Introduction to the Trace Operation used in the Ising Model

Link: https://www.youtube.com/watch?v=2HehOGh0j7M

AMA4004: Statistical mechanics

Model Systems II: The Ising Model

What we now need to do

We need to calculate canonical partition functions for various model Hamiltonians

We need to have a Hamiltonian that we can use to calculate the energy of a microstate.

$$Z = e^{\Psi} = \sum_{j} e^{-\beta H(\mathbf{x}_j, \mathbf{p}_j)}$$

Sum over all possible microstates.

What model Hamiltonians do we look at

	particles on a lattice	independent particles
non-interacting particles		
Interacting particles		

Hamiltonian for Ising model

This Hamiltonian is for the so-called 1D closed Ising Model, which is the simplest interacting Model we can work

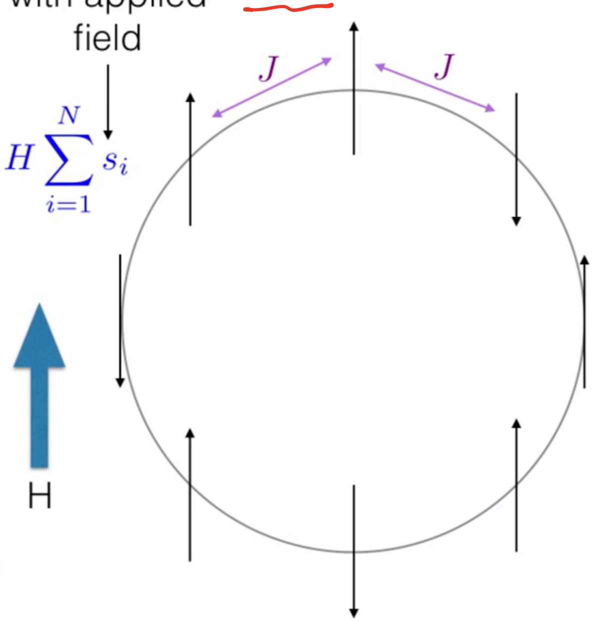
Neighbouring spins interact with each other

Spins interact with applied field

$$H = -J\sum_{i=1}^{N} s_i s_{i+1} - H\sum_{i=1}^{N} s_i$$

$$s_{N+1} = s_1$$

Boundary Condition



Once again each spin can be either spin up or spin down

Bringing it all together

$$\sum_{s_1=0}^{1}\sum_{s_2=0}^{1}\cdots\sum_{s_n=0}^{1}$$

$$H = -J\sum_{i=1}^{N} s_i s_{i+1} - H\sum_{i=1}^{N} s_i$$

$$H = -\sum_{i=1}^{N}\left[J s_i s_{i+1} + H\frac{s_i + s_{i+1}}{2}\right]$$

$$Z = e^{\Psi} = \sum_{j} e^{-\beta H(\mathbf{x}_j, \mathbf{p}_j)}$$

Si could only be either 0 or 1.

$$z(x) = \begin{cases} -1 & \text{if} \quad x = 0 \\ +1 & \text{if} \quad x = 1 \\ 0 & \text{otherwise} \end{cases}$$

$$Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1}\cdots\sum_{s_n=0}^{1}\exp\left(\beta\sum_{i=1}^{N}\left[Jz(s_i)z(s_{i+1}) + H\frac{z(s_i)+z(s_{i+1})}{2}\right]\right)$$

Some simplifications

$$Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1}\cdots\sum_{s_n=0}^{1}\exp\left(\beta\sum_{i=1}^{N}\left[Jz(s_i)z(s_{i+1}) + H\frac{z(s_i)+z(s_{i+1})}{2}\right]\right)$$

$$Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1}\cdots\sum_{s_n=0}^{1}\prod_{i=1}^{N}\exp\left(\beta\left[Jz(s_i)z(s_{i+1}) + H\frac{z(s_i)+z(s_{i+1})}{2}\right]\right)$$

Must be two sums at front as each term in Hamiltonian depends on value of two spins.

$$Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1}\exp\left(\beta\left[Jz(s_1)z(s_2) + H\frac{z(s_1)+z(s_2)}{2}\right]\right)\sum_{s_3=0}^{1}\exp\left(\beta\left[Jz(s_2)z(s_3) + H\frac{z(s_2)+z(s_3)}{2}\right]\right)\dots$$

$$\dots\sum_{s_{n-k}=0}^{1}\exp\left(\beta\left[Jz(s_{n-k-1})z(s_{n-k}) + H\frac{z(s_{n-k-1})+z(s_{n-k})}{2}\right]\right)\dots$$

$$\dots\sum_{s_n=0}^{1}\exp\left(\beta\left[Jz(s_{n-1})z(s_n) + H\frac{z(s_{n-1})+z(s_n)}{2}\right]\right)\exp\left(\beta\left[Jz(s_n)z(s_1) + H\frac{z(s_n)+z(s_1)}{2}\right]\right)$$

There are N terms in the product so final sum must be product of two terms

Simplifying something horrendous

$$Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1} \exp\left(\beta\left[Jz(s_1)z(s_2) + H\frac{z(s_1)+z(s_2)}{2}\right]\right) \sum_{s_3=0}^{1} \exp\left(\beta\left[Jz(s_2)z(s_3) + H\frac{z(s_2)+z(s_3)}{2}\right]\right)\dots$$

$$\dots \sum_{s_{n-k}=0}^{1} \exp\left(\beta\left[Jz(s_{n-k-1})z(s_{n-k}) + H\frac{z(s_{n-k-1})+z(s_{n-k})}{2}\right]\right)\dots$$

$$\dots \sum_{s_n=0}^{1} \exp\left(\beta\left[Jz(s_{n-1})z(s_n) + H\frac{z(s_{n-1})+z(s_n)}{2}\right]\right) \exp\left(\beta\left[Jz(s_n)z(s_1) + H\frac{z(s_n)+z(s_1)}{2}\right]\right)$$

Look at what we are summing over

This term appears second here

But first here

This term looks like a product of matrices

$$Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1} \exp\left(\beta\left[Jz(s_1)z(s_2) + H\frac{z(s_1)+z(s_2)}{2}\right]\right) \sum_{s_3=0}^{1} \exp\left(\beta\left[Jz(s_2)z(s_3) + H\frac{z(s_2)+z(s_3)}{2}\right]\right)$$

$$\dots \sum_{s_{n-k}=0}^{1} \exp\left(\beta\left[Jz(s_{n-k-1})z(s_{n-k}) + H\frac{z(s_{n-k-1})+z(s_{n-k})}{2}\right]\right)\dots$$

$$\begin{array}{c} s_{n-1} \\ \downarrow \end{array} \cdots \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix} \underset{s_1 \longrightarrow}{\begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}}$$

Transfer Matrix ?

Continuing to simplify something horrendous

$$Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1} \exp\left(\beta\left[Jz(s_1)z(s_2) + H\frac{z(s_1)+z(s_2)}{2}\right]\right) \sum_{s_3=0}^{1} \exp\left(\beta\left[Jz(s_2)z(s_3) + H\frac{z(s_2)+z(s_3)}{2}\right]\right)\dots$$

$$\dots \sum_{s_{n-k}=0}^{1} \exp\left(\beta\left[Jz(s_{n-k-1})z(s_{n-k}) + H\frac{z(s_{n-k-1})+z(s_{n-k})}{2}\right]\right)\dots$$

$$\dots \sum_{s_n=0}^{1} \exp\left(\beta\left[Jz(s_{n-1})z(s_n) + H\frac{z(s_{n-1})+z(s_n)}{2}\right]\right) \exp\left(\beta\left[Jz(s_n)z(s_1) + H\frac{z(s_n)+z(s_1)}{2}\right]\right)$$

$\Downarrow$ Rewrite

$$Z = \sum_{s_1=1}^{1} \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix} \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix} \cdots \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}$$

Continuing to simplify something horrendous

$$Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1} \exp\left(\beta\left[Jz(s_1)z(s_2)+H\frac{z(s_1)+z(s_2)}{2}\right]\right)\sum_{s_3=0}^{1}\exp\left(\beta\left[Jz(s_2)z(s_3)+H\frac{z(s_2)+z(s_3)}{2}\right]\right)\dots$$
$$\dots\sum_{s_{n-k}=0}^{1}\exp\left(\beta\left[Jz(s_{n-k-1})z(s_{n-k})+H\frac{z(s_{n-k-1})+z(s_{n-k})}{2}\right]\right)\dots$$
$$\dots\sum_{s_n=0}^{1}\exp\left(\beta\left[Jz(s_{n-1})z(s_n)+H\frac{z(s_{n-1})+z(s_n)}{2}\right]\right)\exp\left(\beta\left[Jz(s_n)z(s_1)+H\frac{z(s_n)+z(s_1)}{2}\right]\right)$$

$$Z = \sum_{s_1=1}^{1}\begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}^N$$

Continuing to simplify something horrendous

$$Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1} \exp\left(\beta\left[Jz(s_1)z(s_2)+H\frac{z(s_1)+z(s_2)}{2}\right]\right)\sum_{s_3=0}^{1}\exp\left(\beta\left[Jz(s_2)z(s_3)+H\frac{z(s_2)+z(s_3)}{2}\right]\right)\dots$$
$$\dots\sum_{s_{n-k}=0}^{1}\exp\left(\beta\left[Jz(s_{n-k-1})z(s_{n-k})+H\frac{z(s_{n-k-1})+z(s_{n-k})}{2}\right]\right)\dots$$
$$\dots\sum_{s_n=0}^{1}\exp\left(\beta\left[Jz(s_{n-1})z(s_n)+H\frac{z(s_{n-1})+z(s_n)}{2}\right]\right)\exp\left(\beta\left[Jz(s_n)z(s_1)+H\frac{z(s_n)+z(s_1)}{2}\right]\right)$$

$$Z = \sum_{s_1=1}^{1}\begin{array}{c} s_1 \longrightarrow \\ \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}^N \end{array} \quad \begin{array}{c} s_1 \\ \downarrow \end{array}$$

Continuing to simplify something horrendous

$$
\begin{aligned}
Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1} \exp\left(\beta\left[Jz(s_1)z(s_2) + H\frac{z(s_1)+z(s_2)}{2}\right]\right) \sum_{s_3=0}^{1} \exp\left(\beta\left[Jz(s_2)z(s_3) + H\frac{z(s_2)+z(s_3)}{2}\right]\right)\dots \\
\dots \sum_{s_{n-k}=0}^{1} \exp\left(\beta\left[Jz(s_{n-k-1})z(s_{n-k}) + H\frac{z(s_{n-k-1})+z(s_{n-k})}{2}\right]\right)\dots \\
\dots \sum_{s_n=0}^{1} \exp\left(\beta\left[Jz(s_{n-1})z(s_n) + H\frac{z(s_{n-1})+z(s_n)}{2}\right]\right) \exp\left(\beta\left[Jz(s_n)z(s_1) + H\frac{z(s_n)+z(s_1)}{2}\right]\right)
\end{aligned}
$$

$$
Z = \sum_{s_1=1}^{1} \begin{array}{c} s_1 \longrightarrow \\ \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}^{N} \end{array} \begin{array}{c} s_1 \\ \downarrow \end{array}
$$

☆ : The $\boxed{\text{trace of the power of matrices}}$ is equivalent to the summation that emerges when we insert the Hamiltonian into the partition function.

Continuing to simplify something horrendous

$$
\begin{aligned}
Z = \sum_{s_1=0}^{1}\sum_{s_2=0}^{1} \exp\left(\beta\left[Jz(s_1)z(s_2) + H\frac{z(s_1)+z(s_2)}{2}\right]\right) \sum_{s_3=0}^{1} \exp\left(\beta\left[Jz(s_2)z(s_3) + H\frac{z(s_2)+z(s_3)}{2}\right]\right)\dots \\
\dots \sum_{s_{n-k}=0}^{1} \exp\left(\beta\left[Jz(s_{n-k-1})z(s_{n-k}) + H\frac{z(s_{n-k-1})+z(s_{n-k})}{2}\right]\right)\dots \\
\dots \sum_{s_n=0}^{1} \exp\left(\beta\left[Jz(s_{n-1})z(s_n) + H\frac{z(s_{n-1})+z(s_n)}{2}\right]\right) \exp\left(\beta\left[Jz(s_n)z(s_1) + H\frac{z(s_n)+z(s_1)}{2}\right]\right)
\end{aligned}
$$

This is useful as we can find the partition function by exploiting various well known techniques from linear algebra

The things we will need: eigenvectors and eigenvalues

Square Matrix

an eigen**vector**

Solutions of: $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$

a matrix

an eigenvalue (a scalar)

For a n*n square matrix A, it will have n eigenvalues & n corresponding eigenvectors.

This square matrix A, can be decomposed into the products of 3 matrices :

$$A = V \Lambda V^{-1}$$

(see below for details).

The things we will need: eigenvectors and eigenvalues

Solutions of: $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$

Matrix of left eigenvectors (one eigenvector per row)

Matrix of right eigenvectors (one eigenvector per column)

$$\mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{-1}$$

Diagonal matrix containing eigenvalues

The things we will need

$$\mathbf{A}^2 = \mathbf{A}\mathbf{A} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{-1}\mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{-1}$$

$$\downarrow$$

$$\mathbf{V}\boldsymbol{\Lambda}\mathbf{I}\boldsymbol{\Lambda}\mathbf{V}^{-1}$$

$$\downarrow$$

$$\mathbf{V}\boldsymbol{\Lambda}^2\mathbf{V}^{-1}$$

Multiplication of diagonal matrices

$$\Lambda^2 = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} = \begin{pmatrix} \lambda_1^2 & 0 \\ 0 & \lambda_2^2 \end{pmatrix}$$

To square a diagonal matrix just square each element on the diagonal

The things we will need

$$\mathbf{A}^2 = \mathbf{A}\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}\mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$$

$$\downarrow$$

$$\mathbf{V}\mathbf{\Lambda}\mathbf{I}\mathbf{\Lambda}\mathbf{V}^{-1}$$

$$\downarrow$$

$$\mathbf{V}\mathbf{\Lambda}^2\mathbf{V}^{-1}$$

The trace of a matrix is equal to the sum of its eigenvalues

$$\mathrm{Tr}[\mathbf{A}^2] = \sum_{i=1}^{N} \lambda_i^2$$

$$\mathrm{Tr}[A^n] = \sum_{i=1}^{N} \lambda_i^n$$

Finding eigenvalues

Come back to the partition function Z

$$Z = \mathrm{Tr}\left[\begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}^N\right] = \lambda_1^N + \lambda_2^N$$

Calculate the eigenvalues of the transfer matrix raised to the power of N.

This matrix's eigenvalues.

λ_1, λ_2

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$$

$$[\mathbf{A} - \lambda\mathbf{I}]\,\mathbf{v} = 0$$

$$\det[\mathbf{A} - \lambda\mathbf{I}] = 0$$

Solving the determinant

$$\det\left[\begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right] = 0$$

$$\Downarrow$$

$$(e^{\beta(J+H)} - \lambda)(e^{\beta(J-H)} - \lambda) - e^{-2\beta J} = 0$$

$$\overbrace{(e^{2\beta J} - e^{-2\beta J})}^{=\, 2\sinh(2\beta J)} - \lambda e^{\beta J} \overbrace{(e^{\beta H} + e^{-\beta H})}^{=\, 2\cosh(\beta H)} + \lambda^2 = 0$$

Solving the determinant

$$\det\left[\begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right] = 0$$

$$(e^{\beta(J+H)} - \lambda)(e^{\beta(J-H)} - \lambda) - e^{-2\beta J} = 0$$

$$2\sinh(2\beta J) - \lambda 2 e^{\beta J} \cosh(\beta H) + \lambda^2 = 0$$

Solving the determinant

$$\det\left[\begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix} - \lambda\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right] = 0$$

$$(e^{\beta(J+H)} - \lambda)(e^{\beta(J-H)} - \lambda) - e^{-2\beta J} = 0$$

Coefficient of the linear term

$$2\sinh(2\beta J) - \lambda \underline{2e^{\beta J}\cosh(\beta H)} + \lambda^2 = 0$$

$$\lambda = e^{\beta J}\cosh(\beta H) \pm \sqrt{e^{2\beta J}\cosh^2(\beta H) - 2\sinh(2\beta J)}$$

Some simplifications

$$\lambda = e^{\beta J}\cosh(\beta H) \pm \sqrt{e^{2\beta J}\cosh^2(\beta H) - 2\sinh(2\beta J)}$$

$$\Downarrow$$

$$\lambda = e^{\beta J}\cosh(\beta H) \pm \sqrt{e^{2\beta J}[\cancel{1} + \sinh^2(\beta H)] - (\cancel{e^{2\beta J}} - e^{-2\beta J})}$$

$$\Downarrow$$

$$\lambda = e^{\beta J}\cosh(\beta H) \pm \sqrt{e^{2\beta J}\sinh^2(\beta H) + e^{-2\beta J}}$$

Some simplifications

$$\lambda = e^{\beta J}\cosh(\beta H) \pm \sqrt{e^{2\beta J}\cosh^2(\beta H) - 2\sinh(2\beta J)}$$

Set: $H = 0$

$$\lambda = e^{\beta J}\cancelto{1}{\cosh(\beta H)} \pm \sqrt{e^{2\beta J}\cancelto{0}{\sinh^2(\beta H)} + e^{-2\beta J}}$$

$$\lambda = e^{\beta J} \pm e^{-\beta J}$$

$$\underline{\lambda_1 = 2\cosh(\beta J)} \qquad \underline{\lambda_2 = 2\sinh(\beta J)}$$

Finally the partition function

$$Z = \mathrm{Tr}\left[\begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}^N\right] = \lambda_1^N + \lambda_2^N$$

For: $H = 0$

$$\lambda_1 = 2\cosh(\beta J) \qquad \lambda_2 = 2\sinh(\beta J)$$

$$Z = 2^N\cosh^N(\beta J) + 2^N\sinh^N(\beta J)$$

Let's summarise

$$Z = \sum_{s_1=0}^{1} \sum_{s_2=0}^{1} \cdots \sum_{s_n=0}^{1} \exp\left(\beta \sum_{i=1}^{N} \left[J z(s_i) z(s_{i+1}) + H \frac{z(s_i) + z(s_{i+1})}{2} \right] \right)$$

We can write this as the trace of a power of a diagonalisable matrix

$$Z = \mathrm{Tr}\left[\begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}^{N} \right]$$

- Find the eigenvalues of the matrix.
- Take Nth powers of eigenvalues.
- Sum powers of eigenvalues to get trace