac{2J}{T}\right), \\ c &= 4e^{J'-J/T}\sinh\frac{2J'}{T}\cos\frac{H}{T}, \quad d = -4\sinh^2\frac{2J'}{T}. \end{aligned} \tag{5}$$

Since he claimed that the partition function given in Equation (2) is exact for any values of N, we may check such a claim for any arbitrary value of N. We do such evaluation for $N=4$. Based on the transfer matrix given in Equation (2), the partition function for $N=4$, $Z(4)$, in terms of the reduced magnetic field $h = B/T$ and spin–spin interaction energies K and K_1, can be calculated by Mathematica. The result is as follows:

$$\begin{aligned} Z(4) = \mathrm{Tr}(W^4) = {} & 4\exp(2h) + 4\exp(-4K_1) + 4\exp(-2(h + K_1)) \\ & + \exp(-4(h - K + K_1))\exp(4(h + K + K_1)) + 2\exp(-4K + 4K_1). \end{aligned} \tag{6}$$

Using Equation (1) for the Hamiltonian, however, the exact partition function for $N=4$ can be obtained as,

$$\begin{aligned} Z[4] = {} & \exp(4K + 4K_1 - 4h) + 4\exp(-2h) + 4\exp(-4K_1) \\ & + 2\exp(-4K + 4K_1) + 4\exp(2h) + \exp(4K + 4K_1 + 4h) \end{aligned} \tag{7}$$

which is obviously different from that given in Equation (6), except for $K_1 = 0$.

It is worth mentioning that the element of the transfer matrix for the model is given by Pini and Rettori [2] as follows,

$$\begin{aligned} T\left(s_1^z, s_2^z; s_3^z s_4^z\right) = {} & \exp\left[1/2\beta J_{Rr}\left(s_1^z s_2^z + 2s_2^z s_3^z + s_3^z s_4^z\right)\right]\exp\left[\beta J_{rr} s_2^z s_4^z\right] \\ & \times \exp\left[\beta/2 g_r \mu_B H\left(s_2^z + s_4^z\right)\right] \end{aligned} \tag{8}$$

from which the transfer matrix may be found as,

$$T_{s_1 s_2, s_3 s_4} = \begin{pmatrix} \exp(2K + 2K_1 + 2h) & \exp(K + h) & \exp(-K + h) & \exp(-2K_1) \\ \exp(h - K) & \exp(-2K + 2K_1) & \exp(-2K_1) & \exp(K - h) \\ \exp(K + h) & \exp(-2K_1) & \exp(-2K + 2K_1) & \exp(-K - h) \\ \exp(-2K_1) & \exp(-K - h) & \exp(K - h) & \exp(2K + 2K_1 - 2h) \end{pmatrix} \tag{9}$$

then, the partition function may be given by,

$$Z = \mathrm{Tr}\left[T^{N/2}\right] = \left(\lambda_1^{N/2} + \lambda_2^{N/2} + \lambda_3^{N/2} + \lambda_4^{N/2}\right) \tag{10}$$

which, for $N=4$, gives the same result as Equation (7).

When $h=0$, there is an analytical solution for the transfer matrix, for which the eigenvalues may be found as,

$$\lambda_1 = 1/2\exp(-2K-4K_1)(\exp(6K_1)+2\exp(2K+2K_1)+\exp(4K+6K_1) + \exp(4K_1)(\exp(2K)+1)\sqrt{4\exp(2K)+\exp(4K_1)-2\exp(2K+4K_1)+\exp(4K+4K_1)} \tag{11a}$$

$$\lambda_2 = 1/2\exp(-2K-4K_1)(\exp(6K_1)+2\exp(2K+2K_1)+\exp(4K+6K_1) - \exp(4K_1)(\exp(2K)+1)\sqrt{4\exp(2K)+\exp(4K_1)-2\exp(2K+4K_1)+\exp(4K+4K_1)} \tag{11b}$$

$$\lambda_3 = 1/2\exp(-2K-4K_1)\Big[\exp(6K_1)-2\exp(2K+2K_1)+\exp(4K+6K_1) - \exp(4K_1)(\exp(2K)-1)\sqrt{-4\exp(2K)+\exp(4K_1)-2\exp(2K+4K_1)+\exp(4K+4K_1)}\Big] \tag{11c}$$

$$\lambda_4 = 1/2\exp(-2K-4K_1)\Big[\exp(6K_1)-2\exp(2K+2K_1)+\exp(4K+6K_1) + \exp(4K_1)(\exp(2K)-1)\sqrt{-4\exp(2K)+\exp(4K_1)-2\exp(2K+4K_1)+\exp(4K+4K_1)}\Big] \tag{11d}$$

however, if $h\neq 0$, there is no analytical solution for the matrix, as mentioned by Pini and Rettori [2].

3. Results and discussion

We have solved the transfer matrix numerically for the model to obtain its largest eigenvalue for 1-D Ising model, including both NN and NNN interactions. Based on a numerical calculation of the partition function, the heat capacity, C_v, is obtained by using the periodic boundary condition for the model in the presence of a magnetic field for different values of the competition factor (ratio of the NNN to NN interaction energies) $n = K_1/K = 0.2$, 0.3, 0.4, 0.5, and 0.6. The results for the reduced heat capacity *versus* temperature for given values of n and $f=0.15$ (the ratio of magnetic field-spin interaction to that of the NN spin–spin interaction energy) are shown in Figure 1. According to Figure 1, on increasing the ratio n, the peak shifts to a higher temperature. Also, the reduced heat capacity *versus* temperature for different values of magnetic field is shown in Figure 2, when $f=0.15$ and $n=0.20$. We should note that, the heat capacity can be analytically obtained when $B=0$ and $N\to\infty$, by taking into account that:

$$Z = \mathrm{Tr}[T]^{N/2} = \left(\lambda_1^{N/2}+\lambda_2^{N/2}+\lambda_3^{N/2}+\lambda_3^{N/2}\right) = \lambda_1^{N/2}\left(1+\frac{\lambda_2^{N/2}}{\lambda_1^{N/2}}+\frac{\lambda_3^{N/2}}{\lambda_1^{N/2}}+\frac{\lambda_4^{N/2}}{\lambda_1^{N/2}}\right) \tag{12}$$

For $N\to\infty$, the partition function is approximately equal to

$$Z = (\lambda_1)^{\frac{N}{2}} \tag{13}$$

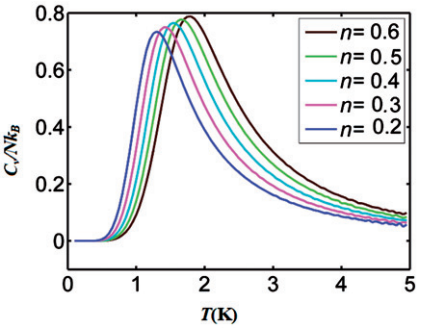

Figure 1. Heat capacity *vs.* temperature for different values of the competition factor (ratio of NNN to NN interaction energies) $n = 0.2$, 0.3, 0.4, 0.5, and 0.6.

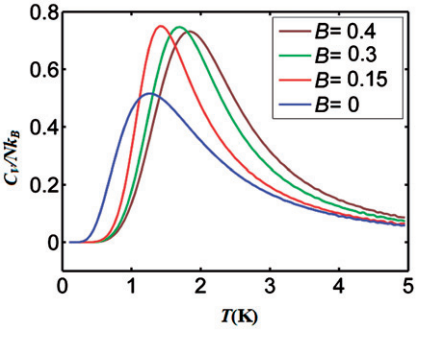

Figure 2. Heat capacity *vs.* temperature for different magnetic fields $B = 0$, 0.15, 0.3, and 0.4.

then

$$\frac{C_v}{Nk} = -T\frac{\partial^2 F}{\partial T^2} = -1/2T\frac{\partial}{\partial T}\frac{\partial}{\partial T}(-T\ln(\lambda_1)). \tag{14}$$

One can use the expression for λ_1 given in Equation (11a), to obtain an analytical expression for C_v at $B = 0$. We notice that, according to Figure 2, the peak in the heat capacity shifts to a higher temperature when B increases. Figure 2 of this study is quite different from the corresponding result of reference [15] (see Figure 9 therein). Having the partition function, one may simply use the formula

$$M = -\frac{\partial F}{\partial H} \tag{15}$$

to calculate magnetization M. The calculated reduced magnetization is shown in Figure 3, as a function of T for different values of B.

As shown in Figure 3, the magnetization goes to zero at a higher temperature when the magnetic field is stronger. At a low temperature, the system is in an ordered state. By raising temperature it becomes partially disordered. The extent of disorder depends on both T and B, as shown in Figure 3. Magnetization *versus* magnetic field is plotted for different values of n as shown in Figure 4.

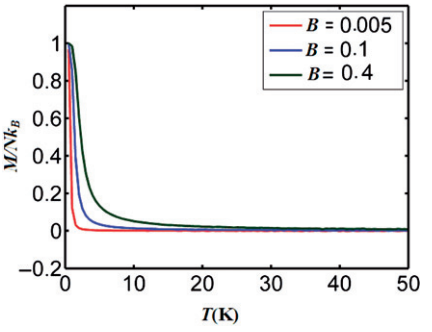

Figure 3. Reduced magnetization *vs.* temperature for given values of the reduced magnetic field $B = 0.005$, 0.1, and 0.4 (in units of tesla).

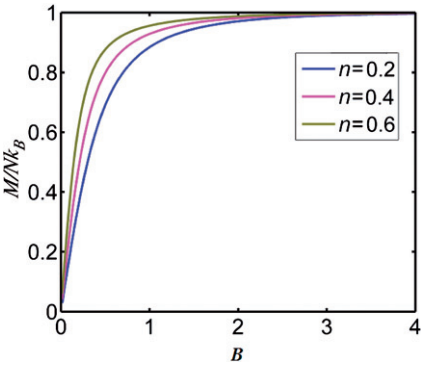

Figure 4. Reduced magnetization *vs.* magnetic field for different values of the competition factor $n = 0.2$, 0.4, and 0.6.

According to Figure 4, the magnetization is zero in zero magnetic field. Increasing the magnetic field, the magnetization increases and the system goes into an ordered state. For a strong magnetic field, the spins in the system do not respond further to the external magnetic field and the magnetization remains constant. Moreover the thermal magnetic susceptibility

$$\chi = -\frac{\partial^2 F}{\partial^2 H} \tag{16}$$

versus temperature, which is given for different values of the competition factor and $f = 0.2$, is shown in Figure 5.

4. Conclusions

A model consisting of a 1-D array of spins interacting through NN and NNN interactions is studied in the thermodynamic limit in the presence of a magnetic field. It is shown that in general there is no analytical solution for the model. Therefore, a numerical approach must be used to solve the transfer matrix. The heat capacity *versus* temperature for

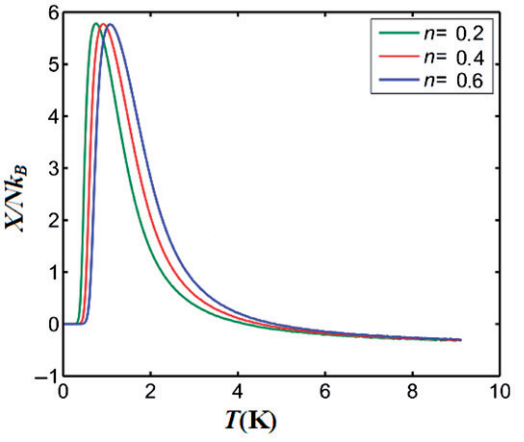

Figure 5. Reduced magnetic susceptibility *vs.* temperature for different values of the competition factor $n = 0.2$, 0.4, and 0.6.

different values of the competition factor and magnetic field are shown (Figures 1 and 2), and it is shown that, by increasing the competition factor and the magnetic field, the peak in the heat capacity shifts to a higher temperature. The magnetization is also calculated *versus* the magnetic field and temperature (Figures 3 and 4). At low temperatures, the magnetization is high and the system is typically in the ordered ferromagnetic phase, while with increasing temperature the magnetization (order parameter) decreases and finally approaches zero. The magnetization in weak magnetic fields is small, but it increases with magnetic field, until it reaches a constant (saturated) state. The thermal magnetic susceptibility is also presented for given values of the competition factor (Figure 5).

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