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ISING MODEL: AN ALTERNATIVE METHOD OF SOLUTION

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ABSTRACT

A new recursive method used to solve the Ising problem in one dimension is presented. The solutions for the open and closed chain with and without external field are worked out.

RESUMEN

Se presenta un nuevo método recursivo usado para resolver el problema de Ising en una dimensión. Son desarrolladas las soluciones para la cadena abierta y cerrada con y sin campo externo.

1. INTRODUCTION

The Ising Model is considered the simplest model that describes

phase transitions in ferromagnetism and binary substitutional alloys and thermal denaturation and polimerization processes of some biological systems[1,2] with an acceptable degree of reality.

The Ising Chain is of interest in Statistical Mechanics because it can be solved exactly[3,4,5,6] and its closed form solutions can be compared with the behaviour of several physical systems. Also they can serve as a guide for analyzing the results of approximate methods in higher dimensions.

We have developed a recursive method which is simple enough that can be used to solve practical applications of the Ising Model with relatively uncomplicated mathematics. In this paper we solve the linear lattice of N sites in the following cases: i) An open chain with and without external field, and ii) A closed chain also with and without external field. We point out that these four cases are difficult to solve by the same method (see for instance Ref. 5).

The main motivation of this work is to present a new iterative method for solving the partition function of the Ising Chain which can stimulate further search for exact solutions of the two and three dimensional Ising problem

2. MATHEMATICAL FORMULATION FOR THE OPEN CHAIN

Let us consider the usual Ising model in one-dimension with N sites:

A configuration $\{\mu\} = (\mu_1, \ldots\ldots\ldots\ldots, \mu_N)$ is a N-vector whose i-th component μ_i denotes the spin value in the i-th site and takes the values +1 or -1. Now for a given configuration $\{\mu\}$, the interaction energy of the system is given by

$$E\{\mu\} = -\tilde{J}\sum_{i=1}^{N-1}\mu_i\mu_{i+1} - \tilde{H}\sum_{i=1}^{N}\mu_i \quad , \qquad (1)$$

where $\tilde{J}$ is the coupling constant and $\tilde{H}$ is the external magnetic field. The partition function Z is the sum over all configurations of exp ($-\beta E\{\mu\}$) and is given by

$$Z = \sum_{\{\mu\}} \exp(-\beta E\{\mu\}) = \sum_{\{\mu\}} \exp\left(\beta\tilde{J}\sum_{i=1}^{N-1}\mu_i\mu_{i+1} + \beta\tilde{H}\sum_{i=1}^{N-1}\mu_i\right) , \qquad (2)$$

where $\beta = 1/kT$, k is Boltzmann's constant and T denotes the absolute temperature.

Using the equality

$$e^x = \sum_{j=0}^{\infty} \frac{x^j}{j!}$$

and noting that $\mu_i^{2n} = 1$ and $\mu_i^{2n+1} = \mu_i$, we obtain

$$Z = K \sum_{\{\mu\}} \prod_{i=1}^{N-1} (1 + \omega_J \mu_i \mu_{i+1}) \prod_{i=1}^{N} (1 + \omega_H \mu_i) \quad , \tag{4}$$

with $J = \beta\tilde{J}$, $H = \beta\tilde{H}$, $\omega_J = \tanh J$, $\omega_H = \tanh H$ and $K = (\cosh J)^{N-1} (\cosh H)^N$.

Let us consider all terms containing μ_1 :

$$Z = K \sum_{\{\mu^2\}} \left[\sum_{\mu_1 = \pm 1} (1 + \omega_J \mu_1 \mu_2)(1 + \omega_H \mu_1) \right] \prod_{i=2}^{N-1} (1 + \omega_J \mu_i \mu_{i+1})$$

$$\cdot \prod_{i=2}^{N} (1 + \omega_H \mu_i) \quad , \tag{5}$$

where the first sum is taken over all the configurations $\{\mu^2\} = \{\mu_2, \mu_3, \ldots, \mu_N\}$. Performing separately the sum over μ_1 in the above expression, we obtain

$$Z = 2\, K \sum_{\{\mu^3\}} \left[\sum_{\mu_2 = \pm 1} (\alpha_1 + \beta_1 \mu_2) \prod_{i=2}^{N-1} (1 + \omega_J \mu_i \mu_{i+1}) \prod_{i=2}^{N} (1 + \omega_H \mu_i) \right]$$

$$= 2\, K \sum_{\{\mu^3\}} \left[\sum_{\mu_2 = \pm 1} (\alpha_1 + \beta_1 \mu_2)(1 + \omega_J \mu_2 \mu_3)(1 + \omega_H \mu_2) \right]$$

$$\cdot \prod_{i=3}^{N-1} (1 + \omega_J \mu_i \mu_{i+1}) \prod_{i=3}^{N} (1 + \omega_H \mu_i) \tag{6}$$

$$= 2^2 K \sum_{\{\mu^3\}} \left[(\alpha_1 + \beta_1 \omega_H) + (\beta_1 \omega_J + \alpha_1 \omega_J \omega_H) \mu_3 \right] \prod_{i=3}^{N-1} (1 + \omega_J \mu_i \mu_{i+1}) \prod_{i=1}^{N} (1 + \omega_H \mu_i),$$

where $\alpha_1 = 1$ and $\beta_1 = \omega_J \omega_H$. Defining

$$\alpha_2 = \alpha_1 + \beta_1 \omega_H \qquad \text{and} \qquad \beta_2 = \beta_1 \omega_J + \alpha_1 \omega_J \omega_H \quad , \tag{7}$$

the partition function becomes

$$Z = 2^2 K \sum_{\{\mu^4\}} \Big[\sum_{\mu_3=\pm 1} (\alpha_2 + \beta_2 \mu_3) \prod_{i=3}^{N-1} (1 + \omega_J \mu_i \mu_{i+1}) \prod_{i=3}^{N} (1 + \omega_H \mu_i) \Big] . \quad (8)$$

Repeating the procedure for μ_3, μ_4, ... up to μ_j with $j < N-1$ one obtains the recursive formulas

$$\alpha_{i+1} = \alpha_i + \beta_i \omega_H \quad \text{and} \quad \beta_{i+1} = \beta_i \omega_J + \alpha_i \omega_J \omega_H \quad . \quad (9)$$

Then, we have

$$Z = 2^j K \sum_{\{\mu^{j+1}\}} (\alpha_j + \beta_j \mu_{j+1}) \prod_{i=j+1}^{N-1} (1 + \omega_J \mu_i \mu_{i+1}) \prod_{i=j+1}^{N} (1 + \omega_H \mu_i), \quad (10)$$

for $j < N-1$. In particular, for $j = N-1$, it follows that

$$\begin{aligned} Z &= 2^{N-1} K \sum_{\mu_N=1} (\alpha_{N-1} + \beta_{N-1} \mu_N)(1 + \omega_H \mu_N) \\ &= 2^N K (\alpha_{N-1} + \beta_{N-1} \omega_H) = 2^N K \alpha_N . \end{aligned} \quad (11)$$

In order to obtain an explicit expression for α_N we note that (9) can be rewritten in the following matrix form

$$\begin{pmatrix} \alpha_{i+1} \\ \beta_{i+1} \end{pmatrix} = \begin{pmatrix} 1 & \omega_H \\ \omega_J \omega_H & \omega_J \end{pmatrix} \begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix} = \begin{pmatrix} 1 & \omega_H \\ \omega_J \omega_H & \omega_J \end{pmatrix}^i \begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix} \quad (12)$$

$$= \mathbf{A}^i \begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix} .$$

We now consider the different cases:

Case i-a: Open chain without magnetic field.

In this case, the solution is straightforward since $\omega_H = 0$. Therefore, from (12)

$$\mathbf{A}^i = \begin{pmatrix} 1 & 0 \\ 0 & \omega_J^i \end{pmatrix} , \tag{13}$$

which gives rise to the partition function

$$Z = 2^N (\cosh J)^{N-1} = 2(2 \cosh J)^{N-1} . \tag{14}$$

This is the well known solution for the linear chain with open ends in zero magnetic field[5,8].

Case i-b: Open chain with magnetic field

To find the partition function, we have to uncouple the matrix **A** given in Eq. (12).

Choosing a non-singular matrix $\mathbb{C}$ such that

$$\mathbb{C}^{-1} \mathbf{A} \mathbb{C} = \Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \tag{15}$$

where λ_1 and λ_2 are the eigenvalues of **A**. They are given by

$$\lambda_{1,2} = \frac{(1 + \omega_J) \pm \sqrt{(\omega_J - 1)^2 + 4 \omega_J \omega_H^2}}{2} . \tag{16}$$

Therefore

$$\mathbf{A}^i = \mathbb{C} \Lambda^i \mathbb{C}^{-1} = \mathbb{C} \begin{pmatrix} \lambda_1^i & 0 \\ 0 & \lambda_2^i \end{pmatrix} \mathbb{C}^{-1} . \tag{17}$$

The α_N can then be determined from Eq. (12).

Case ii: Closed chain

Using the same technique, the partition function for the closed chain is

$$Z = \sum_{\{\mu\}} \exp\left(\sum_{i=1}^{N} J\mu_i\mu_{i+1} + H\,\mu_i\right)$$

$$= K' \sum_{\{\mu\}} e^{J\mu_1\mu_N} \left(\prod_{i=1}^{N-1} e^{H\mu_i + J\mu_i\mu_{i+1}}\right) e^{H\,\mu_N} \quad , \tag{18}$$

where $K' = (\cosh J)^N (\cosh H)^N$ and $\mu_{N+1} = \mu_1$.

The iterative procedure proceeds now as follows:

$$Z = K' \sum_{\{\mu\}} (1 + \omega_J\mu_1\mu_N) \prod_{i=1}^{N-1} (1 + \omega_H\mu_i)\ (1 + \omega_J\mu_i\mu_{i+1})\ (1 + \omega_H\mu_N)$$

$$= K' \sum_{\{\mu^2\}} \left(\sum_{\mu_1=1} (1 + \omega_J\mu_1\mu_N)\ (1 + \omega_J\mu_1\mu_2)\ (1 + \omega_H\mu_1)\right) \prod_{i=2}^{N-1} (1 + \omega_H\mu_i)$$

$$\cdot (1 + \omega_J\mu_i\mu_{i+1})\ (1 + \omega_H\mu_N)$$

$$= 2\,K' \sum_{\{\mu^2\}} (\alpha_1 + \beta_1\mu_2 + \gamma_1\mu_N + \varepsilon_1\mu_2\mu_N) \prod_{i=2}^{N-1} (1 + \omega_H\mu_i)\ (1 + \omega_J\mu_i\mu_{i+1})$$

$$\cdot (1 + \omega_H\mu_N). \tag{19}$$

In the second step above we have performed the sum over μ_1 . Here $\alpha_1 = 1$, $\beta_1 = \omega_J\omega_H$, $\gamma_1 = \omega_J\omega_H$ and $\varepsilon_1 = \omega_J^2$.

Summing over μ_2, in Eq. (19) we obtain

$$Z = 2^2\,K' \sum_{\{\mu^3\}} \Big[(\alpha_1 + \omega_H\beta_1) + (\omega_J\beta_1 + \omega_J\omega_H\alpha_1)\,\mu_3 + (\omega_H\varepsilon_1 + \gamma_1)\mu_N$$

$$+ (\omega_J\varepsilon_1 + \omega_J\omega_H\gamma_1)\,\mu_3\mu_N\Big] \prod_{i=3}^{N-1} (1 + \omega_H\mu_i)\ (H\,\omega_J\mu_i\mu_{i+1})\ (1 + \omega_H\mu_N). \tag{20}$$

Repeating recursivelly the same procedure $j < N-2$ times we have

$$Z = 2^j\,K' \sum_{\{\mu^j\}} (\alpha_j + \beta_j\mu_{j+1} + \gamma_j\mu_N + \varepsilon_j\mu_{j+1}\mu_N) \prod_{i=j+1}^{N-1} (1 + \omega_H\mu_i)$$

$$\cdot (1 + \omega_J\mu_i\mu_{i+1})\ (1 + \omega_H\mu_N), \tag{21}$$

where

$$\begin{pmatrix} \alpha_{j+1} \\ \beta_{j+1} \\ \gamma_{j+1} \\ \varepsilon_{j+1} \end{pmatrix} = \left(\begin{array}{cc|cc} 1 & \omega_H & & \\ \omega_J\omega_H & \omega_J & \multicolumn{2}{c}{0} \\ \hline & & 1 & \omega_H \\ \multicolumn{2}{c|}{0} & \omega_J\omega_H & \omega_J \end{array}\right) \begin{pmatrix} \alpha_j \\ \beta_j \\ \gamma_j \\ \varepsilon_j \end{pmatrix} = \mathbb{B} \begin{pmatrix} \alpha_j \\ \beta_j \\ \gamma_j \\ \varepsilon_j \end{pmatrix}, \qquad (22)$$

thus, the (j+1)-th coefficient can be determined from the h-th coefficients.

For the particular case j = N-2:

$$Z = 2^{N-2} K' \sum_{\{\mu\}_N} \Bigg(\sum_{\mu_{N-1}=\pm 1} (\alpha_{N-2} + \beta_{N-2}\mu_{N-1} + \gamma_{N-2}\mu_N + \varepsilon_{N-2}\mu_{N-1}\mu_N)(1 + \omega_H\mu_{N-1}) \cdot (1 + \omega_J\mu_{N-1}\mu_N) \Bigg) (1 + \omega_H\mu_N)$$

$$= 2^{N-1} K' \sum_{\mu_N=\pm 1} \Big((\alpha_{N-1} + \varepsilon_{N-1}) + (\gamma_{N-1} + \beta_{N-1})\mu_N \Big) (1 + H\,\mu_N) \qquad (23)$$

$$= 2^N K' \Big((\alpha_{N-1} + \varepsilon_{N-1}) + (\gamma_{N-1} + \beta_{N-1})\omega_H \Big) = 2^N K' (\alpha_N + \varepsilon_{N-1} + \omega_H\gamma_{N-1}),$$

where in the first step we performed the sum over μ_{N-1} and in the second step we summed over μ_N.

We now consider the two different cases:

Case ii-a: Closed chain without magnetic field

When the magnetic field H = 0, we have $\omega_H = 0$ and the partition function takes on the simple form.

$$Z = 2^N (\cosh J)^N (\alpha_N + \varepsilon_{N-1}). \qquad (24)$$

To obtain the coefficients α_N and ε_{N-1}, we use Eq. (22):

$$\begin{pmatrix} \alpha_{j+1} \\ \beta_{j+1} \\ \gamma_{j+1} \\ \varepsilon_{j+1} \end{pmatrix} = \left(\begin{array}{cc|cc} 1 & 0 & & \\ 0 & \omega_J & \multicolumn{2}{c}{0} \\ \hline & & 1 & 0 \\ \multicolumn{2}{c|}{0} & 0 & \omega_J \end{array}\right)^j \begin{pmatrix} 1 \\ 0 \\ 0 \\ \omega_J^2 \end{pmatrix}, \qquad (25)$$

from which it follows that $\alpha_N = 1$, $\varepsilon_{N-1} = \omega_J^N$ and

$$Z = 2^N (\cosh J)^N + (\sinh J)^N , \tag{26}$$

which is the well known result for this case[4,5].

Case ii-b: Closed chain with magnetic field

In analogy with the case of an open chain with magnetic field we now have a matrix $\mathbb{D} = \begin{pmatrix} \mathbb{C} & 0 \\ 0 & \mathbb{C} \end{pmatrix}$ which diagonalizes a matrix $\mathbf{B}$ and then uncouples the system (22) by means of the equations

$$\mathbb{D}^{-1} \quad \mathbf{B} \quad \mathbb{D} = \Omega , \tag{27}$$

where

$$\mathbf{B} = \begin{pmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{A} \end{pmatrix} \text{ and } \Omega = \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda \end{pmatrix} . \tag{28}$$

This case then reduces to that of an open chain since

$$\mathbb{C}^{-1} \quad \mathbf{A} \quad \mathbb{C} = \Lambda \tag{29}$$

and the eigenvalues λ_1 and λ_2 follow from Eq. (16).

The elements of the recurrent matrix are related with the eigenvalues $\lambda_{1,2}$ through the equations:

$$\begin{aligned} \varepsilon_j = \beta_j &= \sum_{i=1}^{2} P_i^1 (\lambda_i)^j , \\ \alpha_j = \gamma_j &= \sum_{i=1}^{2} P_i^2 (\lambda_i)^j , \end{aligned} \tag{30}$$

where the coefficients $P_i^{1,2}$ are functions of the elements of the transformation matrices $\mathbb{C}$ and $\mathbb{C}^{-1}$.

Using Eq. (30) we can write the logarithm of the partition function Z, Eq. (23) as follows:

$$\frac{1}{N} \ln Z = \ln 2 + \ln(\cosh J) + \ln(\cosh H) + \ln \lambda_1 +$$

$$+ \frac{1}{N} \ln \left\{ \sum_{i=1}^{2} P_i' \left(\frac{\lambda_i}{\lambda_1}\right)^N + \sum_{i=1}^{2} \frac{P_i^2}{\lambda_1} \left(\frac{\lambda_i}{\lambda_1}\right)^{N-1} + \sum_{i=1}^{2} \frac{P_i^2 \omega_H}{\lambda_1} \left(\frac{\lambda_i}{\lambda_1}\right)^{N-1} \right\} \quad (31)$$

In the thermodynamic limit, and recalling that $\lambda_1 > \lambda_2$, we finally obtain:

$$\lim_{N\to\infty} \frac{1}{N} \ln Z = \tilde{\beta J} + \ln(\cosh \tilde{\beta H} + (\cosh^2 \tilde{\beta H} - 2 \exp(-2 \tilde{\beta J}) \sinh 2\tilde{\beta J})^{0.5}) \,, \quad (32)$$

where we have used Eqs. (16).

Equation (32) is the well known result of this case[7], which leads to the calculation of all thermodynamic function of interest.

3. CONCLUSIONS

We have presented an iterative method for solving the partition function of the Ising Chain. Four cases have been treated: closed and open chains with and without external field. Because these four cases are difficult to handle by the same technique and due to operational advantages over the transfer matrix method, we think that the method describe here provides a new way of searching for analytical solutions of the Ising problem in higher dimensions.

A second and perhaps no less important characteristic of the method describe here is that, according to our experience, it permits a relatively simple treatment of the Ising problem in a Statistical Mechanics course.

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