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Exact eigenvalues of the Ising Hamiltonian in one-, two- and three-dimensions in the absence of a magnetic field

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Abstract

The Hamiltonian of the Ising model in one-, two- and three-dimensions has been analysed using unitary transformations and combinatorics. We have been able to obtain closed formulas for the eigenvalues of the Ising Hamiltonian for an arbitrary number of dimensions and sites. Although the solution provided assumes the absence of external magnetic fields an extension to include a magnetic field along the z -axis is readily extracted. Furthermore, generalisations to a higher number of spin components on each site are possible within this method. We made numerical comparisons with the partition function from the earlier analytical expressions known in the literature for one- and two-dimensional cases. We find complete agreement with these studies. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

In the theory of structural phase transitions [1] description of displacive transitions requires Landau–Ginzburg modelling, while order–disorder transitions make use of the Ising model with an effective spin variable. Such a model has been analysed in an enormous number of papers over many decades. It is based on a regular lattice of N points in an n -dimensional space, with spin variables, S_i , placed at each lattice site and

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interacting with their nearest neighbours (which we denote by $\langle i, j \rangle$) and an external magnetic field H_o , parallel to the z -axis. Its Hamiltonian may be written as

$$H = -J \sum_{\langle i, j \rangle} S_i^z S_j^z - 2\beta H_o \sum_i S_i^z, \quad (1)$$

where S_i^z denotes the z -component of spin at site i and β is the Bohr magneton. As well as being a simple model of magnetic materials such as CoCs_3Br_5 , $\text{Co}(\text{HCOO})_2 \cdot 2\text{H}_2\text{O}$, Rb_2CoF_4 and K_2CoF_4 , the spin $-\frac{1}{2}$ Ising antiferromagnet is directly related to lattice gas theory [2], which provides a crude model for some solid electrolytes [3]. Bienenstock and Lewis [4] utilised the Ising antiferromagnet in a field to describe binary alloys with variable composition. As is well known the Ising model, despite being very simple, is of crucial importance in the understanding of critical phenomena [5]. In one-dimension the free energy [6] is well known but does not result in a finite temperature phase transition. For the two-dimensional case the free energy was obtained analytically by Onsager [7] many years ago, essentially in the thermodynamic limit, following a rather involved algebraic argument. This latter exhibits the typical behaviour of a ferromagnet in that, above a certain critical temperature the elementary spins, in a large sample, are in a disordered state with no net bulk magnetisation. Below the critical temperature the spins tend to order themselves parallel to one another with a net overall magnetisation. Although no exact results have been obtained in three-dimensions, which has so far eluded analytical solution, a number of approximations have been investigated in the literature. For example, the Bragg–Williams approximation assumes that there is no short-range order apart from that which follows from long-range order and is equivalent to a Curie–Weiss-like molecular field approximation. The Bethe–Peierls approximation [5,6] does account for specific short-range order but, although it agrees with the 1D results, it differs from the exact 2D Onsager result. If one allows the couplings between spins to not only be between z -components but all three components, this leads to the Heisenberg model which exhibits no phase transitions in one- and two-dimensional spaces [8].

A model which goes some way towards a three-dimensional Ising model is the so-called spherical model which utilises the Hamiltonian above but imposes the constraint

$$N = \sum_{i=1}^N S_i^z,$$

which is a conserved quantity [9]. In a 3D lattice, it does possess ferromagnetic properties in the low-temperature régime. More relevant to the content of this paper (as we see later), however, is the fact that Stanley [10] proved, by generalising the Ising model to q -component spins, that its free energy approaches that of the spherical model when $q \rightarrow \infty$ (i.e., in the classical limit). Two other generalisations are the X – Y model, in which spins have two components and interact via a bilinear scalar product and the Potts model with its q -components of the spin variable [11].

The mathematical problems associated with the extraction of the physics of co-operative assemblies of spins are formidable. Hence, in the past models were introduced in which, for example, molecular interactions are greatly simplified but maintain the co-operative characteristics of the original assembly. However, even these simplified models, e.g. the Ising model, are notoriously difficult to analyse so a variety of approximations are normally used, as we saw above. Analytical methods, particularly the transfer matrix method [12,13] have been very useful in rigorously studying the statistical mechanics of classical systems such as the Ising model. Finite-size scaling techniques have also been advocated for a spin $-\frac{1}{2}$ antiferromagnetic Heisenberg–Ising chain [14]. In many publications, particular interest is in the determination of critical exponents for which a whole battery of methods have been employed like finite chain extrapolations [15], high-temperature series [16], two-time Green functions [17], Suzuki–Trotter mapping [18], Monte Carlo methods [19,20] and those based on the Bethe ansatz [21,22]. For the ferromagnetic Ising model Majumdar and Ramarao [23] have studied the low-temperature series expansion with temperature grouping polynomials. They have shown that certain roots of these polynomials converge to the critical fields H_c and in certain cases the critical field can be obtained quite accurately, the results being in general agreement with those found from a Padé analysis.

In this paper we make full use of unitary transformations which make the transfer terms diagonal and a one-to-one relationship between the product of N spin states in 1D, N^2 in 2D and N^3 in 3D and a binary or integer base system appropriate to the degeneracy of the spin states at each site. The unitary transformations have been used earlier by one of the authors in the literature to study the interaction of a single s-band with a substitutional potential of arbitrary range [24]. We shall only consider the case in zero field, i.e., $H_o = 0$, although, as the reader will recognise, the method we use is readily applicable to the case when $H_o \neq 0$ providing the magnetic field is along the z -axis. The interaction between spins will be between nearest neighbours only although we point out that the method we adopt can also be used for next nearest neighbours, etc. Our method is applicable in one-, two- *and also in three-dimensions*, provides a unique labelling for both eigenfunctions and eigenvalues and enables explicit determination of all eigenvalues for a system with a finite number of spins, however large, when appropriate periodic boundary conditions are utilised.

2. Nearest-neighbour coupled spins in one-dimension

Here we write the Hamiltonian in a form so that each of its terms involves a sum over *all* spin sites but the whole expression is entirely equivalent to that in Eq. (1). When we do this an $N \times N$ matrix appears which is reminiscent of the Hubbard transfer terms [25] which one knows how to deal with. Let us denote the Hamiltonian by H_1 and write

$$h_1 = \frac{-H_1}{J} = (S_{z1}S_{z2}S_{z3}\dots S_{zN})\mathcal{A}(S_{z1}S_{z2}S_{z3}\dots S_{zN})^+, \quad (2)$$

where we assume there are spins on N sites, the z components of which are denoted by S_{zi} ($i=1-N$). The notation $(\)^+$ denotes a column vector and A is a square $N \times N$ matrix whose main diagonal is bordered with ones and, in addition, there is a one in the top-right and bottom-left, to build in periodic boundary conditions, i.e.,

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdot & \cdot & \cdot & 1 \\ 1 & 0 & 1 & 0 & & & & \\ 0 & 1 & 0 & 1 & & & & \\ 0 & 0 & 1 & 0 & & & & \\ \cdot & \cdot & \cdot & & & & & \cdot \\ \cdot & \cdot & \cdot & & & & & \cdot \\ \cdot & \cdot & \cdot & & & & & 1 \\ 1 & 0 & 0 & & & & 1 & 0 \end{bmatrix} . \tag{3}$$

This form of A incorporates the coupling of spins to nearest neighbours only, the lattice sites being equally spaced in 1D.

It is easily seen that the r th eigenfunction of the matrix A is

$$|r\rangle = \frac{1}{\sqrt{N}} \sum_{s=1}^N \omega^{(r-1)(s-1)} |e_s\rangle \tag{4}$$

where $|e_s\rangle$ denotes an $N \times 1$ column vector whose elements are all zero except the s th which is unity and ω is the N th root of unity, i.e., $\omega = \exp(2\pi i/N)$. In the general $N \times N$ case the eigenvalue of $|r\rangle$ is

$$E_r = 2 \cos \left[\frac{2\pi}{N}(r-1) \right] . \tag{5}$$

Furthermore, the matrix A may be brought into diagonal form, D_1 , with a unitary transformation U_1 given by

$$D_1 = U_1^{-1} A U_1 , \tag{6}$$

where

$$U_1 = \frac{1}{\sqrt{N}} \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \dots & \omega^{N-1} \\ 1 & \omega^2 & \omega^4 & \dots & \omega^{2(N-1)} \\ \cdot & \cdot & \cdot & & \cdot \\ 1 & \omega^{N-1} & (\omega^2)^{N-1} & \dots & (\omega^{(N-1)})^{(N-1)} \end{bmatrix} \tag{7}$$

and U_1^{-1} has elements which are the complex conjugate of those in U_1 .

From Eq. (6) and the Hamiltonian H_1 in Eq. (2) we have

$$\begin{aligned} h_1 &= (S_{z1} S_{z2} S_{z3} \dots S_{zN}) U_1 U_1^{-1} A U_1 U_1^{-1} (S_{z1} S_{z2} S_{z3} \dots S_{zN})^+ \\ &= (S_{z1} S_{z2} S_{z3} \dots S_{zN}) U_1 D_1 U_1^{-1} (S_{z1} S_{z2} S_{z3} \dots S_{zN})^+ \\ &= P_1 D_1 P_1^+ , \end{aligned} \tag{8}$$

where \mathbf{P}_1 is a $1 \times N$ row vector whose r th column is

$$\frac{1}{\sqrt{N}} \sum_{t=1}^N \omega^{(r-1)(t-1)} S_{zt} . \tag{9}$$

Similarly \mathbf{P}_1^+ represents a $N \times 1$ column vector whose r th row is

$$\frac{1}{\sqrt{N}} \sum_{q=1}^N \omega^{(1-r)(q-1)} S_{zq} . \tag{10}$$

Note the coefficients in (10) are the complex conjugates of those in (9). Hence h_1 becomes

$$h_1 = \sum_{r=1}^N \frac{E_r}{N} \left(\sum_{t=1}^N \omega^{(r-1)(t-1)} S_{zt} \right) \left(\sum_{q=1}^N \omega^{(1-r)(q-1)} S_{zq} \right) , \tag{11}$$

where the summations over t and q are over all sites, not just nearest neighbours.

The eigenstates of h_1 are clearly products of kets representing a spin state on each site of the form

$$|m_{s_1}\rangle |m_{s_2}\rangle |m_{s_3}\rangle \cdots |m_{s_N}\rangle , \tag{12}$$

where m_{s_q} is the component of spin on the q th site. We delay the evaluation of the eigenvalues of h_1 in (11) until a later section as similar considerations hold in 2D and 3D and for any value of total spin, assuming that it is the same on each site.

3. Nearest-neighbour coupled spins on a square net in two-dimensions

In this case we assume the square net of lattice sites has N sites in one direction and N in a perpendicular direction so that we have N^2 spins in total. We will denote the Hamiltonian by H_2 and write it as

$$H_2 = (S_{z1} S_{z2} S_{z3} \dots S_{zN^2}) \mathbf{B} (S_{z1} S_{z2} S_{z3} \dots S_{zN^2})^+ , \tag{13}$$

where \mathbf{B} is an $N^2 \times N^2$ matrix. We number the lattice sites as in Fig. 1 and define \mathbf{B} as that matrix which has N diagonal blocks equal to \mathbf{A} with bordering $N \times N$ unity blocks plus an $N \times N$ unit matrix in the top-right and bottom-left of \mathbf{B} , i.e.,

$$\mathbf{B} = \begin{bmatrix} \mathbf{A} & \mathbf{I} & 0 & 0 & \cdot & \cdot & \cdot & \mathbf{I} \\ \mathbf{I} & \mathbf{A} & \mathbf{I} & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & \mathbf{I} & \mathbf{A} & \mathbf{I} & \cdot & \cdot & \cdot & \\ 0 & 0 & \mathbf{I} & & & & & \mathbf{I} \\ \mathbf{I} & 0 & \cdot & \cdot & \cdot & & & \mathbf{I} \mathbf{A} \end{bmatrix} \tag{14}$$

(See Fig. 2 for the illustration of a 2D array for $N = 4$.)

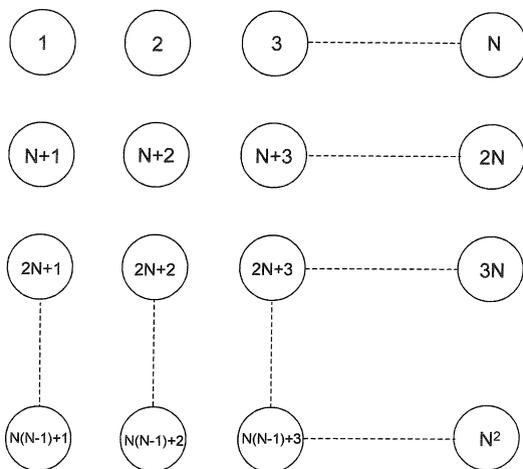


Fig. 1. Numbering of lattice sites in 2D.

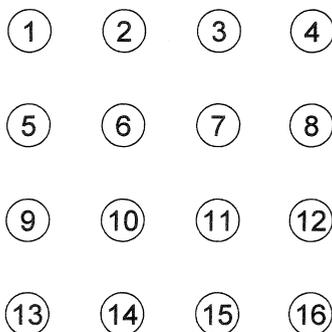


Fig. 2. Numbering of lattice sites of an $N = 4 \times N = 4$ square 2D net.

We now adopt a similar procedure to the 1D case and define an $N^2 \times N^2$ matrix, U_2 , which brings B into diagonal form so that

$$\begin{aligned}
 H_2 &= (S_{z1}S_{z2} \dots S_{zN^2})U_2U_2^{-1}BU_2U_2^{-1}(S_{z1}S_{z2} \dots S_{zN^2})^+ \\
 &= (S_{z1}S_{z2} \dots S_{zN^2})U_2D_2U_2^{-1}(S_{z1}S_{z2} \dots S_{zN^2})^+ \\
 &= P_2D_2P_2^+,
 \end{aligned}
 \tag{15}$$

where P_2 is a $1 \times N^2$ row vector whose (r, r') th column is

$$\frac{1}{N} \sum_{t,t'=1}^N \omega^{(r-1)(t-1)}\omega^{(r'-1)(t'-1)}S_{z,t+(t'-1)N}
 \tag{16}$$

and \mathbf{P}_2^+ is the $N^2 \times 1$ column vector whose elements in the (r, r') th row is

$$\frac{1}{N} \sum_{t''t'''=1}^N \omega^{(1-r)(t''-1)} \omega^{(1-r')(t'''-1)} S_{z,t''+(t'''-1)N} \tag{17}$$

The matrix \mathbf{D}_2 is diagonal and the element (r, r') th down the main diagonal is

$$E_{r,r'} = 2 \left\{ \cos\left(\frac{2\pi}{N}(r-1)\right) + \cos\left(\frac{2\pi}{N}(r'-1)\right) \right\}, \tag{18}$$

i.e., these are the eigenvalues of \mathbf{B} .

To see how the nested structure exhibited in Eqs. (16)–(18) comes about it is instructive to see what \mathbf{U}_2 actually is by performing two component operations. The first makes each diagonal block of \mathbf{B} diagonal but leaves the unit $N \times N$ matrices, \mathbf{I} , unchanged and in the same position. This is easily realised by first premultiplying \mathbf{B} by an $N^2 \times N^2$ matrix whose diagonal $N \times N$ blocks (N of them) are each \mathbf{U}_1^{-1} and postmultiplying by another $N^2 \times N^2$ matrix whose diagonal $N \times N$ blocks are \mathbf{U}_1 . After this is done \mathbf{B} becomes \mathbf{B}_1 , where

$$\mathbf{B}_1 = \begin{bmatrix} \mathbf{U}_1^{-1}\mathbf{A}\mathbf{U}_1 & \mathbf{I} & \mathbf{O} & \mathbf{O} & \dots & \dots & \dots & \mathbf{I} \\ \mathbf{I} & \mathbf{U}_1^{-1}\mathbf{A}\mathbf{U}_1 & \mathbf{I} & \mathbf{O} & \dots & \dots & \dots & \mathbf{O} \\ \mathbf{O} & \mathbf{I} & \mathbf{U}_1^{-1}\mathbf{A}\mathbf{U}_1 & \mathbf{I} & \dots & & & \mathbf{O} \\ & & & & & & & \mathbf{I} \\ \mathbf{I} & \mathbf{O} & \dots & \dots & & & \mathbf{I} & \mathbf{U}_1^{-1}\mathbf{A}\mathbf{U}_1 \end{bmatrix}, \tag{19}$$

i.e., a matrix whose main diagonal $N \times N$ blocks are $\mathbf{U}_1^{-1}\mathbf{A}\mathbf{U}_1$ bordered by $N \times N$ unity blocks, \mathbf{I} , with additional \mathbf{I} blocks in the top-right and bottom-left corners. The matrices \mathbf{O} are each $N \times N$ with zero elements. The matrix $\mathbf{U}_1^{-1}\mathbf{A}\mathbf{U}_1$ is now diagonal, the element in the top left being coupled only to that in the top left of the \mathbf{I} matrix which is second block along on the top row of blocks, i.e., the $(N + 1)$ th position and the element in the top left of the \mathbf{I} matrix in the top-right of \mathbf{B}_1 , i.e., the $N(N - 1) + 1$ the position, etc. The coupled blocks so formed again have the same form and size as \mathbf{A} and the r th will have the form

$$\begin{bmatrix} E_r & 1 & 0 & 0 & \dots & \dots & 0 & 1 \\ 1 & E_r & 1 & 0 & & & & \\ 0 & 1 & E_r & 1 & & & & \\ 0 & 0 & 1 & & & & & \\ 1 & 0 & \dots & \dots & & & 1 & E_r \end{bmatrix}. \tag{20}$$

The associated linear combinations of spin functions, after making \mathbf{A} diagonal, for such a block, will be

$$\frac{1}{\sqrt{N}} \sum_{t=1}^N \omega^{(r-1)(t-1)} S_{zt} = T_1 \tag{21}$$

from the top $N \times N$ block,

$$\frac{1}{\sqrt{N}} \sum_{t'=N+1}^{2N} \omega^{(r-1)(t'-1)} S_{zt'} = T_2 \quad (22)$$

from the second $N \times N$ block down the main diagonal of \mathbf{B}_1 ,

$$\frac{1}{\sqrt{N}} \sum_{t'=2N+1}^{3N} \omega^{(r-1)(t'-1)} S_{zt'} = T_3 \quad (23)$$

from the next block down, etc. The (r') th combination of spin functions to make (20) diagonal, for a given r , will be

$$\frac{1}{N} \sum_{t=1}^N \omega^{(r'-1)(t-1)} \sum_{t'=(t-1)N+1}^{tN} \omega^{(r-1)(t'-1)} S_{zt'} \quad (24)$$

which simplifies to

$$\frac{1}{N} \sum_{t,t'=1}^N \omega^{(r-1)(t'-1)} \omega^{(r'-1)(t'-1)} S_{z,t+(t'-1)N}. \quad (25)$$

The reference to the (r, r') th column above simply designates the r th block after the A 's are diagonalised and r' denotes the combination within it when the r th block is reduced to diagonal form.

To summarise, our 2D Hamiltonian, H_2 , may therefore be expressed as

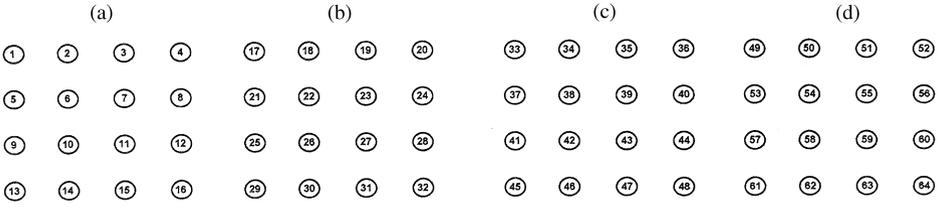
$$H_2 = \sum_{r',r=1}^N \frac{E_{r,r'}}{N^2} \left(\sum_{t,t'=1}^N \omega^{(r-1)(t-1)} \omega^{(r'-1)(t'-1)} S_{z,t+(t'-1)N} \right) \times \left(\sum_{t'',t'''=1}^N \omega^{(1-r)(t''-1)} \omega^{(1-r')(t'''-1)} S_{z,t''+(t'''-1)N} \right). \quad (26)$$

It is clear once again that eigenstates of H_2 are products of N^2 spin states, one from each site, the different eigenstates being the different arrangements of the N^2 spin components. For example, if on each site the spin $S = \frac{1}{2}$, then there will be 2^{N^2} arrangements of spin components in 2D.

4. Nearest-neighbour couplings on a 3D cubic network of sites

Very similar principles hold in this situation when compared with 2D and 1D and we write the Hamiltonian, H_3 , as

$$H_3 = (S_{z1} S_{z2} \dots S_{zN^3}) C (S_{z1} S_{z2} \dots S_{zN^3})^+ \quad (27)$$



END ON VIEW

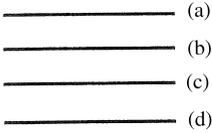


Fig. 3. Numbering of sites in 3D: (a) top layer, (b) next layer down, (c) layer below (b) and (d) layer below (c).

where C is given by

$$C = \begin{bmatrix} \mathbf{B} & \mathbf{I} & \mathbf{O} & \dots & \dots & \mathbf{O} & \mathbf{I} \\ \mathbf{I} & \mathbf{B} & \mathbf{I} & & & & \mathbf{O} \\ \mathbf{O} & \mathbf{I} & \mathbf{B} & & & & \mathbf{O} \\ & & & & & & \mathbf{O} \\ \mathbf{O} & & & & & \mathbf{B} & \mathbf{I} \\ \mathbf{I} & \mathbf{O} & \dots & \dots & \mathbf{O} & \mathbf{I} & \mathbf{B} \end{bmatrix} \tag{28}$$

where \mathbf{I} here is an $N^2 \times N^2$ unit matrix. That is, C , is an $N^3 \times N^3$ matrix with N \mathbf{B} matrices along its main diagonal bordered by $N^2 \times N^2$ unit matrices with an $N^2 \times N^2$ unit matrix in the top-right and bottom-left of C . In the same spirit as the 2D case we may premultiply C by U_3^{-1} and postmultiply by U_3 to make C into a diagonal D_3 so that the Hamiltonian becomes

$$H_3 = (S_{z1}S_{z2} \dots S_{zN^3})U_3U_3^{-1}CU_3U_3^{-1}(S_{z1}S_{z2} \dots S_{zN^3})^+ \\ = (S_{z1}S_{z2} \dots S_{zN^3})U_3D_3U_3^{-1}(S_{z1}S_{z2} \dots S_{zN^3})^+. \tag{29}$$

To illustrate how the lattice sites are numbered in the 3D case we refer the reader to Fig. 3.

The diagonalisation of C again takes two transformations which make up U_3 . The first makes each diagonal block, \mathbf{B} , diagonal, but leaves the unit matrices in the same position and unchanged. This will obviously be enacted by first premultiplying the $N^3 \times N^3$ matrix, C , by an $N^3 \times N^3$ matrix whose diagonal $N^2 \times N^2$ blocks are U_2^{-1}

and postmultiplying by one with diagonal blocks U_2 . The result is a matrix, C_1 , where

$$C_1 = \begin{bmatrix} U_2^{-1}BU_2 & I & O & \dots & \dots & O & I \\ I & U_2^{-1}BU_2 & I & & & & O \\ O & I & U_2^{-1}BU_2 & & & & O \\ & & & & & U_2^{-1}BU_2 & I \\ O & & & & & & I \\ I & O & \dots & \dots & O & I & U_2^{-1}BU_2 \end{bmatrix}. \tag{30}$$

When B is diagonalised, the energies along its main diagonal are $E_{r,r'}$. Thus C_1 may be rearranged into a series of N block matrices which are $N \times N$ for fixed r and r' of the form

$$\begin{bmatrix} E_{r,r'} & 1 & O & O & \dots & O & 1 \\ 1 & E_{r,r'} & 1 & O & \dots & & O \\ O & 1 & E_{r,r'} & 1 & & & \\ O & O & 1 & & & & O \\ & & & & & & 1 \\ 1 & O & O & \dots & O & 1 & E_{r,r'} \end{bmatrix}. \tag{31}$$

The matrix in (31) may then be easily diagonalised, in a second part of the process, using U_1 yet again. The energies of C become

$$E_{r,r',r''} = 2 \left\{ \cos\left(\frac{2\pi}{N}(r-1)\right) + \cos\left(\frac{2\pi}{N}(r'-1)\right) + \cos\left(\frac{2\pi}{N}(r''-1)\right) \right\} \tag{32}$$

and the associated linear combinations of spin functions will now be

$$\frac{1}{N\sqrt{N}} \sum_{t,t',t''=1}^N \omega^{(r-1)(t-1)} \omega^{(r'-1)(t'-1)} \omega^{(r''-1)(t''-1)} S_{z,t+(t'-1)N+(t''-1)N^2}. \tag{33}$$

The 3D Hamiltonian operator, H_3 , now takes the form

$$H_3 = \sum_{r,r',r''=1}^N \frac{E_{r,r',r''}}{N^3} \times \left\{ \sum_{t,t',t''=1}^N \omega^{(r-1)(t-1)} \omega^{(r'-1)(t'-1)} \omega^{(r''-1)(t''-1)} S_{z,t+(t'-1)N+(t''-1)N^2} \right\} \times \left\{ \sum_{t_1,t'_1,t''_1=1}^N \omega^{(1-r)(t_1-1)} \omega^{(1-r')(t'_1-1)} \omega^{(1-r'')(t''_1-1)} S_{z,t_1+(t'_1-1)N+(t''_1-1)N^2} \right\}. \tag{34}$$

The eigenstates of H_3 will be products of N^3 spin states, one for each site, the different eigenstates being the different arrangements of the N^3 spin components. In the next section we analyse these eigenstates in such a way that, for 1D, 2D and 3D lattices we may easily find the energies of H_1, H_2 and H_3 .

5. Eigenstates

5.1. One-dimension

For simplicity, at least at first, we shall assume that on each site the spin $S = \frac{1}{2}$ so each spin has two components $m_s = \mp \frac{1}{2}$. Instead of dragging halves throughout the calculation we designate spin up with unity (1) and spin down (0) so that

$$m_S = +\frac{1}{2} = \text{up} = (1) - \frac{1}{2}$$

and

$$m_S = -\frac{1}{2} = \text{down} = (0) - \frac{1}{2}.$$

We consider the case with $N = 4$ and imagine 2^N rectangular boxes of length N so that the entry in the position (1, 1) is the component of spin on site one, that in (1, 2) is the component on site two, etc. The eigenstates for this simple case may then be represented by 16 boxes occupied as below. One way in which they may be generated is to begin with all four slots in the first box with spin down, the second, third, fourth and fifth boxes are then generated by turning over one spin in turn, i.e.,

$$\begin{aligned} &(0, 0, 0, 0), \\ &(1, 0, 0, 0), \\ &(0, 1, 0, 0), \\ &(0, 0, 1, 0), \\ &(0, 0, 0, 1). \end{aligned} \tag{35}$$

Then we begin with box 2 and generate 1's to the right of the one there already in all possible ways, i.e.,

$$\begin{aligned} &(1, 1, 0, 0), \\ &(1, 0, 1, 0), \\ &(1, 0, 0, 1). \end{aligned} \tag{36}$$

Then repeat this procedure with the third box, i.e.,

$$\begin{aligned} &(0, 1, 1, 0), \\ &(0, 1, 0, 1) \end{aligned} \tag{37}$$

and then the fourth

$$(0, 0, 1, 1). \tag{38}$$

If a box already has a one on the right we ignore it and go back to the first box with two spins up and repeat the process, then the second, etc. Hence, we generate

$$\begin{aligned}
 (0, 0, 0, 0) &\rightarrow 0, \\
 (1, 0, 0, 0) &\rightarrow 1, \\
 (0, 1, 0, 0) &\rightarrow 2, \\
 (0, 0, 1, 0) &\rightarrow 4, \\
 (0, 0, 0, 1) &\rightarrow 8, \\
 (1, 1, 0, 0) &\rightarrow 3, \\
 (1, 0, 1, 0) &\rightarrow 5, \\
 (1, 0, 0, 1) &\rightarrow 9, \\
 (0, 1, 1, 0) &\rightarrow 6, \\
 (0, 1, 0, 1) &\rightarrow 10, \\
 (0, 0, 1, 1) &\rightarrow 12, \\
 (1, 1, 1, 0) &\rightarrow 7, \\
 (1, 1, 0, 1) &\rightarrow 11, \\
 (1, 0, 1, 1) &\rightarrow 13, \\
 (0, 1, 1, 1) &\rightarrow 14, \\
 (1, 1, 1, 1) &\rightarrow 15.
 \end{aligned}
 \tag{39}$$

Each box represents an eigenstate of a linear chain with 4 sites. Although the above will always generate all the possible eigenstates it is not very convenient for (a) labelling the eigenfunction or row or box and (b) whether a spin at the q th position ($1 \leq q \leq N$) is up or down. However, there is an *unique* labelling utilising a binary base. Suppose we represent the given box with a number, b , which we may write in binary

$$b = a_1 2^0 + a_2 2^1 + a_3 2^2 + a_4 2^3,
 \tag{40}$$

where a_1, a_2, a_3 and a_4 are either unity or zero. Clearly (40) then uniquely labels the rows of (39), the number being given to the right of each box in (39). Imagining (39) as a matrix with 2^N rows and N columns we see that the numbering of the i th row is given by

$$i - 1 = \sum_{j=1}^N a_{ij} 2^{j-1},
 \tag{41}$$

the row labelling the particular spin eigenfunction (for the whole chain i.e., a particular product of spin states) and j the N sites associated with it. As we shall see, what we require is an expression for a_{ij} for a particular i and each $1 \leq j \leq N$. We may do this fairly readily by using the Integer Value Function $\text{Int}(x) = n = [x]$ where $n \leq x \leq n + 1$ which extracts from its argument the largest integer that does not exceed the argument. To obtain a_{ij} we begin with the N th spin site and note that

$$a_{i,N} = [(i - 1) / 2^{N-1}].
 \tag{42}$$

Similarly,

$$a_{i,N-1} = [(i - 1 - a_{i,N} 2^{N-1}) / 2^{N-2}]
 \tag{43}$$

and

$$a_{i,N-2} = \left[\frac{i - 1 - a_{i,N}2^{N-1} - a_{i,N-1}2^{N-2}}{2^{N-3}} \right], \tag{44}$$

etc. The general term being

$$a_{i,N-s} = \left[\frac{i - 1 - \sum_{r=0}^{s-1} a_{i,N-r}2^{N-r-1}}{2^{N-s-1}} \right] \tag{45}$$

for $1 \leq s \leq N - 1$ and Eq. (42) for $s = 0$.

As an example let us consider $N = 4$ again and eigenfunction 10 (in (39) this will clearly correspond to that which is numbered 9 since rows are numbered from 1 to 2^N and not 0 to $2^N - 1$). In this case spin 1 is up (i.e., at site one), spins 2 and 3 (at, respectively, sites 2 and 3) are down and spin 4 is up. The action of s_{z2} on this spin product state, i.e.,

$$(1, 0, 0, 1) \equiv |m_{S1} = \frac{1}{2}\rangle |m_{S2} = -\frac{1}{2}\rangle |m_{S3} = -\frac{1}{2}\rangle |m_{S4} = +\frac{1}{2}\rangle$$

is clearly $-\frac{1}{2}(1, 0, 0, 1)$ or simply $(a_{10,2} - \frac{1}{2})(1, 0, 0, 1)$ or s_{z1} on this state is $(a_{10,2} - \frac{1}{2})(1, 0, 0, 1)$.

Thus, $s_{z,k}$ acting on the i th eigenstate simply gives $a_{i,k} - \frac{1}{2}$ multiplied by the same product state. Written in terms of the [...] function this is simply

$$\left[\frac{i - 1 - \sum_{r=0}^{N-k} a_{i,N-r}2^{N-r-1}}{2^{k-1}} \right] - \frac{1}{2} = C(i, k, N, 2) \tag{46}$$

for $1 \leq k < N$, the argument of the [...] function being replaced by that in Eq. (42) when $k=N$. i.e., the element in the i th row and k th column of a $1 \times N$ row matrix when the spin degeneracy on each site is equal to 2. For this special case the corresponding i th eigenvalue of the 1D Hamiltonian will simply be (from Eq. (11)),

$$\sum_{r=1}^N \frac{E_r}{N} \left| \sum_{t=1}^N \omega^{(r-1)(t-1)} C(i, t, N, 2) \right|^2 \quad 1 \leq i \leq N. \tag{47}$$

By using the fact that $E_r = \omega^{(r-1)} + \omega^{-(r-1)}$ the summation over r may be performed since

$$\sum_{r=1}^N \omega^{sr} = (\delta_{s,0} + \delta_{s,+N} + \delta_{s,-N}) \tag{48}$$

The expression in (47) becomes

$$\sum_{t=1}^N C(i, t, N, 2) \{ C(i, t + 1, N, 2) + C(i, t - 1, N, 2) + C(i, t + 1 - N, N, 2) + C(i, t - 1 - N, N, 2) + C(i, 1 + t + N, N, 2) + C(i, t - 1 + N, N, 2) \}, \tag{49}$$

where the second label in each C must be ≥ 1 and $\leq N$ for the C to be non-vanishing. All the C 's for a given i can be clearly evaluated from the identities in Eqs. (42)–(45) and the i th eigenvalue is completely determined.

It is worth pointing out that if the degeneracy of each spin is increased the above analysis can be repeated *and still holds*, when the factor of two is replaced by the degeneracy of the spin. For example, if each spin were $S = 1$ then each slot in what could correspond to (39) – now with 3^N rows – can contain 2,1,0 and the equation which corresponds to Eq. (46) will be of the form [...] with a 2 replaced by 3 and $-\frac{1}{2}$ replaced by -1 . The designation of rows is again unique in this basis of 3. Obviously, any finite basis could be used and the argument would follow through.

5.2. Two-dimensions

Because of the way we have numbered sites we can use the same technique as in 1D but here each rectangular box will be $1 \times N^2$ and, for a spin degeneracy of 2, there will be 2^{N^2} rows [for a degeneracy of 3 there will be 3^{N^2} rows and so on]. Thus, in 2D, from Eq. (26), the i th eigenvalue will be

$$\sum_{r,r'=1}^N \frac{E_{r,r'}}{N^2} \left| \sum_{t,t'=1}^N \omega^{(r-1)(t-1)} \omega^{(r'-1)(t'-1)} C(i, t + (t' - 1)N, N^2, 2) \right|^2 \quad (50)$$

for a spin degeneracy of 2. Note the upper limit of the summations is still N not N^2 . To incorporate increased spin degeneracy the modification is obvious. Furthermore, the sums over r and r' may be carried out using Eq. (48) using the same procedure as in the 1D case. We give this result in Appendix A, the restrictions on the second label in each C coefficient being the same as in the 1D case.

5.3. Three-dimensions

Here our boxes will be $1 \times N^3$ and for a degeneracy of 2 there will be 2^{N^3} rows and the i th eigenvalue, from Eq. (34), will be simply (!)

$$\sum_{r,r',r''=1}^N \frac{E_{r,r',r''}}{N^3} \left| \sum_{t,t',t''=1}^N \omega^{(r-1)(t-1)} \omega^{(r'-1)(t'-1)} \omega^{(r''-1)(t''-1)} \right. \\ \left. \times C(i, t + (t' - 1)N + (t'' - 1)N^2, N^3, 2) \right|^2. \quad (51)$$

Comments concerning increased degeneracy are here also equally obvious. The sums over r, r', r'' may be again performed using Eq. (48), the result we give in Appendix A and the restrictions on the C coefficients is the same as in the 1D and 2D cases.

6. Numerical calculations

In this section we will illustrate the method with several specific examples of finite-size lattices in one- and two-dimensions. We have focused in this paper on a novel analytical approach and the examples given below primarily serve the purpose of an independent check on the correctness of the method.

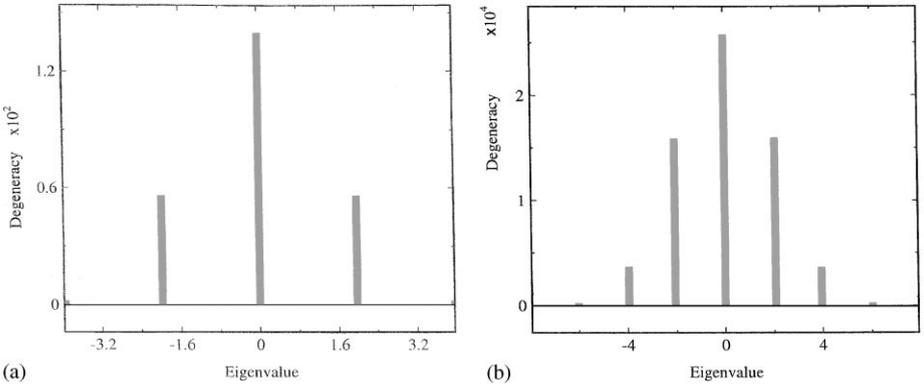


Fig. 4. Distribution of eigenvalues together with the associated degeneracies for (a) a 1D, 8 spin system and (b) a 1D, 16 spin system.

The first example concerns an 8-site 1D Ising system. Fig. 4a is a plot of the degeneracies for the five eigenvalues (0, ±2, ±4) found using Eq. (48). The corresponding degeneracies are 140, 56 and 2, respectively. The resultant partition function can be easily represented as

$$z = 4 \cosh(4\beta) + 112 \cosh(2\beta) + 140. \tag{52}$$

A well-known formula for the Ising model in 1D gives

$$z = \lambda_+^N + \lambda_-^N, \tag{53}$$

where, in the absence of an external magnetic field,

$$\lambda_+ = 2 \cosh(\beta/2), \quad \lambda_- = 2 \sinh(\beta/2). \tag{54}$$

Substituting these expressions into Eq. (53) and taking $N=8$ yields perfect agreement with Eq. (52).

In Fig. 4b we have shown a similar plot of the eigenvalues of the 1D Ising model with $N = 16$ and the eigenvalues are now (0, ±2, ±4, ±6, ±8). In all of the above we have set $2J = 1$.

In Fig. 5 we show the result in the 2D case on a 4×4 lattice. The difficulty in making a comparison with the Onsager result [7] is that the latter gives the free energy per spin for n large, i.e.,

$$F/nkT = -\ln(2 \cosh J\beta) - \frac{1}{2\pi} \int_0^\pi d\phi \ln \left[\frac{1}{2} \left(1 + \sqrt{1 - k^2 \sin^2 \phi} \right) \right], \tag{55}$$

where $n = N^2$ and

$$k = \frac{2 \sinh(\beta J)}{\cosh^2(\beta J)} \tag{56}$$

with $\beta = 1/kT$, k being Boltzmann’s constant (Fig. 6).

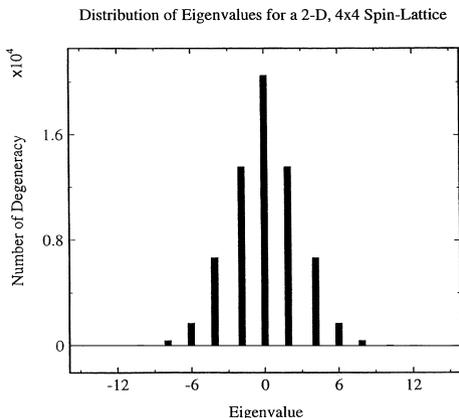


Fig. 5. Degeneracies and eigenvalues for an $N = 4 \times N = 4$ spin system in 2D.

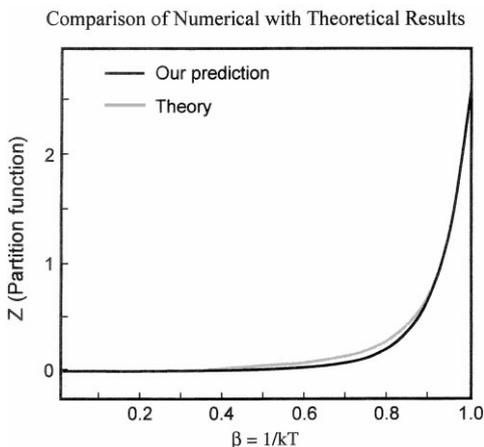


Fig. 6. Comparison of our numerical with earlier results of Onsager in 2D.

In the low-temperature limit the free energy tends to (since $k \rightarrow 0$)

$$F = -nJ . \tag{57}$$

From Eqs. (47), (50) and (51) we see that if all the C coefficients are equal to one-half – corresponding to the low-temperature situation when all sites are occupied – the expressions for the i th eigenvalues reduce to (i) $N/2$ in 1D (ii) N^2 in 2D (iii) $3N^3/2$ in 3D. Therefore, in 2D the zero-Kelvin estimate of the free energy is also given by Eq. (57). Care should be taken to observe that the Hamiltonian defined in Eq. (1) runs over all nearest neighbours of one site ($\langle i, j \rangle$) whereas some conventional

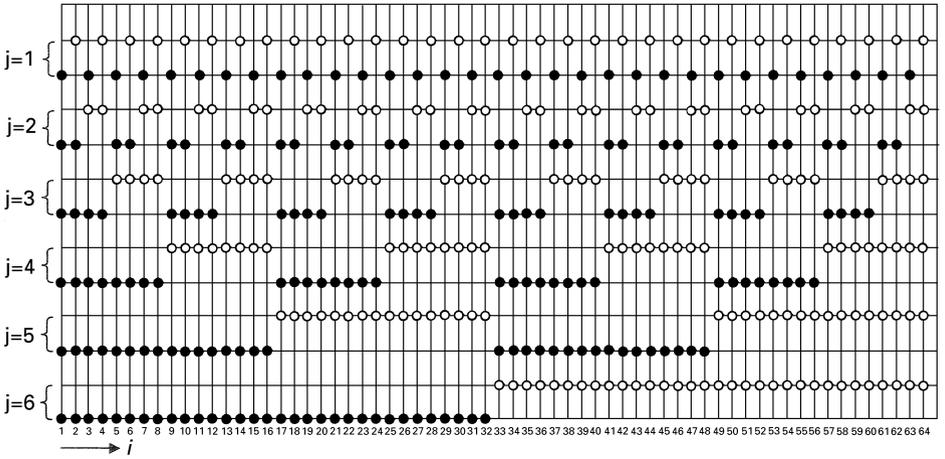


Fig. 7. Periodic occupancies for $N = 6$ in 2D: spin up (\circ) and spin down (\bullet).

literature defines the interaction by $-\varepsilon(\sum_i s_{iz}s_{i+1,z})$ thereby introducing a factor of two between the interaction constant, ε , and our J .

7. Periodic occupancy of spin components in 1D

We have used the base system to designate our states in 1D, 2D and 3D for a number of reasons. Firstly, it is a very succinct method of labelling n spin states in any number of dimensions. Secondly, the adoption of this idea provides a unique numbering of very complicated states. There is a third reason and this is to incorporate the periodic symmetries which it possesses. It is not immediately apparent that such symmetries exist so we have tried to give an example in Fig. 7. Here we have taken the case of $N=6$ sites in 1D and plotted i horizontally, labelling the 64 possible states (the spin on each site being $s = \frac{1}{2}$). Vertically we plot j the ‘box’ number where $j=1$ to $j=6$. When we use our system of labelling states as described in Eqs. (42)–(45) each box j for a given i can contain a spin up, which we denote by \circ , or spin down which we represent by \bullet . Beginning with $j=6$ we see that precisely half the 64 states for the $j=6$ box have spin down and half-spin up, the first 32 all having spin down and the rest spin up. When we go vertically up in Fig. 7 to $j=5$ we see that the first 16 states have spin down, the next 16 spin up, the next 16 spin down and the last 16 spin up. Thus, the period of the spin arrangement has halved in going from $j=6$ to $j=5$. This period is halved yet again in going from $j=5$ to 4. When we get to the top of Fig. 7 and $j=1$, $i=1$ is spin down, $i=2$ is spin up, $i=3$ is spin down, etc. The system of labelling for states we have adopted therefore possesses a periodic arrangement of spins with i (the label for the state), the period gradually being reduced as j is reduced from $j=6$ to 1.

8. Summary and outlook

This paper has been concerned with a derivation of analytical expressions for the eigenvalues and eigenstates of the Ising Hamiltonian in one-, two- and three-dimensional lattices of arbitrary size. The method employed relied on transfer matrix properties and diagonalisations using the N th roots of unity. Although the resultant expressions are simple looking their implementation using computer codes is very time consuming. Due to time constraints we have only explored several manageable cases in one- and two-dimensions and the results agree with earlier exact calculations known in the literature (see Fig. 6). Although we have not carried out any calculations for a 3D lattice yet our paper provides an exact formula in this case also. We intend to pursue the question of computer code optimisation in the near future. One natural line of attack would be a Monte Carlo sampling method.

Having found an analytical formula for the eigenvalues of the Ising Hamiltonian solves the problem only in principle. What is needed in statistical applications is the partition function. The straightforward summation over all states can now be carried out numerically since we know the energy values for each state. However, the problem of running over *all* states will very quickly become virtually insurmountable since the number of states grows as 2^N where N is the number of lattice sites. The alternative of summing over the energies requires the knowledge of the degeneracy for each state which just places the key difficulty on another quantity. Lastly, and perhaps most practically, one could resort to a numerical approach, such as the Monte Carlo method [26], in conjunction with the formula which we derived here. We propose for future applications the use of the Metropolis algorithm for a finite size, finite temperature system. In this procedure, a final state, $\{S\}_f$ is obtained from an initial state, $\{S\}_i$ by flipping one or more spins. The probability of moving from state i to f is given by

$$P(\{S\}_i \rightarrow \{S\}_f) = \begin{cases} e^{-\beta(E_f - E_i)} & \text{if } E_f > E_i, \\ 1 & \text{if } E_f < E_i, \end{cases}$$

where E_f and E_i are the corresponding eigenenergies, which have been, of course, calculated here. It is hoped that with the formula for the eigenvalues provided here, one can overcome the size barrier of $(128)^3$ and finite – size scaling analysis can be extended to larger systems. It is also expected that an independent test can be provided for the estimate of the critical temperature of the 3D Ising model given as $J/kT_c = 0.221650(5)$ [26]. Since the values of the critical exponents for these 3D Ising model are not known with impressive precision, this offers an added value of such a numerical undertaking which we plan to execute in the near future.

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Appendix A

A.1. Two-dimensions

Using Eqs. (50) and (48), the i th eigenvalue, E_i , becomes

$$\begin{aligned}
 E_i = & \sum_{t,t'=1}^N C(i,t+(t'-1)N,N^2,2)[C(i,1+t+(t'-1)N,N^2,2) \\
 & + C(i,1+t-N+(t'-1)N,N^2,2) \\
 & + C(i,t-1+(t'-1)N,N^2,2) + C(i,t-1+N+(t'-1)N,N^2,2) \\
 & + C(i,t+t'N,N^2,2) + C(i,t+(t'-1)N,N^2,2) \\
 & + C(i,t+(t'-2)N,N^2,2) + C(i,t+(t'+N-2)N,N^2,2)].
 \end{aligned}$$

A.2. Three-dimensions

Using Eqs. (51) and (48), the i th eigenvalue, E_i , becomes

$$\begin{aligned}
 E_i = & \sum_{t,t',t''=1}^N C(i,t+(t'-1)N+(t''-1)N^2,N^3,2) \\
 & \times [C(i,1+t+(t'-1)N+(t''-1)N^2,N^3,2) \\
 & + C(i,1+t-N+(t'-1)N+(t''-1)N^2,N^3,2) \\
 & + C(i,t-1+(t'-1)N+(t''-1)N^2,N^3,2) \\
 & + C(i,t-1+N+(t'-1)N+(t''-1)N^2,N^3,2) \\
 & + C(i,t+t'N+(t''-1)N^2,N^3,2) \\
 & + C(i,t+(t'-N)N+(t''-1)N^2,N^3,2) \\
 & + C(i,t+(t'-2)N+(t''-1)N^2,N^3,2) \\
 & + C(i,t+(t'+N-2)N+(t''-1)N^2,N^3,2) \\
 & + C(i,t+(t'-1)N+t''N^2,N^3,2) \\
 & + C(i,t+(t'-1)N+(t''-N)N^2,N^3,2) \\
 & + C(i,t+(t'-1)N+(t''-2)N^2,N^3,2) \\
 & + C(i,t+(t'-1)N+(t''+N-2)N^2,N^3,2)].
 \end{aligned}$$

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