SAKARYA UNIVERSITY
JOURNAL OF SCIENCE

e-ISSN: 2147-835X
http://www.saujs.sakarya.edu.tr

Received
20-04-2018
Accepted
15-10-2018

Doi
10.16984/saufenbilder.417384

Investigation of Magnetic Properties of Spin 5/2 Ising Chain by Using Transfer Matrix Method

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Abstract

A magnetic property of the one dimensional spin 5/2 Ising model under the magnetic field has been investigated by means of transfer matrix method. Thermodynamic response functions are also obtained for varying values of temperature (in K) and scaling magnetic field. Entropy and heat capacity of the system were calculated by benefiting from the temperature dependencies of Helmholtz free energy. We observed that the heat capacity tends to shift to the relatively higher temperature regions as the strength of the magnetic field is increased, and these findings are consistent with previous results for the low spin values in one dimensional Ising systems.
Keywords: Magnetic properties, Ising chain, Transfer matrix method, Low dimensional systems

1. INTRODUCTİON

Recent years, the thermodynamic properties of magnetic materials have been studied in many experimental and theoretical studies because of their potentials in nanotechnology industry [1-3]. These materials can be produced in the laboratory and their magnetic properties can be experimentally measured to use in industrial applications such as storage devices, industrial magnets and sensors [1-3].

The size of the nanomaterial affects significantly the magnetic properties in small-scale applications. Many theoretical models such as mean field theory [4], effective field theory [5], Monte Carlo simulation method [6], Green's function formalism [7] and transfer matrix method [8] have been used to investigate the unique properties of these materials in one-dimensional (1D) and two-dimensional (2D) systems. Ising model [9], can be used to describe the material properties such as phase transition and temperature dependent magnetization.

Recent works are mainly focused on exactly solvable spin 1/2 and spin 1 systems based on Monte Carlo and Ising models [10, 11]. This kind of spin chain compounds shows a 1D ferromagnetic behavior modeled by spin chains [12]. In many theoretical studies on the thermodynamic properties, the spin 1/2 Ising system is used for the 1D chain structures.

The exact solution for the 1D Ising systems under external magnetic field was reported in previous work by Kassan-Ogly [13] including nearest neighbor and next-nearest neighbor interactions. The temperature behavior of the spin-correlation function in 1D spin 1 Ising model has been still studied in many theoretical works [11, 14]. Using only spin 1/2 and 1 is too idealized in theoretical studies, and this cannot represent the magnetic materials used in industrial applications such as permanent magnet. Therefore, the studies are expanded to higher spin systems greater than spin

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1. It is well known that the analysis of spin systems becomes difficult for the higher spin values.
The investigation of higher-order spin systems has been theoretically studied many decades ago by Anderson [15] and Kittel [16]. Then, in many experimental studies, the higher-order spin couplings have been observed in some magnetic compounds such as MnO and NiO [17]. The magnetic properties of this kind of complex systems were originally introduced by Iwashita et al. [18]. To understand the spin interactions for magnetic materials, the investigation of higher-order spin system such as 1D spin 2 or 5/2 systems becomes important. For instance, the disordered $Fe_{(1-q)}$ Al_q alloys show higher-order spin values, spin 2 and spin 5/2, for Fe^{+2} and Fe^{+3}, respectively [19], and these spin 5/2 systems have been modeled by using different theoretical methods [20-22].
In this work, we study the spin 5/2 in 1D chain system by using Ising model with transfer matrix method (TMM). This model is successfully applied to investigate numerically the magnetic properties of 1D system due to the hardness of exactly solving the higher-order spin systems.

2. MODEL AND METHOD

The Hamiltonian for the 1D spin 5/2 Ising model with the presence of an external field is given by

$$\mathcal{H} = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j - H\sum_i\sigma_i \tag{1}$$

where J denotes the exchange coupling of ferromagnetic type (J > 0), $\langle ij\rangle$ represents nearest neighbor interaction and the field H is units of energy. σ spin values can be taken as

$$\sigma = \pm\frac{5}{2}, \pm\frac{3}{2}, \pm\frac{1}{2} \tag{2}$$

The partition function constructed by using periodic boundary conditions is given as

$$Z = \sum_{\{\sigma_i\}} e^{-\beta\mathcal{H}(\{\sigma_i\})} = \sum_{\{\sigma_i\}} e^{\beta J\sum_i\left(\sigma_i\sigma_{i+1} + \beta H\left(\frac{\sigma_i+\sigma_{i+1}}{2}\right)\right)} \tag{3}$$

Here $\beta = 1/k_BT$, k_B is the Boltzmann constant. We have used the transfer matrix method (TMM) [23, 24] to perform the statistical analysis of the considered system. The matrix elements of transfer matrix can be defined by

$$\langle\sigma_i|TM|\sigma_{i+1}\rangle = exp\left\{\beta\left[J\sigma_i\sigma_{i+1} + \frac{1}{2}H(\sigma_i + \sigma_{i+1})\right]\right\} \tag{4}$$

Transfer matrix of the 1D spin 5/2-system is given as

$$TM \equiv \begin{pmatrix} e^{\frac{25}{4}\tilde{\beta}\tilde{J}+\frac{5}{2}\tilde{\beta}h} & e^{\frac{15}{4}\tilde{\beta}\tilde{J}+2\tilde{\beta}h} & e^{\frac{5}{4}\tilde{J}\tilde{\beta}+\frac{3}{2}\tilde{\beta}h} & e^{-\frac{5}{4}\tilde{J}\tilde{\beta}+\tilde{\beta}h} & e^{-\frac{15}{4}\tilde{J}\tilde{\beta}+\frac{1}{2}\tilde{\beta}h} & e^{-\frac{25}{4}\tilde{J}\tilde{\beta}+\tilde{\beta}h} \\ e^{\frac{15}{4}\tilde{\beta}\tilde{J}+2\tilde{\beta}h} & e^{\frac{9}{4}\tilde{\beta}\tilde{J}+\frac{3}{2}\tilde{\beta}h} & e^{\frac{3}{4}\tilde{\beta}\tilde{J}+\tilde{\beta}h} & e^{-\frac{3}{4}\tilde{\beta}\tilde{J}+\frac{1}{2}\tilde{\beta}h} & e^{-\frac{9}{4}\tilde{\beta}\tilde{J}+\tilde{\beta}h} & e^{-\frac{15}{4}\tilde{\beta}\tilde{J}-\frac{1}{2}\tilde{\beta}h} \\ e^{\frac{5}{4}\tilde{\beta}\tilde{J}+\frac{3}{2}\tilde{\beta}h} & e^{\frac{3}{4}\tilde{\beta}\tilde{J}+\tilde{\beta}h} & e^{\frac{1}{4}\tilde{\beta}\tilde{J}+\frac{1}{2}\tilde{\beta}h} & e^{-\frac{1}{4}\tilde{\beta}\tilde{J}} & e^{-\frac{3}{4}\tilde{\beta}\tilde{J}-\frac{1}{2}\tilde{\beta}h} & e^{-\frac{5}{4}\tilde{\beta}\tilde{J}-\frac{3}{2}\tilde{\beta}h} \\ e^{-\frac{5}{4}\tilde{\beta}\tilde{J}+\tilde{\beta}h} & e^{-\frac{3}{4}\tilde{\beta}\tilde{J}+\frac{1}{2}\tilde{\beta}h} & e^{-\frac{1}{4}\tilde{\beta}\tilde{J}} & e^{\frac{1}{4}\tilde{\beta}\tilde{J}-\frac{1}{2}\tilde{\beta}h} & e^{\frac{3}{4}\tilde{\beta}\tilde{J}-\tilde{\beta}h} & e^{\frac{5}{4}\tilde{\beta}\tilde{J}-\frac{3}{2}\tilde{\beta}h} \\ e^{-\frac{15}{4}\tilde{\beta}\tilde{J}+\frac{1}{2}\tilde{\beta}h} & e^{-\frac{9}{4}\tilde{\beta}\tilde{J}} & e^{-\frac{3}{4}\tilde{\beta}\tilde{J}-\frac{1}{2}\tilde{\beta}h} & e^{\frac{3}{4}\tilde{\beta}\tilde{J}-\tilde{\beta}h} & e^{\frac{9}{4}\tilde{\beta}\tilde{J}-\frac{3}{2}\tilde{\beta}h} & e^{\frac{15}{4}\tilde{\beta}\tilde{J}-2\tilde{\beta}h} \\ e^{-\frac{25}{4}\tilde{\beta}\tilde{J}} & e^{-\frac{15}{4}\tilde{\beta}\tilde{J}-\frac{1}{2}\tilde{\beta}h} & e^{-\frac{5}{4}\tilde{\beta}\tilde{J}-\tilde{\beta}h} & e^{\frac{5}{4}\tilde{\beta}\tilde{J}-\frac{3}{2}\tilde{\beta}h} & e^{\frac{15}{4}\tilde{\beta}\tilde{J}-2\tilde{\beta}h} & e^{\frac{25}{4}\tilde{\beta}\tilde{J}-\frac{5}{2}\tilde{\beta}h} \end{pmatrix} \tag{5}$$

where we use the dimensionless parameters for numerical simplicity.
We scale our parameter with J so $\tilde{J} = \frac{J}{J} = 1.0$, where $h = H/J$ scaling field parameter and $\tilde{\beta} = J/k_BT$ scaling inverse thermodynamic temperature.
Since the matrix is identical for $(\sigma_1\sigma_2)$, $(\sigma_2\sigma_3)$ and so on, the partition function is then given by

$$Z = \sum_{\{\sigma_i\}}(TM)^N = Tr\,(TM)^N = \sum_{i=1}^{6}\lambda_i^N \tag{6}$$

while $N \gg 1$ the Helmholtz free energy is $F = -k_BTln(\lambda^>)$ where $\lambda^>$ is the biggest eigenvalues of TM in equation (5). We can construct thermodynamic expressions as internal energy E equation (7), ferromagnetic order parameter (magnetization) m equation (8), the magnetic susceptibility χ equation (9), entropy S equation (10) and the specific heat C equation (11) by using Helmholtz free energy F.

$$E = -\left(\frac{\partial ln(\lambda^>)}{\partial\beta}\right)_h \tag{7}$$

$$m = -\left(\frac{\partial F}{\partial h}\right)_T \tag{8}$$

$$\chi = -\left(\frac{\partial^2 F}{\partial h^2}\right)_T = \left(\frac{\partial m}{\partial h}\right)_T \tag{9}$$

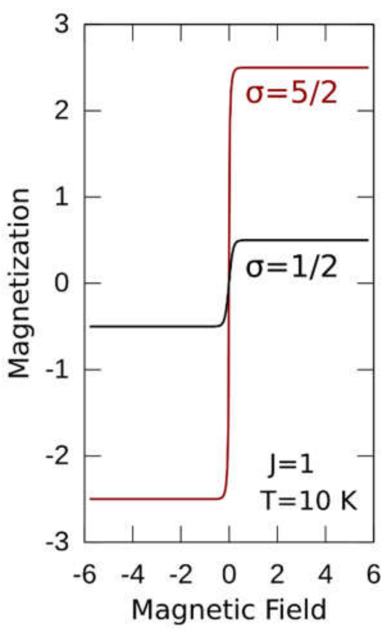
$$S = -\left(\frac{\partial F}{\partial T}\right)_h \tag{10}$$

$$C = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_h = T\left(\frac{\partial S}{\partial T}\right)_h \tag{11}$$

3. RESULTS

We studied the magnetic properties of 1D spin 5/2 system by using the transfer matrix method. In 1D Ising model (N >> 1) the phase transition to the ferromagnetic behavior happens at the critical temperature 0. Free energy is clearly analytic for finite temperature, and there can not be seen any phase transition at any finite temperature (T > 0). Thus in the linear-chain Ising model, spontaneous magnetization is not possible.

We have performed the magnetization behavior as a function of applied magnetic field to understand the differences between the low spin order and higher order spin systems, see Figure 1. It is easy to say that the maximum magnetization value for the spin 1/2 system is 0.5, while the maximum magnetization value for the spin 5/2 system is 2.5 as we expected.



The magnetizations were calculated at T = 5, 100 and 300 K as functions of reduced magnetic field. The magnetization (m) behavior at lower (T=5, 100 K) and higher temperatures (T=300 K), and the magnetization as a function of dimensionless magnetic field (h) and temperature are given in Figure 2.

The magnetization for any value of h at absolute zero is equal to the saturation value 5/2, which implies ferromagnetic order in considering system. This means that phase transition occurs at T=0, and no phase transition occurs at any finite temperature. At low temperature the spins align easily but contrary at high temperature to align the spins a strong magnetic field should be applied. We observed that the magnetization behavior with the change of magnetic field becomes more smooth and wider with the increase of the temperature, see Figure 2 a). When the temperature is close the critical temperature, the response of magnetization to the field becomes sharper. The magnetization becomes a step function at T=0 K ($\beta \rightarrow \infty$). In 1-D system the critical temperature is 0 K, and the linear response of magnetization for a small magnetic field infinitely sharp. The changes in temperature determine how sharply magnetization saturates with the change of applied magnetic field. Results show that the saturation at low temperature requires a small magnetic field, but at higher temperature values it requires ha igher magnetic field.

a) b)

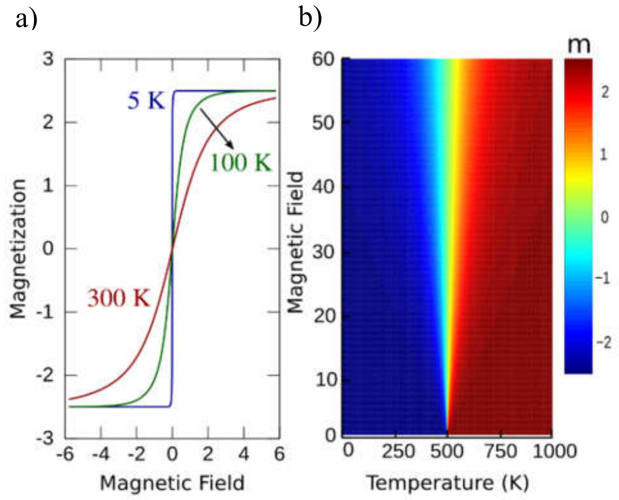


Figure 2. a) Magnetization behavior of 1D spin 5/2 system
aFigure 1. Magnetization as a function of dimensionless bmagnetic field (h) for spin 1/2 and 5/2 at 10 K. The 1exchange copuling parameter (J) is 1.

It is worth mentioning that the magnetization responds extremely sensitive to the applied magnetic field in the limit of the low temperature values.

We have also observed that the magnetization can be controlled by tuning the energy (E) and entropy (S). The energy favors the largest possible value of m which is aligned with the applied field. Therefore, the equilibrium m value can be minimized by the Helmholtz free energy (F), see Figure 3.

The equilibrium value of m is that minimizes F. In Figure 3, we see that only one minimum for all different temperature values and the free energy is minimum at m = 0. This supports the reason of being only one phase for the considering system. The ferromagnetic system can either have +5/2 or -5/2 values and thus, the F would choose only one favorite value.

The changes in entropy and internal energy of considered system with respect to temperature for different magnetic field (h = 0.1, 1.0 and 2.5) are given in Figure 4.

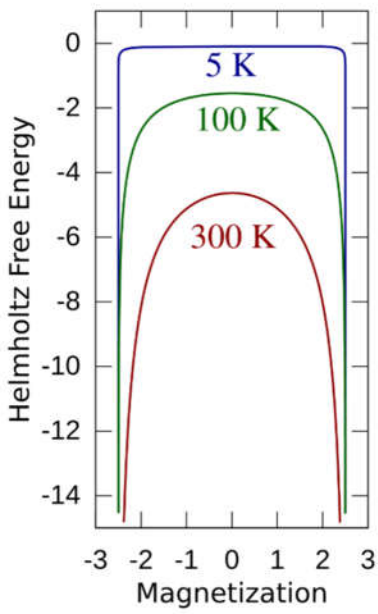


Figure 3. Helmholtz free energy as a function of magnetization at T=5, 100 and 300 K.

Results show that the higher h values (h=2.5) at critical temperature give rise to higher internal energy, and the internal energy converges to the zero at higher temperature values. At low T and h, the entropy becomes constant rapidly, while the energy becomes constant at higher temperatures for higher h values, see Figure 4 a).

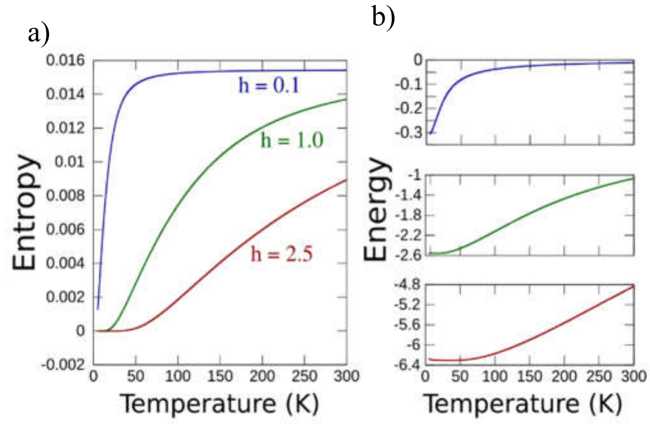


Figure 4. a) Entropy and b) Energy as a function of temperature for h=0.1, 1.0 and 2.5.

In the limit of T→0 entropy goes to zero S →0. An ideal Ising chain would certainly obtain all its entropy of ordering above 0 K. To increase the temperature of the system, one needs to apply heat and adding heat to the system increases its entropy. As the field increases, more thermal energy is required to achieve saturation values of entropy (see Figure 4).

The magnetic susceptibility (χ) of the system is calculated by the derivative of magnetization. The magnetic field dependence of the susceptibility is reported in Figure 5 in the case of T=5, 100 and 300 K. The susceptibility peaks show that the maximum of χ is larger for low temperature value. The critical point is h=0 and diverges as T→0. However, it is important to note that the singularity is not of the power law type instead it is exponential [22].

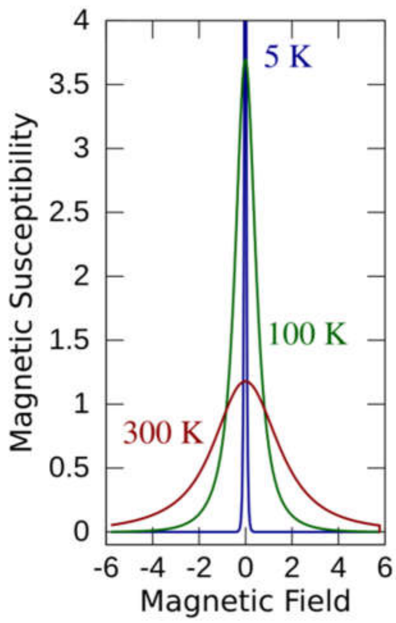


Figure 5. Magnetic susceptibility as a function of magnetic field at 5, 100 and 300 K.

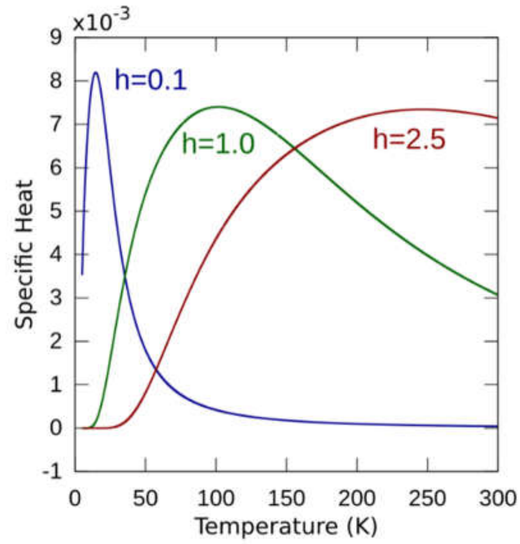


Figure 6. Specific heat as a function of temperature for h=0.1, 1.0 and 2.5.

We know how much energy changes with increasing of the temperature from the specific heat (C). The specific heat is a smooth function of temperature (finite at all temperatures) and vanishing at zero temperature. As expected there is no critical point at a finite temperature which corresponds to the singular behavior of specific heat. Specific heat values at T=15, 102 and 246 K are presented with the maximum for h=0.1, 1.0 and 2.5, respectively in Figure 6. If the magnetic field is increased, the peak of the specific heat at constant volume is shifted to higher temperature region as seen in Figure 6.

4. CONCLUSİON

Equilibrium properties of one dimensional spin 5/2 Ising system under magnetic field were studied by using transfer matrix method. Thermodynamic response functions are obtained for varying values of temperature and scaled magnetic field. We obtained the internal energy and specific heat as a function of temperature. Our numerical results show that heat capacity tends to shift to the relatively higher temperature regions as the magnetic field is increased and the curves are a broad maximum for higher magnetic field values. We have presented the graph in a magnetization-free energy (m-F) plane for different temperature values. Because of Helmholtz free energy has only one minimum, there is one phase for the considering system. Our results are conceptually consistent with the previous results for the lower spin systems in one dimensional Ising chain.

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