Exact solution for the one-dimensional third-neighbour Ising model

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Following the transfer matrix approach, we compute the exact solution for the one-dimensional Ising model with interactions up to third neighbours. We write the result in a compact form, and we show that it coincides with earlier numerical computations.

Keywords: Ising model; exact solutions; distant neighbors.

Utilizando el formalismo de la matriz de transferencia, se determina la solución exacta para el modelo de Ising unidimensional con interacción a terceros vecinos. Es obtenida una expresión para el resultado en forma compacta y mostramos que coincide con resultados numéricos anteriores.

Descriptores: Modelo de Ising; solución exacta; vecinos distantes.

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1. Introduction

The Ising model was proposed and solved in its simplest form by the German physicist Ernst Ising in his PhD thesis in 1924 [1]. As mentioned by him in his paper, the study of this model had been suggested to him by his advisor Wilhelm Lenz, who had proposed it in 1920 [2,3]. It seems that the name was given to the model by R. Peierls in 1936. Actually, considering these facts, there are authors who recognize Lenz's priority in this work [4]. Although Ising never published any other scientific works, his model is a widely used standard model of statistical physics and continues to be frequently cited not only in physics, but also in chemistry, biology, mathematics, sociology, etc.

The computation Ising carried out is the calculation of the partition function for a linear chain of spins with first-neighbour interactions, in an external constant magnetic field [1]. Since then, the calculation of exact solutions for the partition function has continued to be an important problem. In fact, the higher dimensional case has been studied independently by Kramers and Wannier [5] and by Montroll [6], who developed the transfer matrix formulation, in which the problem reduces to finding the maximal eigenvalue of this matrix. This formulation relies on the observation that in the thermodynamic limit, the addition of one finite number of nodes to the system, keeping its geometry, does not affect its partition function. E. Montroll has developed a formulation for a layered array in such a way that each layer is represented by a node of an effective one-dimensional system. Each of the nodes has a self energy which represents all the inner interactions of the layer, and its interaction modes with the neighbouring nodes correspond to the interactions between the layers. The additional assumption of periodicity, which does not modify the partition function either, leads to an expression given by the trace of the transfer matrix. Montroll [7] applied this approach to the one-dimensional approach with second-neighbour interactions in the absence of external fields.

If we stay at the one-dimensional case, the next problem will be to find the solution for third neighbours, whose formulation has been tackled by Green [8] and Fisher [9]. This problem has been also considered regarding the ordering in the ground state by Katsura and Narita [11], Bundaru *et al.* [12] and Morita [10]. In his analysis, Fisher established that the framework of the transfer matrix is the one with fewest algebraic difficulties. However, the eigenvalue for this case, of third neighbours, has not been computed. This problem has been also tackled and numerically solved by Dobson [13]. It seems that no more significant progress regarding exact solutions for higher order neighbours has been made since then [14,15].

In this paper, following the formalism of Kramers-Wannier-Montroll, the exact solution to the third-neighbour Ising model is worked out. It is given in a compact form and is compared with the numerical results of Dobson. In the second section the general setting is sketched, in the third section the results are presented and in the fourth section some conclusions are drawn.

2. One-dimensional Ising model with distant neighbours

Thompson [16] has analized the phase transition problem for the one-dimensional IM. He developed the transfer matrix formalism, defining blocks with a length determined by the rank of the interaction. Let us denote the spin variable associated with each node of the lattice by $\{S\}$. If the interaction

rank is k, and $N = kM$, then the lattice is restructured in M blocks each of length k, with an effective spin $\{\tilde{S}\}$, as shown in Fig. 1.

Let us consider a linear chain with $N = nM$ nodes, where n is the interaction rank. On the node i there is a spin variable S_i which can take the values ± 1. The configuration of the system is characterized by the total spin variable

$$\tilde{S} = \{S_1, S_2, \ldots, S_N\}, \tag{1}$$

which has 2^N different values. We arrange this chain in M blocks containing n elements each, as shown in Fig. 1. Thus, the configuration of the block number j can be caracterized by the block spin $\mathbf{S}_j = \{S_{(j-1)n+1}, S_{(j-1)n+2}, ..., S_{jn}\}$, which has 2^n different values, and whose components can be relabeled as in Fig. 1,

$$\mathbf{S}_j = \{S_1^{(j)}, S_2^{(j)}, ..., S_n^{(j)}\}. \tag{2}$$

With these notations, the total spin of the chain is given by $\tilde{S} = \{\mathbf{S}_1, \ldots, \mathbf{S}_M\}$.

Thus, if the interacting energy between two spins is given by $J_j S_i S_{i+j}$, then the total energy of the system in configuration (1) is given by

$$E(\tilde{S}) = -\sum_{i=1}^{N}\sum_{k=1}^{n} J_k S_i S_{i+k} - \mu B \sum_{i=1}^{n} S_i, \tag{3}$$

where the values containing spins S_i, with $i > N$, must be omitted. Moreover, the interaction strengths must decay under a certain distance dependent law. Separating the terms of this expression into self energy contributions, *i.e.* due to the interactions among elements of the same block, and the contributions of spins of neighbouring blocks, we get, in the notations (2),

$$E(\tilde{S}) = -\sum_{j=1}^{M}\left[\mu B \sum_{i=1}^{n} S_i^{(j)} + \sum_{k=1}^{n-1} J_k \sum_{i=1}^{n-k} S_i^{(j)} S_{i+k}^{(j)}\right] - \sum_{j=1}^{M-1}\sum_{k=1}^{n} J_k \sum_{i=n-k+1}^{n} S_i^{(j)} S_{i-n+k}^{(j+1)}; \tag{4}$$

then, if we define the self energy of the block j as

$$\mathcal{M}(\mathbf{S}_j) = -\mu B \sum_{i=1}^{n} S_i^{(j)} - \sum_{k=1}^{n-1} J_k \sum_{i=1}^{n-k} S_i^{(j)} S_{i+k}^{(j)}, \tag{5}$$

and the interaction energy between the blocks j and $j+1$ as,

$$\mathcal{M}(\mathbf{S}_j, \mathbf{S}_{j+1}) = -\sum_{k=1}^{n} J_k \sum_{i=n-k+1}^{n} S_i^{(j)} S_{i-n+k}^{(j+1)}, \tag{6}$$

then we have,

$$E(\tilde{S}) = \sum_{j=1}^{M} \mathcal{M}(\mathbf{S}_j) + \sum_{j=1}^{M-1} \mathcal{M}(\mathbf{S}_j, \mathbf{S}_{j+1}) = \frac{1}{2}\mathcal{M}(\mathbf{S}_1) + \sum_{j=1}^{M-1} V(\mathbf{S}_j, \mathbf{S}_{j+1}) + \frac{1}{2}\mathcal{M}(\mathbf{S}_M), \tag{7}$$

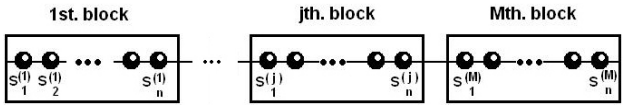

FIGURE 1. Block structure of a linear chain with nth order interactions.

where

$$V(\mathbf{S}, \mathbf{S}') = \frac{1}{2}\mathcal{M}(\mathbf{S}) + \mathcal{M}(\mathbf{S}, \mathbf{S}') + \frac{\mathbf{1}}{\mathbf{2}}\mathcal{M}(\mathbf{S}'). \tag{8}$$

Thus the partition function will be given by

$$Z_M = \sum_{\tilde{S}} e^{-\beta E(\tilde{S})} = \sum_{\mathbf{S}_1} \cdots \sum_{\mathbf{S}_M} U(\mathbf{S}_1) D(\mathbf{S}_1, \mathbf{S}_2) \cdots \times D(\mathbf{S}_{M-1}, \mathbf{S}_M) U(\mathbf{S}_M) \tag{9}$$

where

$$U(\mathbf{S}) = \exp\left[-\left(\frac{\beta}{2}\right)\mathcal{M}(\mathbf{S})\right]$$

are the components of a column matrix U, corresponding to the 2^n configurations of the block spin $\mathbf{S}$, and

$$D(\mathbf{S}, \mathbf{S}') = e^{-\beta V(\mathbf{S}, \mathbf{S}')}, \tag{10}$$

are the components of a $2^n \times 2^n$ matrix D, the transfer matrix. Thus the partition function can be written as

$$Z_M = U^T D^{M-1} U. \tag{11}$$

(See for example Huang) [17]. Montroll [6] has considered a layered medium, such that the range of atoms in one layer did not exceed the atoms in the next layer. Thus each layer has been represented by a block, with a self energy due to its internal interactions, and an effective interaction with the next neighbour blocks. In this way, this medium could be considered as effectively 1-dimensional. He computed the partition function by a change of spin variables in such a way that the matrix D would be diagonalized. Thus, in the thermodynamic limit, he obtained that the partition function is proportional to λ_{max}, with a factor given by the square module of the corresponding eigenfunction.

Following Thompson (1971), we impose periodic boundary conditions on the chain $S_{i+N} = S_i$, which do not modify the results in the thermodynamic limit. Thus we have $\mathbf{S}_{M+1} = \mathbf{S}_1$. In this case interaction terms between the last block and the first one must be added to the energy, and (7) becomes

$$E(\tilde{S}) = \sum_{j=1}^{M} [\mathcal{M}(\mathbf{S}_j) + \mathcal{M}(\mathbf{S}_j, \mathbf{S}_{j+1})] = \sum_{j=1}^{M} V(\mathbf{S}_j, \mathbf{S}_{j+1}), \tag{12}$$

and the partition function is now given by

$$Z_M = TrD^M. \tag{13}$$

If the eigenvalues of the transfer matrix are $\{\lambda_1, \ldots, \lambda_{2^n}\}$, in general they are complex numbers, according to Aguilar *et al*. [15,18], then due to the fact that the partition function is real,

$$\begin{aligned} Z_M &= \sum_{k=1}^{2^n} |\lambda_k^M| = \sum_{k=1}^{2^n} |\lambda_k|^M \\ &= |\lambda_{max}|^M \sum_{k=1}^{2^n} \frac{|\lambda_k|^M}{|\lambda_{max}|^M}, \end{aligned} \tag{14}$$

where $|\lambda_{max}|$ is the maximal eigenvalue modulus. Then in the thermodynamic limit $N \to \infty$, the spin partition function is given by

$$\begin{aligned} L(T) &= \lim_{N\to\infty} \frac{1}{N} \log Z_M \\ &= \lim_{N\to\infty} \frac{1}{N} \log |\lambda_{max}|^M = \frac{1}{n} \log |\lambda_{max}|, \end{aligned} \tag{15}$$

n being the interaction range.

As pointed out by Montroll [7], this system has spin reversal symmetry, that is under the inversion of the values of all the spin variables. That means that each configuration appears twice and if properly arranged, the transfer matrix will have the block form,

$$D = \begin{pmatrix} P & Q \\ Q & P \end{pmatrix}, \tag{16}$$

where P and Q are $2^{n-1} \times 2^{n-1}$ blocks. In this case, by a similarity transformation with

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} I & I \\ -I & I \end{pmatrix}, \tag{17}$$

we get

$$D \to \frac{1}{2} SDS^{-1} = \begin{pmatrix} P+Q & 0 \\ 0 & P-Q \end{pmatrix}. \tag{18}$$

Therefore, the computation of the eigenvalues of D is reduced to the computation of the eigenvalues of the half size matrices $P \pm Q$, which can simplify considerably the problem, in particular in the third-neighbour case, which will be studied in this work. Moreover, the elements of the transfer matrix (10) are exponentials, hence positive numbers. Thus the entries of the matrix $P+Q$ will have also positive values, and its trace will be bigger than the trace of $P-Q$. Therefore, λ_{max} will be an eigenvalue of $P+Q$.

3. Third-neighbour interactions

Let us consider now the case of third-neighbour interactions, $n = 3$, as shown in Fig. 2. In this case the transfer matrix is of order eight, and the matrix $P+Q$ is of order four.

If we define the adimensional variables $x{=}\beta J_1$, $y{=}\beta J_2$ and $z{=}\beta J_3$, a rather cumbersome computation shows that,

$$P = \begin{vmatrix} e^{3\,x+3\,y+3\,z} & e^{2\,x+2\,y+z} & e^{x+y+z} & e^{z} \\ e^{z} & e^{-x-y+3\,z} & e^{-2\,x+2\,y-z} & e^{x-3\,y-z} \\ e^{x+y+z} & e^{-z} & e^{-\,x-y+3\,z} & e^{-2\,x+2\,y-z} \\ e^{2\,x+2\,y+z} & e^{x+y-z} & e^{-z} & e^{-x-y+3\,z} \end{vmatrix}, \tag{19}$$

and

$$Q = \begin{vmatrix} e^{x-y-3\,z} & e^{-2\,y-z} & e^{-x+y-z} & e^{2\,x-z} \\ e^{2\,x-z} & e^{x-y-3\,z} & e^{-2\,y+z} & e^{-x+y+z} \\ e^{-x+y-z} & e^{-2\,x+z} & e^{-3\,x+3\,y-3\,z} & e^{-2\,y+z} \\ e^{-2\,y-z} & e^{-x-3\,y+z} & e^{-2\,x+z} & e^{x-y-3\,z} \end{vmatrix}. \tag{20}$$

Thus, the eigenvalue equation of $P+Q$ is,

$$\lambda^4 + a\lambda^3 + b\lambda^2 + c\lambda + d = 0, \tag{21}$$

where the coefficients can be computed to be given by

$$\begin{aligned} a &= -e^{-3x-y-3z}(3e^{4x} + e^{4y} + 3e^{2x+6z} + e^{6x+4y+6z}), \\ b &= -e^{-6y} + 3e^{-2y} - 3e^{2y} + e^{6y} + 3e^{2x-2y-6z} + 3e^{-2x+2y-6z} + 3e^{-2(x+y-3z)} - 3e^{2x-2y-2z} \\ &\quad - 3e^{-2(x+y-z)} - 3e^{-2(x-y+z)} - 3e^{2(x+y+z)} + 3e^{2(x+y+3z)}, \\ c &= -e^{-3(x+y+3z)}(-1 + e^{4z})^3(-e^{6x} - 3e^{2x+4y} + e^{6z} + 3e^{4x+4y+6z}), \\ d &= e^{-12z}(-1 + e^{4z})^6. \end{aligned}$$

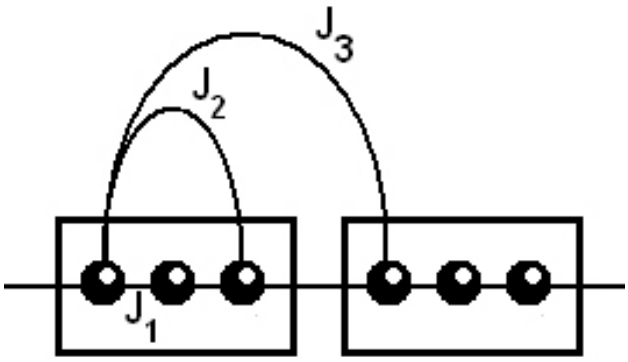

FIGURE 2. Third order interactions.

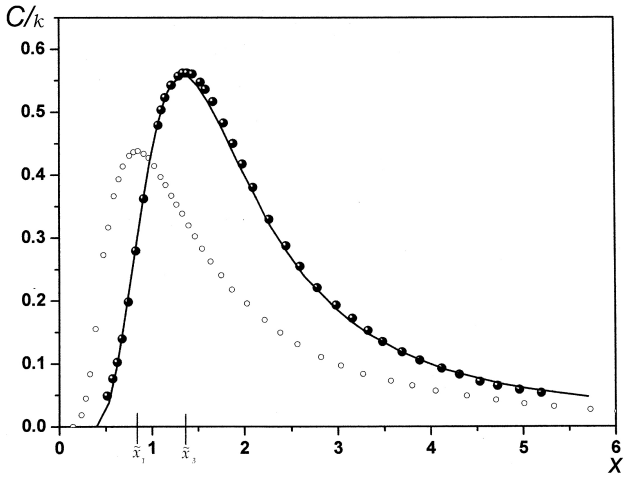

FIGURE 3. The continuous curve corresponds to our result with third neighbors, the black dotted curve is Dobson's and the white dotted curve corresponds to the case with first-neighbor interactions. (The positions of the maxima are indicated by $\tilde{x}_1$ and $\tilde{x}_3$).

The eigenvalues of this Eq. (21) can be written as

$$\lambda_{1,2} = -\frac{a}{4} \pm \frac{\sqrt{A}}{2} + \frac{1}{2}\sqrt{3\delta - A \pm \frac{\gamma}{4\sqrt{A}}}, \qquad (22)$$

$$\lambda_{3,4} = -\frac{a}{4} \pm \frac{\sqrt{A}}{2} - \frac{1}{2}\sqrt{3\delta - A \pm \frac{\gamma}{4\sqrt{A}}}, \qquad (23)$$

where

$$A = \frac{\alpha^{\frac{1}{3}}}{32^{\frac{1}{3}}} + \frac{2\beta^{\frac{1}{3}}}{3^3\alpha^{\frac{1}{3}}} + \delta,$$

$$\alpha = \eta + \sqrt{-4\beta^3 + \eta^2},$$

$$\beta = b^2 - 3ac + 12d,$$

$$\gamma = -a^3 + 4ab - 8c,$$

$$\delta = \frac{a^2}{4} - \frac{2b}{3},$$

$$\eta = 2b^3 - 9abc + 27c^2 + 27a^2d - 72bd.$$

A numerical computation shows us that the maximal eigenvalue is given by λ_1, as could be expected from the signs in Ec. 22 and (23). It is interesting to note that the numerical evaluation gives a real result for it, as well as for λ_2, and the other two eigenvalues get nonvanishing imaginary parts. It would be very difficult to get this result from the given form of these eigenvalues. However, having this exact form for the eigenvalues, the numerical evaluation can be done reliably.

This result is in very good agreement with the numerical results of Dobson (1969), who has computed the heath capacity for third and even higher neighbours, with spin interactions decaying under the Kac-Thompson law, $J_n = J_1/n^\alpha$, as shown for $\alpha = 2$, in Fig. 3. The heath capacity is obtained from,

$$\frac{C(T)}{k} = \frac{1}{3}\left[\frac{\beta^2}{\lambda_{max}}\frac{\partial^2\lambda_{max}}{\partial\beta^2} - \left(\frac{\beta}{\lambda_{max}}\frac{\partial\lambda_{max}}{\partial\beta}\right)^2\right]. \qquad (24)$$

4. Conclusions

We have started from the general problem of the computation of the partition function for the Ising model with distant neighbour interactions of any order. This problem was initially tackled and solved in general by Kramers and Wannier [5] and by Montroll [6,7]. They have shown that the solution to this problem amounts to computing the maximal eigenvalue of the transfer matrix.

We have obtained the exact solution for the one-dimensional Ising model with third-neighbour interactions. The partition function, given by the maximal solution of (21), is given in a compact form in Eq. 22, which requires yet to be transformed into a much simpler form in order to be useful for purely analytic computations. However, this result allows computations of thermodynamic quantities, such as that of heath capacity (24), by means of symbolic manipulation programs[i], from which a subsequent numerical study can be done. We obtain also, in the case of third neighbours, that two of the eigenvalues are real, including the maximal one as should be the case, but the other two have nonvanishing imaginary parts.

The transfer matrix approach can be applied to other one-dimensional problems, in which distant nodes along the chain are now near due to the geometical setting, *e.g.* such as DNA [14], one-dimensional proteins or polymers [19,20]. In particular cases of this type, exact solutions to fourth or fifth order neighbour interactions can be given. Moreover, chains with polyatomic nodes can be considered, *i.e.* in which there are different types of interactions. Some of these topics will appear in Martínez and Ramírez [21].

5. Acknowledgments

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i. Mathematica 3.0, Copyright 1988-1996 Wolfram Research

1. E. Ising, *Z. Phys.* **31** (1925) 253.
2. S.G. Brush, *Rev. Mod. Phys.* **39** (1967) 883.
3. C. Stutz, Conley, and B. Williams, *Physics Today* **52** (1999) 106.
4. J.L. Morán-López, F. Aguilera-Granja, and J.M. Sánchez, *Phys. Rev. B* **48** (1993) 3519.
5. H.A. Kramers and G. Wannier, *Phys. Rev. B* **60** (1941) 252.
6. E.W. Montroll, *J. Chem. Phys.* **9** (1941) 706.
7. E.W. Montroll, *J. Chem. Phys.* **10** (1942) 61.
8. H.S. Green, *Rev. Mod. Phys* **32** (1960) 129.
9. M.E. Fisher and I. Temperley *Rev. Mod. Phys.* **32** (1960) 1029.
10. T. Morita, *J. Phys. A* **7** (1974) 289.
11. S. Katsura and A. Narita, *Progr. Theor. Phys.* **50** (1973) 1428.
12. M. Bundaru, N. Angelescu, and G. Nenciu, *Phys. Lett.* **43** (1973) 5.
13. J.F. Dobson, *J. Math. Phys.* **10** (1969) 40.
14. D.A. Lavis and G.M. Bell, *Statistical Mechanics of Lattice Systems 1: Closed Form and Exact Solutions* (Springer, 1999).
15. A. Aguilar and E. Braun, *Phys. A* **170** (1991) 643.
16. C.J. Thompson, *Mathematical Statistical Mechanics*, (Macmillan, New York, 1971).
17. K. Huang, *Statistical Machanics* (John Wiley, 1985).
18. A. Aguilar and E. Braun, *Phys. A* **178** (1991) 551.
19. J.S. Helman, *Phys. Rev. Lett.* **53** (1984) 1195.
20. R. Medjani, *Physica A* **206** (1994) 332.
21. P. Martínez and C. Ramírez (article in preparation).