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Exact solutions of the one-dimensional, two-dimensional, and three-dimensional Ising models

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ABSTRACT

According to the traditional solutions, there is no magnetisation in the one-dimensional Ising model in the absence of external magnetic field. It is shown that there is a mistake within them. In them, local order of spins was not taken into account and the partition function and the correlation function were calculated wrongly. In this paper, that mistake is improved and a new solution is presented. According to it, there is ferromagnetism in that model. Analogously, solutions of the two-dimensional and three-dimensional Ising models are obtained.

KEYWORDS

Magnetic materials;
Nanostructures;
Magnetic properties;
Magnetic structure;
Phase transitions.

INTRODUCTION

There is a well-known result in physics of phase transitions: the one-dimensional Ising model in the absence of external magnetic field has no magnetic phase transition. It has been a paradox since the predictions of Weiss' mean field theory are independent of lattice dimensionality and hence the linear chain is predicted to undergo a phase transition at non-zero temperature.[1-3] However, it is shown that there are mistakes in the traditional solutions in the calculation of the correlation function and the partition function. Another method for solving this problem is proposed. Using it, one can show that the one-dimensional Ising model displays spontaneous magnetisation which decreases asymptotically to zero with the temperature. The new method is applied to the two-dimensional and three-dimensional problems and exact solutions are obtained. They also produce magnetisation which decreases asymptotically to zero with the temperature.

THEORY

Lest us consider the one-dimensional Ising model in the absence of external magnetic field.[1] The Hamiltonian of a chain of N atoms is of the form

$$\hat{\mathbf{H}} = -\sum_{i=1}^{N-1} \mathbf{J}_i \mathbf{s}_i \mathbf{s}_{i+1} \qquad (1)$$

where the spins s_i are one-dimensional unit vectors assuming only the discrete values +1 and -1 and J_i is the interaction energy between spins situated on sites i and $i + 1$. Positive J_i favours parallel and negative J_i antiparallel alignment of the spins. The partition function is

$$\mathbf{Z}_N = \mathbf{Z}_N(\mathbf{J}_1, \mathbf{J}_2, ..., \mathbf{J}_{N-1}) = \sum_{s_1=-1}^{1} \sum_{s_2=-1}^{1} ... \sum_{s_N=-1}^{1} \exp\left(\sum_{i=1}^{N-1} \beta \mathbf{J}_i \mathbf{s}_i \mathbf{s}_{i+1} \right) \qquad (2)$$

Where $\beta = \frac{1}{kT}$.

For a chain of 2 spins the Hamiltonian will be

$$\hat{H} = -J_1 s_1 s_2 \quad (3)$$

The partition function is

$$Z_2 = Z_2(J_1) = \sum_{s_1=-1}^{1} \sum_{s_2=-1}^{1} \exp(\beta J_1 s_1 s_2) = 4\cosh(\beta J_1) \quad (4)$$

Now we can calculate the nearest-neighbour correlation function for a chain of two spins:

$$\Gamma_1(1) \equiv \langle s_1 s_2 \rangle = Z_2^{-1} \sum_{\{s\}} s_1 s_2 \exp(\beta J_1 s_1 s_2) = \tanh(\beta J_1) \quad (5)$$

where summation is over spins s_1 and s_2. In Ref. 1, using a more tedious derivation it was shown that for a chain of N spins

$$\Gamma_k(1) = \tanh(\beta J_k) \quad (6)$$

Indeed, the expression for $\Gamma_k(1)$ does not depend on the number of spins in the chain.

In Ref. 1, the two-spin correlation function for a chain of N spins was calculated:

$$\Gamma_k(r) \equiv \langle s_k s_{k+r} \rangle = Z_N^{-1} \sum_{\{s\}} s_k s_{k+r} \exp\left(\sum_{i=1}^{N-1} \beta J_i s_i s_{i+1} \right) \quad (7)$$

where the symbol $\{s\}$ denotes the N-fold summation of Eq. (2). Here r is the distance between spins, in units of a lattice constant. It equals

$$\Gamma_k(r) = \tanh(\beta J_k) \tanh(\beta J_{k+1}) ... \tanh(\beta J_{k+r-1}) = \prod_{i=1}^{r} \tanh(\beta J_{k+i-1}) \quad (8)$$

Now we can find the temperature at which long-range order sets in, i.e. the temperature at which the two-spin correlation function falls off sufficiently slowly with the interspin distance r that the magnetisation becomes non-zero. The squared normalized zero-field magnetisation is:[1]

$$\sigma^2 = \frac{M(T, H=0)^2}{M(T=0, H=0)^2} = \lim_{r \to \infty} \Gamma_k(r) \quad (9)$$

From Eq. (8) we see that the hyperbolic tangents are less than one and hence the products approach zero in the limit of infinite r. The linear chain therefore displays zero spontaneous magnetisation for all non–zero values of the temperature. Nevertheless, there is a mistake in the proof given by Eqs. (8) and (9). Consider a chain consisting of 100 spins, $J_k = J$ for all k, and $\Gamma_k(1) = 0.99$. Its squared magnetisation from Eqs. (8) and (9) is $\sigma^2 \sim 0.37$. Now let us assume that $J_{50} = 0$. Then from Eqs. (8) and (9), $\sigma^2 = 0$. It is a wrong result. In reality the chain will split into two chains with $\sigma^2 \sim 0.61$ each. It proves that the previous solution is wrong.

There is a flaw in the proof given by Eqs. (8) and (9). Let us assume theoretically that the correct solution of the Ising model exists and, according to it, in the chain 90% of the spins are up and 10% are down. (Stanley in Ref. 1 presented the same argument: "Suppose the contrary, namely that there exists a phase transition with $T_c > 0$. Then for some $T < T_c$ let us 'flip' half the chain to assume an opposite polarity.") Then Eqs. (8) and (9) predict that magnetisation of this chain is zero.

Eq. (8) is of the form

$$\Gamma_k(r) = \langle s_1 s_2 \rangle \langle s_2 s_3 \rangle \langle s_3 s_4 \rangle ... \quad (10)$$

where every factor is less than unity. Imagine an infinite chain of vectors which is constructed by the following rule: orientation of a vector depends on that of its left neighbour: if the neighbour is up then with the probability 90% the vector is up. If the neighbour is down then with the probability 9 0% the vector is up. Eq. (10) predicts that the long range correlation function for this chain is zero, which is wrong.

Consider an infinite Ising chain with a strong correlation, for example, $\Gamma_k(1) = 0.99$. It means that almost all neighbour spins are aligned so as the central one, k. Two cases are possible. The first one: a chain with about 99% of the spins turned up and only about 1% of them turned down. Such chain will possess magnetisation according to the definition of the correlation function, although the previous solution results in no magnetisation in it. The second case is: the chain consists of domains, each one consists in average of 50 spins. In some of the domains the spins are turned up, and in others they are turned down. The net magnetisation is zero. If $\Gamma_k(1) = 0.999$ then the chain consists of domains of about 500 spins, etc. It is already a new result. If there is no magnetisation at all, then such chain has equal number of spins up and down, and they are oriented randomly, that is its correlation $\Gamma_k(1) = 0$. It contradicts the definition of the problem: $\Gamma_k(1) = 0.99$ and, from Eq. (6), $\Gamma_k(1) = 0$ only at $J_k = 0$ or $T \to \infty$.

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One can suppose that the first case takes place because $\Gamma_k(1)$ is identical for every k, and the directions of spins must be also identical for all $k \neq j$ (j is the index of spins directed down, they are about 1% of the total spin number) due to symmetry of the problem.

The magnetisation of an Ising chain will be equal to that of an averaged elementary cell. The elementary cell consists of a spin and its nearest neighbour. The magnetisation of the chain is,

$$\sigma^2 = \frac{\sum_{i=1}^{N-1} \tanh(\beta J_i)}{N-1} \approx \tanh(\beta < J_i >) \quad (11)$$

here $< J_i >$ is an average interaction energy. In the uniform case, $J_i = J$, the squared normalized zero-field magnetisation is

$$\sigma^2 = \tanh(\beta J) \quad (12)$$

And

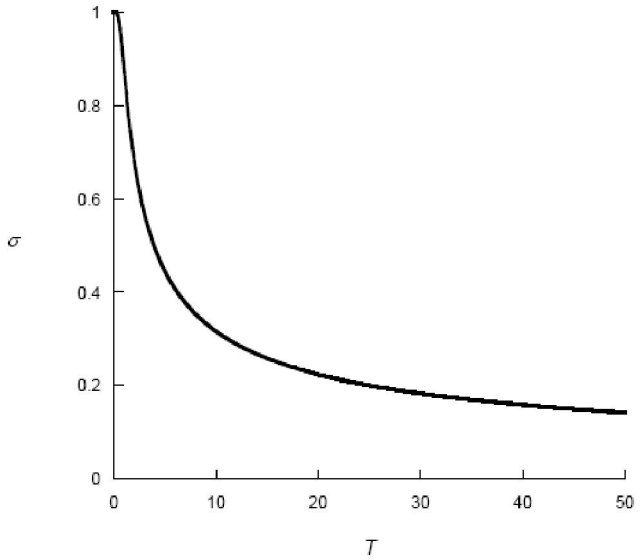

Figure 1: Dependence of the spontaneous magnetisation per spin σ on temperature *T* for the one-dimensional Ising model, Eq. (13), *J* = 1.

$$\sigma = [\tanh(\beta J)]^{0.5} \quad (13)$$

The plot of this function is given in Figure 1. The magnetisation decreases from unity at $T = 0$ and asymptotically tends to zero with the temperature. Mean field theory predicts that the Ising model acquires magnetism at $T \leq T_c$ [1, 3] where T_c can be found from

$$kT_c = zJ \quad (14)$$

Here z is the number of nearest neighbours. This formula is valid for all dimensions. Mean field theory produces the following equation:

$$\sigma = \tanh(z\beta J\sigma) \quad (15)$$

If we denote the magnetisation of an elementary cell of the crystal lattice by M_i then the magnetisation of the two- and three-dimensional Ising lattices is

$$M = \frac{\sum_{i=1}^{N_{cells}} M_i}{N_{cells}} \quad (16)$$

where N_{cells} is the number of the elementary cells. In the uniform case of equal J, the normalized magnetisation σ is equal to that of one elementary cell. For that case, σ for hexagonal lattice, square lattice and simple cubic lattice can be written as

$$\sigma = \left[\frac{\sum_{k=1}^{3} \Gamma_k(1)}{3}\right]^{0.5} \quad (17)$$

$$\sigma = \left[\frac{\sum_{k=1}^{4} \Gamma_k(1)}{4}\right]^{0.5} \quad (18)$$

and

$$\sigma = \left[\frac{\sum_{k=1}^{12} \Gamma_k(1)}{12}\right]^{0.5} \quad (19)$$

respectively. To calculate $\Gamma_k(1)$, one must find the partition function of the elementary cell. The energy of the hexagonal lattice is

$$\hat{H} = E_1 + E_2 + E_3 + \ldots = \frac{-J_1 s_1 s_2 - J_2 s_2 s_3 - J_3 s_3 s_1}{2} + \frac{-J_4 s_2 s_4 - J_5 s_4 s_3 - J_2 s_3 s_2}{2} + \ldots \quad (20)$$

Here the first term on the right hand side is the contribution of the first elementary cell, the second term is that of the adjacent cell, etc. The Hamiltonian of one cell in a lattice differs from that of a single triangle by division by 2 because every term in the numerator is taken twice ($J_2 s_2 s_3$ and $J_2 s_3 s_2$ in Eq. (20)). For the cubic lattice, it differs from that of a single cube by division by 4. The partition function of the hexagonal lattice

in the uniform case is:

$$Z_{hex} = \sum_{\{s\}} \exp[\beta(E_1 + E_2 + E_3 + ...)] = Z_1 Z_2 Z_3 ... \quad (21)$$

where Z_1, Z_2, Z_3, ... are the partition functions of the elementary cells. The partition function of a cell in the hexagonal lattice in the uniform case is:

$$Z_i = 2\exp(1.5J) + 6\exp(-0.5J) \quad (22)$$

Now let us find the nearest-neighbour correlation function between spin 1 and spin 2, $\Gamma_1(1)$, it equals all other nearest-neighbour correlation functions:

$$\Gamma_1(1) = \frac{\sum_{\{s\}} s_1 s_2 \exp[\beta(E_1 + E_2 + E_3 + ...)]}{Z_{hex}} =$$

$$\frac{\sum_{\{s\}} s_1 s_2 \exp(\beta E_1) \sum_{\{s\}} \exp(\beta E_2) \sum_{\{s\}} \exp(\beta E_3) ...}{Z_1 Z_2 Z_3 ...} = \quad (23)$$

$$\frac{\sum_{\{s\}} s_1 s_2 \exp(\beta E_1)}{Z_1}$$

where E_1, E_2, E_3, ... are defined in Eq. (20). So, this correlation function is

$$\Gamma_1(1) = \Gamma_k(1) = \frac{2\exp(1.5J) - 2\exp(-0.5J)}{2\exp(1.5J) + 6\exp(-0.5J)} \quad (24)$$

and the magnetisation is:

$$\sigma = \left[\frac{\exp(1.5J) - \exp(-0.5J)}{\exp(1.5J) + 3\exp(-0.5J)}\right]^{0.5} \quad (25)$$

The plot of this function is given in Figure 2.

Using this method initially developed in Ref. 1, one can easy show that the long range correlation function is

$$\Gamma_k(r) = [\Gamma_1(r)]^r \quad (26)$$

It tends to zero with r and, therefore, according to Ref. 1, the hexagonal two-dimensional lattice possesses no spontaneous magnetisation. This result contradicts the traditional solution for the two-dimensional case and is another evidence that the proof proposed in Ref. 1 (Eqs. (8), (9)) is untenable.

Analogously, one can show that the partition function of a cell in the square lattice in the uniform case is:

$$Z_i = 4\cosh(2J) + 12 \quad (27)$$

the nearest-neighbour correlation function is

$$\Gamma_k(1) = \frac{4\sinh(2J)}{4\cosh(2J) + 12} \quad (28)$$

and the magnetisation is:

$$\sigma = \left[\frac{\sinh(2J)}{\cosh(2J) + 3}\right]^{0.5} \quad (29)$$

Again, the long range correlation function is $[\Gamma_1(r)]^r$ and the magnetisation of this lattice must be zero according to Ref.1. The plot of this σ is shown in Figure 2.

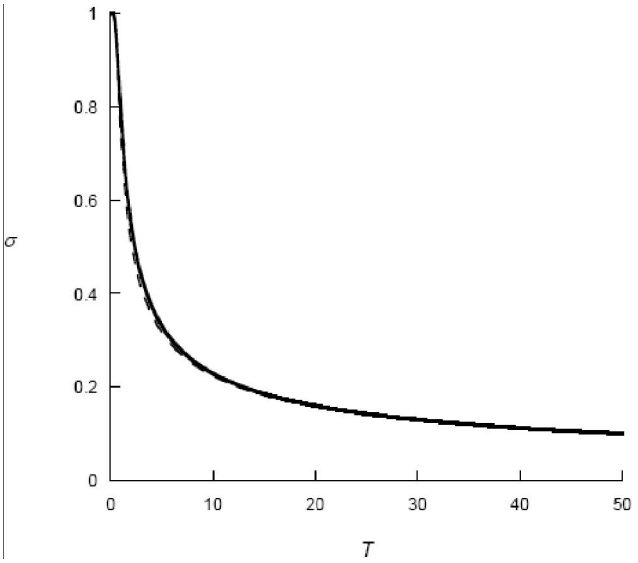

Figure 2 : Dependence of the spontaneous magnetisation per spin σ on temperature T for the two-dimensional hexagonal lattice (solid line) and two-dimensional square lattice (dashed line) Ising models, Eqs. (25) and (29), J = 1. The both curves almost coincide

It practically coincides with that of Eq.(25). The magnetisation decreases asymptotically to zero with the temperature from the maximum value at $T = 0$.

Using the same method, one can find the partition function of a cell in the simple cubic lattice for the uniform case:

$$Z_i = \frac{}{4\cosh(3J) + 32\cosh(1.5J) + 60\cosh(J) + 96\cosh(0.5J) + 64} \quad (30)$$

The nearest-neighbour correlation function is

$$\Gamma_k(1) = \frac{\sinh(3J) + 4\sinh(1.5J) + 5\sinh(J) + 4\sinh(0.5J)}{\cosh(3J) + 8\cosh(1.5J) + 15\cosh(J) + 24\cosh(0.5J) + 16} \quad (31)$$

and the magnetisation is:

$$\sigma = \left[\frac{\sinh(3J) + 4\sinh(1.5J) + 5\sinh(J) + 4\sinh(0.5J)}{\cosh(3J) + 8\cosh(1.5J) + 15\cosh(J) + 24\cosh(0.5J) + 16}\right]^{0.5} \quad (32)$$

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The plot of this result is shown in Figure 3.

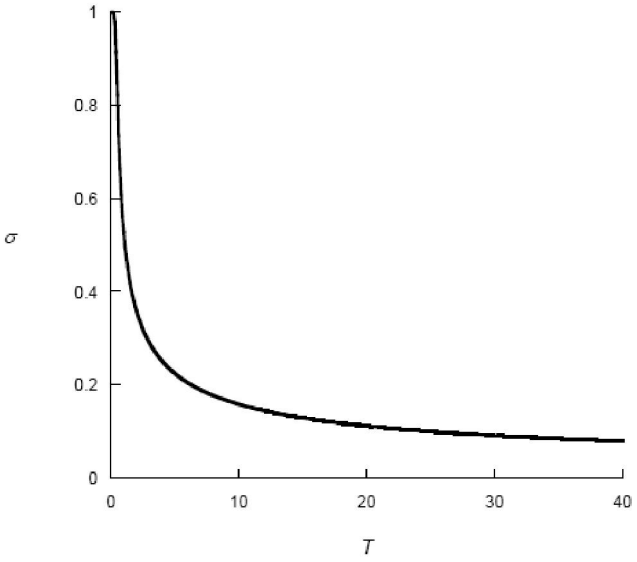

Figure 3 : Dependence of the spontaneous magnetisation per spin σ on temperature *T* for the three-dimensional Ising model, Eq. (32), *J* = 1.

Ising proposed another solution of the one-dimensional Ising model.[4] He considered a chain of N spins and used the expression

$$\sigma = kT\frac{\partial}{\partial H}\ln Z \qquad (33)$$

where H is the external magnetic field and Z is the partition function. In the partition function, the summation is over all configurations with N_1 spins up and $N - N_1$ spins down, where N_1 changes from 0 to N. However, if $\Gamma_k(1) = 0.99$ and the case 1 described above takes place, then $N - N_1$ is of the order 1% and configurations with $N - N_1 >> 1\%$ are impossible and may not be taken into account.

If one knows $\Gamma_k(1)$ one can calculate exactly the number of spins up and down in the infinite chain. In the calculation of the partition function only the configurations with that number of spins up and down must be taken. As the directions up and down have equal rights, one must take also the configurations with N_1 spins down and $N - N_1$ spins up. Such partition function will be exact and calculations with it will produce correct result. Other configurations are impossible and may not be taken into account in calculation of Z. In Refs. 1, 3 - 12, other solutions of the one-dimensional, two-dimensional, and three-dimensional Ising models were given. They also use Eq. (33) and summation over all configurations, and, therefore, are wrong.

CONCLUSIONS

Earlier it has been thought that the Ising model, unlike the mean field theory, predicts no phase transition for a linear chain system in the absence of external magnetic field. It is shown that this traditional result is wrong because it is based on a wrong calculation of the correlation function or taking redundant terms in the partition function. Another solution is obtained which does predict magnetisation. It acquires its maximum value at $T = 0$ and decreases asymptotically to zero with the temperature. It has been proven that the solution of the one-dimensional case is exact. Using this method, exact solutions of the two-dimensional and three-dimensional Ising models are obtained. They also acquire their maximum values at $T = 0$ and decrease asymptotically to zero with the temperature. It is shown that there is a mistake in the former solutions of the two- and three-dimensional Ising models.

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