Appendix A: Explanations of 1-D and 2-D Ising Models

Ferromagnetism in some metals and alloys (e.g., Fe and Ni), is a consequence of spontaneous polarization in a finite fraction of spins of atoms in the same direction. This phenomenon gives rise to a macroscopic magnetic field only if the temperature is below a characteristic value, known as the Curie temperature $T_c$. At and above $T_c$, the spins lose their ordered orientation and their ordering becomes random. Consequently, the net macroscopic magnetic field becomes vanishingly small. As $T_c$ is approached from both sides, the specific heat of the material tends to infinity.

The Ising Model [Ising 1925] is an extremely simplified but effective, representation of the structural behavior of ferromagnetic substances. Its main impact is that a 2-dimensional Ising model yields a mathematically tractable representation of phase transition in statistical mechanics.

First let us start with a 1-dimensional Ising Model. [Note: The 1-dimensional Ising model does not represent phase transitions.] Let us consider an array of $N$ fixed points, called lattice sites in the physics literature, that form $n$-dimensional periodic lattice, $n=1,2,3$. For example, the geometric structure of a lattice may be cubic or hexagonal. There is a spin variable, $S_i$, $i=1,2,\ldots,N$, associated with each lattice. Let us restrict $S_i$ such that $S_i \in \{-1,0,1\}$. We call $S_i = 1$ as the spin up, and $S_i = -1$ as the spin down. Thus, a sequence $\{S_i\}$ configures a system, whose (Ising) energy (denoted by the subscript $I$ in $E_I$) is defined to be:

$$E_I(\{S_i\}) = -\sum_{\langle i,j \rangle} \varepsilon_{ij} S_i S_j - H \sum_{i=1}^{N} S_i$$
where \( \langle i,j \rangle \) denotes a nearest neighbor pair of spins and there is no distinction between \( \langle i,j \rangle \) and \( \langle j,i \rangle \); thus, the sum over \( \langle i,j \rangle \) contains \( bN/2 \) terms, \( b \) being the number of nearest neighbors of any given site. [Note: \( b = 2 \) for 1-D site, \( b = 4 \) for 2-D square lattice, \( b = 6 \) for 3-D cubic lattice, and \( b = 8 \) for 3-D body-centered cubic lattice.]

\( E_{ij} \) is the interaction energy which is an a priori known constant.

The effects of the lattice structure are realized through the parameter \( \epsilon \) and \( E_{ij} \). For isotropic homogeneous materials, \( E_{ij} \) is reduced to a constant \( \epsilon \).

\( H \) is a constant external magnetic field.

Then, for isotropic homogeneous materials, Ising energy is:

\[
E(I) = \sum_{\langle i,j \rangle} E_{ij} - H \sum_{i=1}^{N} \lambda_i
\]

For \( \epsilon > 0 \), the material is called ferromagnetic.

For \( \epsilon < 0 \), the material is called antiferromagnetic.

Let us consider only ferromagnetic materials, i.e., \( \epsilon > 0 \).

Let us define a partition function

\[
Z^N_I(\beta) = \sum_{\lambda_1, \ldots, \lambda_N} \exp(-\beta E(I, \lambda))
\]

where \( \lambda_i \) ranges independently over \( \pm 1, \pm i \). Hence, there are a total of \( 2^N \) terms in the summation of Eq. (2). Then, the Helmholtz free energy is obtained in the Ising setting as:

\[
F_I(\beta) = \lim_{N \to \infty} \frac{1}{\beta N} \ln \left( Z^N_I(\beta) \right)
\]

and the magnetization

\[
M_I(\beta) = -\frac{2}{\beta H} \left( \beta F_I(H, \beta) \right)
\]

Denoting \( \langle \cdot \rangle \) as expectation of \( \cdot \), it follows from (4) that

\[
M_I(\beta) = \langle \sum_{i=1}^{N} \lambda_i \rangle
\]

The quantity \( M_I(\beta) \big|_{H=0} \) is called the spontaneous magnetization.

For ferromagnetic materials, \( M_I(\beta) \big|_{H=0} \neq 0 \).
Given the spin \( s \in \{ -1, 1 \} \), let us define an injective map
\[
\sigma : \{ -1, 1 \} \to \{ 0, 1 \} \times \{ 0, 1 \} \quad \text{such that} \quad \sigma (-1) = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \text{and} \quad \sigma (1) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}
\]
Let us define a scalar-valued function \( \nu : \{ -1 \} \times \{ -1 \} \to [0, \infty) \) with real parameters \( \beta, \varepsilon \) and \( H \) as
\[
\nu (\beta, \varepsilon) = e^{\beta \varepsilon} \left( \beta e^{\beta \varepsilon} + \frac{1}{2} \beta H (\beta + 2) \right)
\]
that yields
\[
\begin{align*}
\nu (+1, +1) &= e^{\beta (\varepsilon + H)} \\
\nu (+1, -1) &= e^{\beta \varepsilon} \\
\nu (-1, +1) &= e^{-\beta \varepsilon} \\
\nu (-1, -1) &= e^{-\beta (\varepsilon - H)}
\end{align*}
\]
Now, we define a \((2 \times 2)\) matrix
\[
V (\beta, \varepsilon, H) = \begin{bmatrix}
\nu (+1, +1) & \nu (+1, -1) \\
\nu (-1, +1) & \nu (-1, -1)
\end{bmatrix} = \begin{bmatrix}
e^{\beta (\varepsilon + H)} & -\beta e^{\beta \varepsilon} \\
e^{-\beta \varepsilon} & e^{\beta (\varepsilon - H)}
\end{bmatrix}
\]
In vector notation, \( \nu (\beta, \varepsilon) = \sigma (\beta)^T V \sigma (\beta) \)
In an alternative notation, \( \nu (\beta, \varepsilon) = \begin{bmatrix} \beta_1 \\ V \end{bmatrix} \sigma (\beta) \)
We define a partition function for nearest-neighbor interactions as
\[
Z_N^N = \sum_{\lambda_1, \ldots, \lambda_N} \sigma (\lambda_1)^T V \sigma (\lambda_2) \sigma (\lambda_2)^T V \sigma (\lambda_3) \ldots \sigma (\lambda_N)^T V \sigma (\lambda_1)
\]
\[
= \sum_{\lambda_1 \in \{ -1, 1 \}} \left( \sigma (\lambda_1)^T V \left( \sum_{\lambda_2 \in \{ -1, 1 \}} \sigma (\lambda_2) \sigma (\lambda_2)^T \right) \right) V \left( \sum_{\lambda_3 \in \{ -1, 1 \}} \sigma (\lambda_3) \sigma (\lambda_3)^T \right) \ldots \sigma (\lambda_N)^T V \sigma (\lambda_1)
\]
Since, for every \( \lambda_k \in \{ -1, 1 \} \)
\[
\sum_{\lambda_k \in \{ -1, 1 \}} \sigma (\lambda_k) \sigma (\lambda_k)^T = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}
\]
\[
\sum_{\lambda_k \in \{ -1, 1 \}} \sigma (\lambda_k)^T \sigma (\lambda_k) = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}
\]
we have
\[
Z_N^N = \sum_{\lambda_1 \in \{ -1, 1 \}} \sigma (\lambda_1)^T V \sum_{\lambda_2 \in \{ -1, 1 \}} \sigma (\lambda_2) \sigma (\lambda_2)^T V \ldots \sigma (\lambda_N)^T V \sigma (\lambda_1)
\]
\[
= (2, 2) \text{ element of } V^N + (1, 1) \text{ element of } V^N = \text{Trace } (V^N)
The partition function is now expressed as:

$$Z_{N}^{N} (\beta, \varepsilon, H) = \sum_{\mathbf{S}} \exp \left( \beta \left( \sum_{k=1}^{N} \varepsilon_{k} \delta_{k,1} + \frac{1}{2} H (\delta_{k,1} + \delta_{k,1}) \right) \right)$$

because of the circular boundary condition $\delta_{N+1} = \delta_{1}$.

Focusing on nearest neighbor interactions only, we find

$$\langle S_{i} \rangle = \langle V_{i} V_{i+1} \rangle = \exp \left( \beta \varepsilon_{i} S_{i} + \frac{1}{2} \beta H (S_{i} + S_{i+1}) \right)$$

and

$$\mathbf{V} = \begin{bmatrix} e^{\beta \varepsilon} & e^{-\beta \varepsilon} \\ e^{-\beta \varepsilon} & e^{\beta \varepsilon} \end{bmatrix}$$

which is a self-adjoint operator.

**Result #1**

$$Z_{N}^{N} (\beta, \varepsilon, H) = \text{Trace} \left( \mathbf{V}^{N} \right)$$

**Result #2**

$$\text{Trace} \left( \mathbf{V}^{N} \right) = \lambda_{+}^{N} + \lambda_{-}^{N}$$

where

$$\lambda_{\pm} = e^{\beta \varepsilon} \left( \cosh (\beta H) \pm \sqrt{\sinh^{2} (\beta H) + e^{-4 \beta \varepsilon}} \right)$$

**Result #3**

Free energy $F_{N} (\beta, \varepsilon, H) \equiv \frac{1}{\beta N} \ln Z_{N}^{N} (\beta, \varepsilon, H)$ is given by:

$$\lim_{N \to \infty} \frac{1}{\beta N} \ln Z_{N}^{N} (\beta, \varepsilon, H) = -\frac{1}{\beta H} \left( \beta \frac{d}{dH} (\lambda_{+}^{N}) \right)$$

**Result #4**

Magnetization $M_{z} (\beta, \varepsilon, H)$ can be obtained as:

$$M_{z} (\beta, \varepsilon, H) = \langle \sum_{i=1}^{N} \delta_{i} \rangle$$

in the thermodynamic limit $N \to \infty$.

**Result #5**

Restricting to the ferromagnetic materials, $M_{z} (\beta, \varepsilon, H) \big|_{H=0} \neq 0$.

**Remark:** The Ising model notation can be extended to Potts model, where $\sigma : \{0, 1, \ldots, q \} \to \{0, 1, \ldots, q \}$, for $q \in \mathbb{N} \setminus \{2\}$ as

$$\sigma (a_{1} a_{2} \ldots a_{q}) = \underbrace{\sigma (a_{1}) \sigma (a_{2}) \cdots \sigma (a_{q})}_{q \times q}$$

Then

$$\mathbf{Z}^{q} \mathbf{0}_{\underbrace{0 \ 0 \ \cdots \ 0}_{q \times q}}^{T} = \begin{bmatrix} 1 & 1 & 0 \\ 0 & \ddots & \ddots \\ 0 & \cdots & 1 \end{bmatrix}$$

denoted as $I_{q}$.
Equivalence of the Ising Model to other Models

The Ising model is based on the concept of ferromagnetism. The underlying concept of Ising model can be used for simulation of other physical systems such as lattice gas and binary alloy.

Lattice Gas: A lattice gas is a collection of atoms whose positions are allowed to take only discrete values. Although the lattice gas model does not directly correspond to any real system, it can represent an ideal gas.

The discrete values form a lattice of a geometry with $l$ nearest neighbors to each lattice site that can be occupied by at most one particle as seen in the figure on the right.

Neglecting the kinetic energy of a particle and considering interactions with the nearest neighbor only, the interactions between a pair of nearest neighbors is assumed to be a constant $\epsilon$.

Then, the potential energy of the system is equivalent to that of a gas in which the atoms are located only on lattice sites and interact through a two-body potential $v(d(\vec{r}_i, \vec{r}_j))$ with

$$v(r) = \begin{cases} \epsilon & \text{for } r = 0 \\ 0 & \text{otherwise} \end{cases}$$

Let $N$ be the total number of lattice sites; $Na (0 \leq Na \leq N)$ be total number of particles; and $Na_0$ be total number of nearest neighbor pairs of particles. Then, the total energy of the lattice gas is:

$$E_G = \epsilon Na_0$$

and the partition function is:

$$Z_G^N(\beta) = \frac{1}{Na_0!} \sum a! \exp(-\beta Ena_0)$$

where the sum $\sum a$ represents $Na_0$ distinguishable particles on $N$ lattice sites.
If the volume of a unit cell of the lattice is chosen to be unity, then the volume of the lattice system is \( N \) and the grand partition function is defined as:

\[
\Omega_G(N, \beta) = \sum_{N \geq 0} \frac{Z_G(3, \beta)}{N^3} Z_G(\beta)
\]

and

\[
\Omega_G(3, \beta) = \lim_{N \to \infty} \Omega_G(3, \beta)
\]

To establish a correspondence between the lattice gas and the Ising model, let the occupied sites be analogous to spins up and empty sites to spins down, i.e., given \( N \), we have \( N_+ = N \).

In the Ising model, a set \( \{s_1, s_2, \ldots, s_N\} \) defines a specific configuration. In contrast, an enumeration of \( N_+ \) occupied sites determines \( N_+! \) configurations instead of a single configuration. This difference occurs from the fact that the atoms are supposed to be able to move from site to site.

**Binary Alloy:**

A binary alloy, such as \( \beta \)-brass, is a body-centered cubic lattice made of Zn and Cu atoms, as seen in the figure on the right. As the temperature is increased, some of the Zn atoms exchange their places with Cu atoms. Below the critical temperature \( T_c = 742^\circ K \), the probability of finding a Zn atom in its correct place is more than \( \frac{1}{2} \). Above \( 742^\circ K \), the Cu and Zn atoms are thoroughly mixed and the probability of finding a Zn atom in its correct place is \( \frac{1}{2} \).

Neglecting kinetic energy, the system energy is:

\[
E_A(N_{11}, N_{22}, N_{12}) = \epsilon_1 N_{11} + \epsilon_2 N_{22} + \epsilon_{12} N_{12}
\]

\[
= (\epsilon_1 + \epsilon_2 - 2\epsilon_{12}) N_{11} + (\epsilon_{12} - \epsilon_2) N_{12} + \epsilon_{12} N_{12}
\]

where \( Y = \# \) of nearest neighbors to each lattice site.

<table>
<thead>
<tr>
<th>( Y N_{11} = 2 N_{11} + N_{12} )</th>
<th>( Y N_{22} = 2 N_{22} + N_{12} )</th>
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<tbody>
<tr>
<td>( Y N_{12} = 2 N_{12} + N_{11} )</td>
<td>( N_{11} + N_{22} = N )</td>
</tr>
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</table>

\[
N_{12} = \frac{Y N_{11}}{2} + N_{11}
\]

\[
N_{22} = \frac{Y N_{11}}{2} - N_{11}
\]

where \( N_{11} = \# \) of atoms of type 1

\( N_{22} = \# \) of atoms of type 2

\( N_{11} = \# \) of pairs of type 1

\( N_{22} = \# \) of pairs of type 2

\( N_{12} = N_{21} = \# \) of pairs of types 1 and 2
Two-dimensional Ising Model

An exact solution of the 2-D Ising model was formulated by Onsager. Considering a square lattice of \( n \) rows and \( n \) columns, the total number of spins \( N = n^2 \). Having \( n+1 \) spins in both rows and columns, this boundary condition yields the topology of a torus. Let \( \mu_k, k = 1, \ldots, n \) be the collection of all spin coordinates of the \( k \)-th row.

\[
\mu_k = \{ S_k^1, \ldots, S_k^n \} \quad \text{for the } k\text{-th row}
\]

The toroidal boundary condition implies that \( \mu_{n+1} = \mu_1 \).

The entire lattice is specified by \( \{ \mu_1, \ldots, \mu_n \} \).

The \( k \)-th row interacts with \( (k-1) \)-th and \( (k+1) \)-th rows. Then,

\[
E(\mu, \mu') = -\epsilon \sum_{k=1}^{n} S_k S_{k+1} \quad \text{(Interaction between two neighboring rows)}
\]

\[
E(\mu, H) = -\sum_{k=1}^{n} S_k S_{k+1} - H \sum_{k=1}^{n} S_k \quad \text{(Interaction energy of spins belonging to a given row and their interacting topology of 2-D Ising Lattice with external field H)}
\]

where \( \mu = \{ S_1, \ldots, S_n \} \), \( \mu' = \{ S_1', \ldots, S_n' \} \), and the toroidal boundary condition implies \( S_{n+1} = S_1 \) in each row.

The total energy for the configuration \( \{ \mu_1, \ldots, \mu_n \} \) is

\[
E^N(\mu, H) = \sum_{k=1}^{n} \left[ E(\mu_k, \mu_{k+1}) + E(\mu_k, H) \right] \quad \text{(3)}
\]

and the partition function

\[
Z^N(\mu, \beta) = \sum_{\mu_1, \ldots, \mu_n} \exp \left( -\beta \sum_{k=1}^{n} \left[ E(\mu_k, \mu_{k+1}) + E(\mu_k, H) \right] \right) \quad \text{(4)}
\]

Let \( P \in \mathbb{R}^{2n \times 2n} \) be defined such that the elements are defined as:

\[
\langle \mu | P | \mu' \rangle = \exp \left( -\beta \left( E(\mu, \mu') + E(\mu, H) \right) \right) \quad \text{(5)}
\]

where \( \mu = \{ \mu_1, \ldots, \mu_n \} \) and \( \mu' = \{ \mu_1', \ldots, \mu'_n \} \).

and \( \langle \mu | P | \mu' \rangle \) is the Dirac bracket notation.
The (scalar-valued) partition function is

\[ Z_I^n (\beta, H) = \sum_{\mu_1} \cdots \sum_{\mu_n} \langle \mu_1 | P | \mu_2 \rangle \langle \mu_2 | P | \mu_3 \rangle \cdots \langle \mu_n | P | \mu_1 \rangle \]

\[ = \sum_{\mu_1} \langle \mu_1 | P^n | \mu_1 \rangle = \text{Trace} (P^n) \]  

(6)

\[ \Rightarrow Z_I^n (\beta, H) = \sum_{i=1}^{2^n} \left( \lambda_i \right)^n \]  

where \( \lambda_i \)'s are (non-negative) real eigenvalues of \( P \).

Then, \( (\lambda_{\text{max}})^n \leq Z_I^n (\beta, H) \leq 2^n (\lambda_{\text{max}})^n \)

or

\[ \frac{\ln Z_I^n}{n} \leq \frac{\ln \lambda_{\text{max}}}{n} \leq \frac{\ln Z_I^n}{n} \]

(7)

As \( n \to \infty \),

\[ \lim_{N \to \infty} \frac{1}{N} \ln Z_I = \lim_{n \to \infty} \frac{1}{n} \ln \lambda_{\text{max}} \]  

where \( N = n^2 \)

How to find \( P \):

\[
\langle \vec{x}_1, \ldots, \vec{x}_n | P | \hat{\vec{x}}_1, \ldots, \hat{\vec{x}}_n \rangle = \prod_{k=1}^{n} \exp \left( \beta H x_k \right) \exp \left( \beta \sum \delta_{x_k, \hat{x}_k} \right) \exp \left( \beta \sum \delta_{\hat{x}_k, x_k} \right)
\]

from (1), (2), and (5)

Define \( 2^n \times 2^n \) matrices matrices \( V_1 \), \( V_2 \) and \( V_3 \) as:

\[
\langle \vec{x}_1, \ldots, \vec{x}_n | V_1 | \hat{\vec{x}}_1, \ldots, \hat{\vec{x}}_n \rangle = \prod_{k=1}^{n} \exp \left( \beta \sum \delta_{x_k, \hat{x}_k} \right)
\]

(9)

\[
\langle \vec{x}_1, \ldots, \vec{x}_n | V_2 | \hat{\vec{x}}_1, \ldots, \hat{\vec{x}}_n \rangle = \delta_{x_1, \hat{x}_1} \cdots \delta_{x_n, \hat{x}_n} \prod_{k=1}^{n} \exp \left( \beta \sum \delta_{x_k, \hat{x}_k} \right)
\]

\[
\langle \vec{x}_1, \ldots, \vec{x}_n | V_3 | \hat{\vec{x}}_1, \ldots, \hat{\vec{x}}_n \rangle = \delta_{x_1, \hat{x}_1} \cdots \delta_{x_n, \hat{x}_n} \prod_{k=1}^{n} \exp \left( \beta + \delta_{x_k, \hat{x}_k} \right)
\]

where \( \delta_{x_i, \hat{x}_j} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases} \)

Note that \( V_2 \) and \( V_3 \) are diagonal matrices.

Comparison of (8) and (9) shows that

\[ P = V_3 V_2 V_1 \]

in the usual sense of matrix multiplication.

Next we use the kronecker product, also known as direct product, of matrices

\[ A \otimes B = \begin{bmatrix} a_{11} B & \cdots & a_{1m} B \\ \vdots & \ddots & \vdots \\ a_{m1} B & \cdots & a_{mm} B \end{bmatrix} \in \mathbb{R}^{m A \times n B} \text{ if } A \in \mathbb{R}^{m A \times n A} \text{ and } B \in \mathbb{R}^{m B \times n B} \]
If dimensions are compatible (for square matrices of same dimensions), then
\[(A \otimes B)(C \otimes D) = (AC) \otimes (BD)\] \hspace{1cm} (12)

**Spin Matrices**

Let us introduce special matrices to express \(V_1, V_2\) and \(V_3\).

Three \(2 \times 2\) spin matrices, known as Pauli matrices, are denoted as:
\[
X = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \text{and} \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \] \hspace{1cm} (13)

that have the following properties:
\[
X^2 = I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad Y^2 = I, \quad Z^2 = I, \\
XY + YX = 0 = ZX + XZ, \quad YZ + ZY = 0.
\] \hspace{1cm} (14)

Now, three sets of \(2^n \times 2^n\) matrices \(X_k, Y_k, Z_k, \ k = 1, 2, \ldots, n\) are defined as:
\[
X_k = I \otimes I \otimes \cdots \otimes I \otimes X \otimes I \otimes \cdots \otimes I \quad (n \text{ factors}), \\
Y_k = I \otimes I \otimes \cdots \otimes I \otimes Y \otimes I \otimes \cdots \otimes I \quad (n \text{ factors}), \] \hspace{1cm} (15)
\[
Z_k = I \otimes I \otimes \cdots \otimes I \otimes Z \otimes I \otimes \cdots \otimes I \quad (n \text{ factors}).
\]

For \(j \neq k\), the commutators, defined as \([A, B] = AB - BA\), are:
\[
[X_j, X_k] = [Y_j, Y_k] = [Z_j, Z_k] = 0, \\
[X_j, Y_k] = [X_j, Z_k] = [Y_j, Y_k] = 0.
\] \hspace{1cm} (16)

For any \(k = 1, 2, \ldots, n\), the \(2^n \times 2^n\) matrices \(X_k, Y_k, Z_k\) satisfy the relations (14).

**Note:** If \(X^2 = I\), then \(e^{\theta X} = \sum_{k=0}^{\infty} \frac{\theta^k}{k!} X^k = I + (\cos \theta) I + (\sin \theta) X\) for any \(\theta \in \mathbb{R}\).

because \(e^{\theta X} = \sum_{k=0}^{\infty} \frac{\theta^k}{k!} X^k = \sum_{k=0}^{\infty} \frac{(\theta^2)^k}{(2k)!} I + \sum_{k=0}^{\infty} \frac{\theta^{2k+1}}{(2k+1)!} X\) \hspace{1cm} (17)

This holds true for \(X, Y, Z\), for \(j = 1, 2, \ldots, n\).
Now we evaluate matrices $V_1$, $V_2$, and $V_3$.

$V_1$ is a Kronecker product of $n$ $(2 \times 2)$ identical matrices

$$V_1 = \underbrace{\alpha \otimes \cdots \otimes \alpha}_{n \text{ times}}$$

where

$$\alpha = \begin{bmatrix} e^{\beta e} & e^{-\beta e} \\ e^{-\beta e} & e^{\beta e} \end{bmatrix} = e^{\beta e} I + e^{-\beta e} X$$

Using (17) it follows that

$$\alpha = \sqrt{2 \sinh (2 \beta e)} \ e^{\theta X} \ \text{where} \ \text{tanh} \ \theta = e^{-2 \beta e}$$

Hence,

$$V_1 = \left[ 2 \sinh (2 \beta e) \right]^{n/2} \underbrace{e^{\theta X} \otimes \cdots \otimes e^{\theta X}}_{n \text{ times}}$$

Note that

$$e^{\theta X} \otimes \cdots \otimes e^{\theta X} = \prod_{k=1}^{n} e^{\theta X_k} = e^{\exp \left( \theta \sum_{k=1}^{n} X_k \right)}$$

Applying (22) in (21), we have

$$V_1 = \left[ 2 \sinh (2 \beta e) \right]^{n/2} \exp \left( \theta \sum_{k=1}^{n} X_k \right)$$

and standard matrix calculations yield

$$V_2 = \prod_{k=1}^{n} \exp \left( \beta \in Z_k Z_{k+1} \right)$$

$$V_3 = \prod_{k=1}^{n} \exp \left( \beta \in \mathbb{Z}_k \right) \ \text{with the boundary condition} \ Z_{n+1} = \mathbb{Z}_n$$

Note: for $H = 0$, $V_3 = I$

Now, the $(2^n \times 2^n)$ matrix is obtained as:

$$P = V_3 V_2 V_1$$
Summary: Ising model in one dimension with nearest-neighbor interactions

Ernst Ising presented a particle interaction model for ferromagnetism in his Ph.D. thesis in 1925, and this model has since come to be known by his name [1]. In this work, Ising modeled a one-dimensional ferromagnet as an infinitely long chain of magnetic sites, where each site represented a magnetic dipole moment generated by the atomic spin. If the atomic spins are aligned, the magnetic moments add up, resulting in the magnetic nature of a ferromagnetic material. On the other hand, if the spins are not aligned, such as at high temperatures, the magnetic nature is lost. The phase transition between these two behaviors of a ferromagnetic material occurs at the Curie temperature. The goal of Ising’s thesis was to study if the interaction between neighboring spins was the underlying mechanism for such behavior of ferromagnetic materials.

Model description In this model, atomic spins are denoted by $\sigma$. The atomic spins can be in one of two states, i.e. $\sigma \in \{-1, +1\}$. The actual values of the spins do not hold any physical significance, except for the fact that they simplify some of the following analysis. Specifically, if two adjacent atomic spins are aligned in the same direction, they could be modeled as either $\{-1, -1\}$ or $\{+1, +1\}$, with no change in the ensuing analysis. Similarly, if two adjacent spins are not aligned, they could either be represented by $\{-1, +1\}$ or $\{+1, -1\}$. Now, the state of the magnet is collectively represented by the atomic spins at each site of the one-dimensional $N$-long chain of magnets as $\sigma = \{\sigma_1, \sigma_2, \ldots, \sigma_N\}$, which is known as the system microstate, where $N$ is a large positive integer. The energy associated with the microstate $\sigma$ for a one-dimensional Ising model with only nearest-neighbor interactions is given by the Hamiltonian:

$$H(\sigma) = -B \sum_{i=1}^{N} \sigma_i - \sum_{<i,j>} J_{ij} \sigma_i \sigma_j$$

(1)

where $B$ represents an external magnetic field, $<i,j>$ represents a nearest-neighbor site pair (i.e., $j = i + 1$), and $J_{ij}$ denotes the interaction strength between sites $i$ and $j$. The interaction strength is assumed to be constant (i.e. $J_{ij} = J$) in this paper.

In order to further simplify the analysis, the one-dimensional model is assumed to have periodic boundary conditions, so that $\sigma_{N+1} = \sigma_1$. While this assumption does not affect the thermodynamic properties of the $N$-long chain with $lim N \to \infty$, it does allow a symmetric representation of the Hamiltonian as follows:

$$H(\sigma) = -\frac{B}{2} \sum_{i=1}^{N} (\sigma_i + \sigma_{i+1}) - J \sum_{i=1}^{N} \sigma_i \sigma_{i+1}$$

(2)

Partition function The partition function plays a very important role in the field of statistical mechanics and can be used to determine the aggregated properties of a system. It derives its name from the fact that it encodes the occurrence of a particular microstate $\sigma$ is given by:

$$P(\sigma) = \frac{1}{Z} e^{-\beta H(\sigma)}$$

(3)

where $Z$ denotes the partition function that serves as a normalizing constant, $\beta = 1/k_B T$, where $k_B$ denotes the Boltzmann constant, and $T$ denotes the temperature. The partition function $Z$ is thus defined as:

$$Z = \sum_{\sigma_1=-1}^{+1} \sum_{\sigma_2=-1}^{+1} \cdots \sum_{\sigma_N=-1}^{+1} e^{-\beta H(\sigma)}$$

(4)

which can be written as:

$$Z = \sum_{\sigma_1=-1}^{+1} \cdots \sum_{\sigma_N=-1}^{+1} \exp \left\{ \beta \sum_{i=1}^{N} \left( \frac{B}{2} (\sigma_i + \sigma_{i+1}) + J \sigma_i \sigma_{i+1} \right) \right\}$$

(5)

Transfer matrix In order to evaluate the partition function, Kramers and Wannier suggested the use of transfer matrices [1, pp. 476]. The right-hand side of (5) can be expressed as a product of $2 \times 2$ matrices as explained below. Consider a situation with only two adjacent sites $\sigma_i$ and $\sigma_{i+1}$. Then, in accordance with (2), the Hamiltonian $H(\sigma)$ yields:

$$e^{-\beta H(\sigma)} = \begin{cases} e^{\beta(B+J)}, & \sigma_i = +1, \sigma_{i+1} = +1 \\ e^{\beta(-B+J)}, & \sigma_i = -1, \sigma_{i+1} = -1 \\ e^{-\beta J}, & \text{otherwise} \end{cases}$$

(6)

Now, for a vector representation of the spins, let the spins $+1$ and $-1$ be denoted as vectors $q_1 = [1 \ 0 \ ]$ and $q_2 = [0 \ 1 \ ]$, respectively. If the transfer matrix $P$ is given by:

$$P = \begin{bmatrix} e^{\beta(B+J)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(-B+J)} \end{bmatrix}$$

(7)
the operation \( (\sigma_i P \sigma_{i+1}) \) yields the same results as in (6), i.e.

\[
(\sigma_i P \sigma_{i+1}) = \begin{cases}
  e^{\beta(B+J)}, & \sigma_i = q_1, \sigma_{i+1} = q_1^T \\
  e^{\beta(-B+J)}, & \sigma_i = q_2, \sigma_{i+1} = q_2^T \\
  e^{-\beta J}, & \text{otherwise}
\end{cases}
\]  

Solution of the partition function Using the transfer matrix representation, the partition function is re-written as:

\[
Z = \sum_{\sigma_1 = -1}^{+1} \cdots \sum_{\sigma_{N-1} = -1}^{+1} (\sigma_1 P \sigma_2)(\sigma_2 P \sigma_3) \cdots (\sigma_N P \sigma_1) \\
= \sum_{\sigma_1 = -1}^{+1} (\sigma_1 P^N \sigma_1) = Tr(P^N) \\
= \lambda_a^N + \lambda_b^N
\]  

where the eigenvalues of \( P \) are represented as \( \lambda_a \) and \( \lambda_b \) in an ordered way (i.e., \( \lambda_b < \lambda_a \)). In the absence of an external field (i.e., \( B = 0 \)), the eigenvalues are found to be:

\[
\lambda_a = 2 \cosh(\beta J) \\
\lambda_b = 2 \sinh(\beta J)
\]

which yield a solution of the partition function. With knowledge of the partition function, several other statistics (e.g., free energy and magnetization per spin) can be evaluated along with their trends as a function of inverse temperature \( \beta \).

References