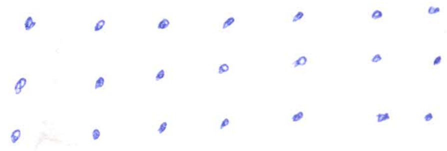
Ising Model

7/3/06

"Cubic" lattice in any dimension.

D = 1: 

D = 2: Square 

Dynamical variables

'Spin' on each lattice site

↳ s takes values ± 1.

$$E(s_1, \ldots, s_N) = -J \sum_{\langle ij \rangle} s_i s_j - K \sum_i s_i$$

$\langle ij \rangle$ implies nearest neighbour pairs

J, K constants

On each lattice site we have a dynamical variable

Example

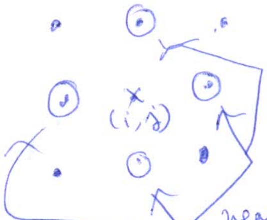
① $D = 1$

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

What do we mean by S_{N+1}?
⇒ Periodic boundary condition:- $s_{N+1} = s_1$

② $D = 2$

$$E = -J \sum_{i,j=1}^{N} s_{i,j} - \ldots$$



nearest neighbours

Periodic boundary ~~calc~~ condn makes calculation simpler

⇓ to make it more symmetric

$$-\frac{J}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} (s_{i,j} s_{i+1,j} + S$$

Could have written
$\sum s_i s_{i-1}$
$+ \sum s_i s_{i+1}$

But under a shift of i, the first sum will also be of the form $\sum s_i s_{i+1}$

$$E = -\frac{J}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \left(s_{i,j} s_{i+1,j} + s_{i,j} s_{i,j+1} + s_{i,j} s_{i-1,j} + s_{i,j} s_{i,j-1} \right) - K \sum_{i=1}^{M} \sum_{j=1}^{N} s_{i,j}$$

Periodic boundary conditions :- $\begin{cases} S_{N+1,j} = S_{1,j} \\ S_{i,N+1} = S_{i,1} \end{cases}$

Motivation :-

→ A Model for ferromagnetism.

Take a lattice & at each lattice site we have a magnetic dipole.

At i^{th} site,

$$\vec{\mu} = \mu_0 (\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i)$$

Direction cosines of the dipole

∴ the Hamiltonian of the system is

$$\mathcal{H} = \sum_i \left(\frac{p_{\theta_i}^2}{2I} + \frac{p_{\phi_i}^2}{2I \sin^2\theta_i} \right) - a \sum_{\langle i,j \rangle} \vec{\mu_i} \cdot \vec{\mu_j} - \vec{B} \cdot \sum \vec{\mu_i}$$

i itself is a collection of 3 indices

$\vec{B}$ → External magnetic field $(0, 0, B)$

$$Z = \int \prod_{i=1}^{N} \left(d\theta_i \, d\phi_i \, dp_{\theta_i} \, dp_{\phi_i} \right) e^{-\beta H}$$

$$= C (kT)^N \int \prod_{i=1}^{N} \left(d\theta_i \, d\phi_i \sin\theta_i \right) e^{-\beta \left(-a \sum_{\langle i,j \rangle} \vec{\mu_i} \cdot \vec{\mu_j} - B \sum \mu_{iz} \right)}$$

C → constant

Approximation :-

Replace the angular integration by a sum over two values: $\theta = 0$ & $\theta = \pi$.

$$\mu_i = \mu_0 s_i (0, 0, 1) \qquad s_i = 1 \text{ or } -1$$

$$Z \rightarrow c (kT)^N \sum_{s_1 = \pm 1, s_2 = \pm 1, \dots s_N = \pm 1} e^{-\beta H'}$$

$$H' = -a \mu_0^2 \sum_{\langle ij \rangle} s_i s_j - B \mu_0 \sum_i s_i$$

Ising model Hamiltonian

$\vec{\mu}_i \cdot \vec{\mu}_j = \mu_0^2 s_i s_j$

$\vec{B} \cdot \vec{\mu}_i = \mu_0 B s_i$

The integral over the entire solid angle 4π, we allow the spin to point in 2 dirns (North pole & South pole)

Picking up these 2 pts. is like picking up 2 extremes - we hope that this approxmn captures the behaviour of the integral

This may capture qualitative features of what is happening

The values may not be accurate but features like ferromagnetism should show up

Analysis of one dimensional ising model

$$E = -J \sum_{i=1}^{N} s_i s_{i+1} - \underbrace{K \sum_{i=1}^{N} s_i}$$

$$-K \sum_{i=1}^{N} \frac{s_i + s_{i+1}}{2}$$

Canonical partition fn.

$$Z = \sum_{s_1 = \pm 1} \sum_{s_2 = \pm 1} \cdots \sum_{s_N = \pm 1} e^{\beta J \sum_{i=1}^{N} s_i s_{i+1} + \frac{\beta K}{2} \sum_{i=1}^{N} (s_i + s_{i+1})}$$

i.e., $$Z = \sum_{s_1 = \pm 1} \sum_{s_2 = \pm 1} \cdots \sum_{s_N = \pm 1} e^{\beta J \sum_{i=1}^{N} s_i s_{i+1} + \beta K/2 \sum_{i=1}^{N} (s_i + s_{i+1})}$$

Define :—

$$T_{ss'} = e^{\beta J ss' + \beta K/2 (s+s')}$$

We may write

$$Z = \sum_{s_1=\pm1}\sum_{s_2=\pm1}\cdots\sum_{s_N=\pm1} \prod_{i=1}^{N} e^{\beta J s_i s_{i+1} + \beta K/2 (s_i + s_{i+1})}$$

$$= \sum_{s_1=\pm1}\sum_{s_2=\pm1}\cdots\sum_{s_N=\pm1} T_{s_1 s_2} T_{s_2 s_3} T_{s_3 s_4} \cdots T_{s_{N-1} s_N} T_{s_N s_1}$$

($T_{ss'}$ can be thought of as a 2×2 matrix bcos $s=\pm1$ & $s'=\pm1$)

$$\Rightarrow Z = \mathrm{Tr}\,(T^N)$$

Here

$$T = \begin{array}{cc} s=1,s'=1 & s=1,s'=-1 \\ s=-1,s'=+1 & s=-1,s'=-1 \end{array} \begin{pmatrix} e^{\beta J + \beta K} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta K} \end{pmatrix}$$

It is called the transfer matrix.

$$\Rightarrow Z = \lambda_1^N + \lambda_2^N \qquad \lambda_1, \lambda_2 \text{ are eigenvalues of } T.$$

Eigenvalue eqn

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

Soln

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

$$\Downarrow$$

$$e^{2\beta J}\cosh^2\beta K - e^{2\beta J} + e^{-2\beta J}$$

$$= e^{2\beta J}\sinh^2\beta K + e^{-2\beta J} > 0$$

$\Rightarrow$ Both eigenvalues are real.

$$Z = \left(\lambda_1^N + \lambda_2^N\right)$$

$$F = -kT \ln Z$$
$$= -kT \ln\left(\lambda_1^N + \lambda_2^N\right)$$
$$= -kT\left\{\ln \lambda_1^N + \ln\left(1 + (\lambda_2/\lambda_1)^N\right)\right\}$$
$$\xrightarrow[N\to\infty]{} -kT \ln \lambda_1^N$$
$$= -NkT \ln \lambda_1$$

Take λ_1 to be the bigger eigenvalue:–

$$e^{\beta J}\cosh\beta K + \sqrt{e^{2\beta J}\cosh^2\beta K - 2\sinh 2\beta J}$$

~~$F = -NkT \ln\left[e^{\beta J}\cosh\beta K\right.$~~

$$F = -NkT \ln\left[e^{\beta J}\cosh\beta K + \sqrt{e^{2\beta J}\cosh^2\beta K - 2\sinh 2\beta J}\right]$$
$$= -NkT\left[\beta J + \ln\left\{\cosh\beta K + \sqrt{\underbrace{\cosh^2\beta K - 2e^{-2\beta J}\sinh 2\beta J}_{>0}}\right\}\right]$$

So no branch pt. from here. Also argument of log is always +ve $\rightarrow$ no branch pt. from there.

$\Rightarrow$ F is never singular.

$\Rightarrow$ no phase transition

Total magnetic moment

$$M = \mu_0 \sum_{i=1}^{N} s_i$$

$$\langle M\rangle = \frac{\sum\limits_{s_1=\pm1}\sum\limits_{s_2=\pm1}\cdots e^{-\beta E}\mu_0\sum\limits_{i=1}^{N} s_i}{\sum\limits_{s_1=\pm1}\sum\limits_{s_2=\pm1}\cdots e^{-\beta E}}$$

$$Z = \sum_{s_1=\pm1}\sum_{s_2=\pm1}\cdots e^{\beta J\sum_{i=1}^{N} s_i s_{i+1} + \beta K\sum_{i=1}^{N} s_i}$$

$$\frac{1}{Z}\frac{\partial Z}{\partial K} = \beta \left\langle \sum_{i=1}^{N} S_i \right\rangle = \frac{\beta}{\mu_0}\langle M \rangle$$

$$\langle M \rangle = \frac{\mu_0}{\beta}\frac{\partial}{\partial K}\ln Z$$

$$= -\mu_0 \frac{\partial F}{\partial K}$$

$$\boxed{\begin{aligned} F &= -kT \ln Z \\ &= -\frac{1}{\beta}\ln Z \end{aligned}}$$

Exercise :- Show that

$$\langle M \rangle = \mu_0 N \frac{\sinh(\beta K)}{\sqrt{\cosh^2 \beta K - 2e^{-2\beta J}\sinh 2\beta J}}$$

$$-\partial F/\partial K = NkT\beta\left[\frac{\sinh\beta K + \frac{\cosh\beta K \sinh\beta K}{\sqrt{\cosh^2\beta K - 2e^{-2\beta J}\sinh 2\beta J}}}{\cosh\beta K + \sqrt{\cdots}}\right]$$

$$= \frac{N\sinh\beta K}{\sqrt{\cdots}} \times \frac{\sqrt{\cdots} + \cosh\beta K}{\sqrt{\cdots} + \cosh\beta K}$$

$$\therefore \langle M \rangle = \mu_0 \frac{N\sinh\beta K}{\sqrt{\cdots}}$$

Properties :-

① $\langle M \rangle \longrightarrow -\langle M \rangle$ under $K \to -K$

$K = \mu_0 B$

(Magnetization flips sign on switching the mag. field in the opp. dir$^{\underline{n}}$)

② $\langle M \rangle = 0$ for $K = 0$ for any β. ~~spontaneous magnetization.~~

~~$\Rightarrow$ there is no spontaneous~~

$$\lim_{K\to 0^+}\langle M \rangle = 0.$$

Ferromag. depends on the previous application of mag. field - you need to switch on mag. field & then reduce it to zero.

So, we need to calculate the limit

Suppose

$$\langle M \rangle = C\,\frac{\sinh\beta K}{|\sinh\beta K|}$$

$$\lim_{K\to 0^+}\langle M \rangle = C$$

$$\lim_{K\to 0^-}\langle M \rangle = -C$$

Exactly at $K = 0$, $\langle M \rangle$ is ill-defined

(This is the way you see spontaneous magnetization)

$\Longrightarrow$ no spontaneous magnetization

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Equivalence of Ising model with other systems

Consider a cubic lattice.

σ_i : variable associated with i^{th} lattice site which can take two values $\sigma^{(1)}, \sigma^{(2)}$.

Examples :- ① Random alloy :→ a cubic lattice where the i^{th} site may have an atom ~~molecule~~ of type A or type B.

② Lattice gas :- A cubic lattice where the i^{th} site is either occupied or vacant.

$\{\sigma_i\} \rightarrow$ labels a configuration

Suppose

$$E(\{\sigma_i\}) = \sum_{\langle ij\rangle} E^{(0)}(\sigma_i, \sigma_j) + \sum_i E^{(1)}(\sigma_i)$$

$\langle ij\rangle \hookrightarrow$ sum over nearest neighbours

We'll now map this to the ising ~~mode~~ model.

Introduce a new lattice variable s_i for each site.

$$s_i = 1 \text{ for } \sigma_i = \sigma^{(1)}$$
$$= -1 \text{ for } \sigma_i = \sigma^{(2)}$$

$$\{s_i\} \xleftrightarrow[\text{complete info. about}]{\text{contains}} \{\sigma_i\}$$

Consider a new function :-

$$\tilde{E}(\{s_i\}) = -J\sum_{\langle ij\rangle} s_i s_j - K\sum_i s_i + \text{constant}$$

σ_i is not even a no. — it assigns atom A or atom B

We add a constant piece & nothing changes

$$= \sum_{\langle ij\rangle}\left(-J\, s_i s_j - \tfrac{K}{n}(s_i + s_j)\right)$$

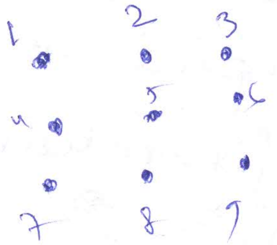
$+$ constant

n = number of nearest neighbours of a given atom

$K\sum_i s_i$
$\Downarrow$
sum over indiv. lattice sites

$$\tfrac{K}{n}\sum_{\langle ij\rangle}(s_i + s_j) = \frac{K}{n}\sum_{\langle ij\rangle} s_i + \tfrac{K}{n}\sum_{\langle ij\rangle} s_j$$

$\sum_{\langle ij\rangle} = \frac{1}{2}\sum_i \sum_{j\,(n.n.)}$
$= \frac{1}{2}\sum_i (n)$
$= \frac{n}{2}\sum_i$
$\Rightarrow \sum_i = \frac{2}{n}\sum_{\langle ij\rangle}$



$$\sum_{\langle ij\rangle} = \frac{1}{2}\sum_i \sum_{j \text{ nearest neighbour of } i}$$

$$\sum_i E^{(1)}(\sigma_i) = \sum_i \frac{1}{n}\sum_{\substack{\text{nearest}\\ \text{neighbour}\\ \text{of } i}} E^{(1)}(\sigma_i) = \frac{1}{n}\sum_i \sum_{\substack{\text{nearest}\\ \text{neighbour}\\ \text{of } i}} E^{(1)}(\sigma_i)$$

$$= \frac{1}{n}\times 2\sum_{\langle ij\rangle} E^{(1)}(\sigma_i)$$

$$\frac{2}{n}\sum_{\langle ij\rangle} E^{(1)}(\sigma_i) = \frac{1}{n}\sum_{\langle ij\rangle} E^{(1)}(\sigma_i) + \frac{1}{n}\sum_{\langle ij\rangle} E^{(1)}(\sigma_j)$$

$$= \frac{1}{n}\sum_{\langle ij\rangle}\left(E^{(1)}(\sigma_i) + E^{(1)}(\sigma_j)\right)$$

$$E(\{\sigma_i\}) = \sum_{\langle ij\rangle}\left\{E^{(2)}(\sigma_i, \sigma_j) + \frac{1}{n}\left(E^{(1)}(\sigma_i) + E^{(1)}(\sigma_j)\right)\right\}$$

manifestly it is sym. under i, j exchange

we can choose $E^{(2)}(\sigma_i, \sigma_j)$ to be sym. bcos antisym. won't contribute anyway

Consider the ising model energy:

$$\tilde{E}(\{s_i\}) = -J\sum_{\langle ij\rangle} s_i s_j - K\sum_i s_i$$

$$= \sum_{\langle ij\rangle}\left\{-J s_i s_j - K/n\,(s_i + s_j)\right\}$$

$$\Rightarrow \sum_{\langle ij\rangle}\left\{-J s_i s_j - K/n\,(s_i + s_j) + \underbrace{A}_{\text{constant}}\right\}$$

has no relevance to stat. mech.

not going to affect the thermodynamics

For each pair, the energy should match for both the problems

Goal:- Choose J, K & A such that the pair energy in the original ~~matrix~~ model matches the pair energy in the ising model.

① $\sigma_i = \sigma^{(1)}$, $\sigma_j = \sigma^{(1)} \leftrightarrow s_i = 1$, $s_j = 1$

$$E^{(0)}(\sigma^{(1)}, \sigma^{(1)}) + \frac{2}{n}E^{(1)}(\sigma^{(1)}) = -J - 2K/n + A$$

② $\sigma_i = \sigma^{(1)}$, $\sigma_j = \sigma^{(2)} \longleftrightarrow s_i = 1$, $s_j = -1$

$$E^{(0)}(\sigma^{(1)}, \sigma^{(2)}) + \frac{1}{n}\left[E^{(1)}(\sigma^{(1)}) + E^{(1)}(\sigma^{(2)})\right]$$

$$= J + A$$

③ $\sigma_i = \sigma^{(2)}$, $\sigma_j = \sigma^{(2)} \leftrightarrow s_i = -1$, $s_j = -1$

$$E^{(0)}(\sigma^{(2)}, \sigma^{(2)}) + 2/n\, E^{(1)}(\sigma^{(2)}) = -J + 2K/n + A$$

We have 3 eqns for 3 unknowns J, K & A

$\Rightarrow$ Solve for J, K, A.

$\xrightarrow[\text{gives you}]{\text{this}}$ an exact map betw. the original model & ising model.

Ising model :- $\sum_{\{s_i\}}$

Each s_i takes the value ± 1

There is no restriction

Total no. of α & total no. of β are separately fixed

Original model :- $\sum_{\{\sigma_i\}}$

total no. of A − total no. of B = fixed = L

Each lattice site is either a or b

But in alloy, there is a restriction

corresponds to

$\sum S_i$ = fixed in the ising model

Of course total no. of (A+B) = fixed ⟹ no. of lattice sites − fixed in both cases

$$\sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1}$$

$$\sum S_i = L$$

So it's not exactly the gan. part. fn. of ising model

Ising model Canonical ensemble $\xrightarrow{\text{is}}$ equivalent to grand canonical ensemble of the system with $\mu = K +$ constant

Role of the ~~ma~~ mag. field or parameter K is the chem. pot. in the alloy system

Ising model on two dimensional square lattice with periodic boundary condition

$$E = -J \sum_{i=1}^{M} \sum_{j=1}^{N} \left(s_{i,j}\, s_{i,j+1} + s_{i,j}\, s_{i+1,j} \right) - K \sum_{i=1}^{M}\sum_{j=1}^{N} s_{i,j}$$

$$= -J \sum_{i=1}^{M} \sum_{j=1}^{N} \left\{ s_{i,j}\, s_{i+1,j} + \frac{1}{2} s_{i,j}\, s_{i,j+1} + \frac{1}{2} s_{i+1,j}\, s_{i+1,j+1} \right\}$$

$$- \frac{K}{2} \sum_{i=1}^{M} \sum_{j=1}^{N} \left\{ s_{i,j} + s_{i+1,j} \right\}$$

$$Z = \sum_{\{s_{ij}=\pm 1\}} e^{-\beta E}$$

$$= \sum_{\{s_{ij}=\pm 1\}} \prod_{i=1}^{M} \underbrace{\exp\left\{\left[\beta J \sum_{j=1}^{N} s_{i,j} \cdot s_{i+1,j} + \frac{1}{2}\beta J \sum_{j=1}^{N} \left(s_{i,j}\, s_{i,j+1} + s_{i+1,j}\, s_{i+1,j+1}\right) + \frac{1}{2}\beta K \sum_{j=1}^{N} \left(s_{i,j} + s_{i+1,j}\right)\right]\right\}}_{T(\vec{\sigma}^{(i)}, \vec{\sigma}^{(i+1)})}$$

Suppose $\vec{\sigma}, \vec{\sigma}'$ are two N dimensional vectors.

$$\vec{\sigma} = (\sigma_1, \ldots, \sigma_N), \quad \vec{\sigma}' = (\sigma_1', \ldots, \sigma_N')$$

Define :- $$T(\vec{\sigma}, \vec{\sigma}') = \exp\left[\beta J \sum_{j=1}^{N} \sigma_j \sigma_j' + \frac{1}{2}\beta J \sum_{j=1}^{N} \left(\sigma_j \sigma_{j+1} + \sigma_j' \sigma_{j+1}'\right) + \frac{1}{2}\beta K \sum_{j=1}^{N} \left(\sigma_j + \sigma_j'\right)\right]$$

$$T(\vec{\sigma}, \vec{\sigma}') = T(\vec{\sigma}', \vec{\sigma})$$

Define :-

$\vec{\sigma}^{(i)}$: N dimensional vector for each $i = 1, \ldots, M$

$$\vec{\sigma}^{(i)} = (s_{i,1}, s_{i,2}, \ldots, s_{i,N})$$

$$\left(\vec{\sigma}^{(i)}\right)_j = s_{i,j}$$

jth component of the vector $\vec{\sigma}^{(i)}$

$$\sum_{\{S_{i,j}=\pm 1\}} \rightarrow \sum_{\{\vec{\sigma}^{(i)}\}} \qquad \vec{\sigma}^{(i)} = (\pm 1, \pm 1, \ldots, \pm 1)$$

Each $\vec{\sigma}^{(i)}$, takes 2^N values

$$Z = \sum_{\{\vec{\sigma}^{(i)}\}} \prod_{i=1}^{M} T\left(\vec{\sigma}^{(i)}, \vec{\sigma}^{(i+1)}\right)$$

$$T\left(\vec{\sigma}^{(1)}, \vec{\sigma}^{(2)}\right) T\left(\vec{\sigma}^{(2)}, \vec{\sigma}^{(3)}\right) T\left(\vec{\sigma}^{(3)}, \vec{\sigma}^{(4)}\right)$$

$$\cdots\; T\left(\vec{\sigma}^{(M-1)}, \vec{\sigma}^{(M)}\right) T\left(\vec{\sigma}^{(M)}, \vec{\sigma}^{(1)}\right)$$

(Each T can be thought of as $2^N \times 2^N$ matrix bcos each of $\vec{\sigma}^{(i)}$'s can take 2^N values)

$$Z = \mathrm{Tr}\left(T^M\right)$$

T : $2^N \times 2^N$ matrix

$$Z = \underbrace{\sum_{\alpha}}_{\text{sum over eigenvalues}} \lambda_\alpha^M$$

λ_{max} has no explicit dep. on N, but it depends on N bcos T is $2^N \times 2^N$

$$= \left(\lambda_{max}\right)^M \left\{ 1 + \sum_{\alpha}{}' \left(\frac{\lambda_\alpha}{\lambda_{max}}\right)^M \right\}$$

$\sum'$: sum over all α except the maximum e.v.

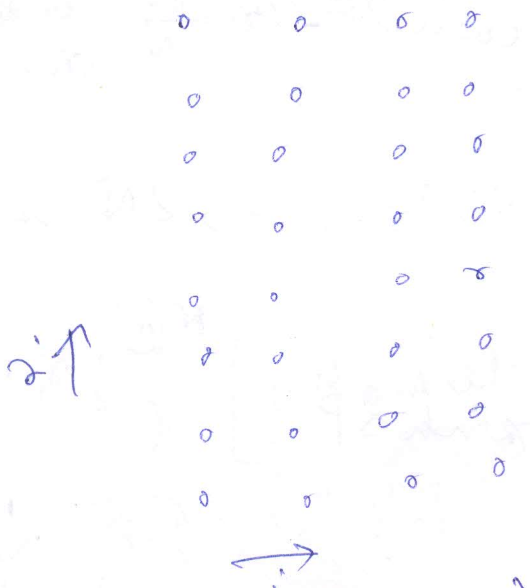
$$F = -kT \ln Z$$

$$= -kT\left\{ \ln \lambda_{max}^M + \ln\left(1 + \sum_{\alpha}\left(\frac{\lambda_\alpha}{\lambda_{max}}\right)^M\right)\right\}$$

$$\xrightarrow[M \to \infty]{} -MkT \ln \lambda_{max}$$

Problem reduces to calculating the maximum eigenvalue of the transfer matrix.

[Transfer matrix does the job that the 2 sums that sum over j is translated ~~into~~ into a matrix prodt. & the problem reduces to diagonalizing a matrix]



$T(\sigma^{(i)}, \vec{\sigma}^{(i+1)})$

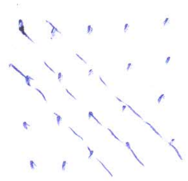
T in a sense is transferring from one column to another — can think it of as an ~~xxxx~~ operator — evolving one column to another

encoding interaction betn 2 columns

$\Downarrow$

So it is called the Column transfer matrix

Similarly, we'll have row transfer matrix



$\Rightarrow$ Sometimes one uses corner transfer matrix

Reorganizing the lattice sum into slices — Transfer matrix

$\Downarrow$

a general notion which has wide applications

Result for λ_{max} (For $K=0$)

Problem is solvable only for $K=0$; for $K\neq 0$ we have to use perturbation theory

Define $\phi = \beta J$, $\theta = \tanh^{-1} e^{-2\phi}$

$$\gamma_k = \cosh^{-1}\left\{\cosh 2\phi \cosh 2\theta - \cos\frac{\pi k}{N} \sinh 2\phi \sinh 2\theta\right\}$$

$k = 0, 1, 2, \ldots, 2N-1$

Cosh has an ambiguity bcos it is an even fn.

You have 2 values for $\cosh^{-1}$ for each argument

the positive value

$$\lambda_{max} = \left[2\sinh 2\beta J\right]^{N/2} e^{\frac{1}{2}(\gamma_1+\gamma_3+\gamma_5+\cdots+\gamma_{2N-1})}$$

this is also N-dep. bcos there are N terms in the sum

$Z = Tr(T^M)$

T: $2^N \times 2^N$ matrix

$$T(\vec{\sigma},\vec{\sigma}') = \exp\left[\beta J \sum_{j=1}^{N} \sigma_j \sigma_j' + \frac{1}{2}\beta J \sum_{j=1}^{N} (\sigma_j \sigma_{j+1} + \sigma_j' \sigma_{j+1}') + \frac{1}{2}\beta K \sum_{j=1}^{N} (\sigma_j + \sigma_j')\right]$$

$\vec{\sigma} = (\sigma_1, \ldots, \sigma_N)$, $\sigma' = (\sigma_1', \ldots, \sigma_N')$

$\sigma_i = \pm 1$, $\sigma_i' = \pm 1$

$$Z = \sum_\alpha \lambda_\alpha^M$$

$\hookrightarrow$ eigenvalues of T

$$F = -kT \ln Z = -kT \ln \sum_\alpha \lambda_\alpha^M$$

$$\xrightarrow[M \to \infty]{} -kT \ln \lambda_{max}^M = -MkT \ln \lambda_{max}$$

We need to find λ_{max}

<u>Result for λ_{max}</u> (This is for zero magnetic field)

Define $\phi = \beta J$, $\tanh \theta = e^{-2\phi}$

$$\cosh \gamma_k = \cosh(2\phi)\cosh(2\theta) - \cos\frac{\pi k}{N} \sinh(2\phi) \sin(2\theta)$$

$$k = 0, 1, 2, \ldots, 2N-1$$

$$\gamma_k \geq 0$$

$$\lambda_{max} = [2 \sinh 2\beta J]^{N/2} e^{1/2(\gamma_1 + \gamma_3 + \cdots + \gamma_{2N-1})}$$

$$F = -MkT\left[\frac{N}{2} \ln(2\sinh 2\beta J) + \frac{1}{2}\sum_{i=1}^{N} \gamma_{2i-1}\right]$$

$$= -\frac{1}{2} MNkT \left[\ln(2 \sinh 2\beta J) + \frac{1}{N}\sum_{i=1}^{N} \gamma_{2i-1}\right]$$

There are MN sites — ∴ to calculate some intrinsic prop., we need to evaluate f

$$f \underset{\text{defn}}{=} \frac{F}{MN} = -\frac{1}{2}kT\left[\ln(2\sinh 2\beta J) + \frac{1}{N}\sum_{i=1}^{N}\gamma_{2i-1}\right]$$

For N large, $\cosh \gamma_k$ will be a smooth fn. of k becos as k changes by unity $\pi k / N$ changes very little

Define $u = i/N$

$i = Nu$

$$\gamma_{2i-1} = \gamma_{2Nu-1} \simeq \gamma_{2Nu}$$

$$f \underset{N\to\infty}{=} -\frac{1}{2} kT \left[\ln(2 \sinh 2\beta J) + \int_0^1 du\, \gamma_{2Nu} \right]$$

$$\cosh \gamma_{2Nu} = \cosh(2\phi) \cosh(2\theta) - \cos(2\pi u) \sinh(2\phi) \sinh(2\theta)$$

Once we write $\gamma_{2Nu} = \cosh^{-1}(\ldots)$, there is no N-dependence & we get a smooth fn.

Ex. Show that

$$\int_0^1 du\, \gamma_{2Nu} = \ln\left(\frac{2\cosh^2 2\beta J}{\sinh 2\beta J}\right) + \frac{1}{\pi} \int_0^{\pi} d\theta \ln\left\{\frac{1}{2}\left(1 + \sqrt{1 - K^2 \sin^2\theta}\right)\right\}$$

where

$$K = \frac{2}{\cosh(2\phi)\coth(2\phi)}$$

Ising model is indep. under the interchange $M \leftrightarrow N$; nothing for e.g. depends on the ratio M/N

Average total energy $\bar{E} = -\frac{\partial}{\partial\beta}\ln Z$

$$= -\frac{\partial}{\partial\beta}(-\beta F)$$

$$\boxed{\beta = \frac{1}{kT}}$$

$$= \frac{\partial}{\partial\beta}(\beta f) \times MN$$

$$e = \frac{\bar{E}}{MN} = \frac{\partial}{\partial\beta}(\beta f)$$

Average energy per site (Av. energy / site)

$$f = -kT\left[\ln(2\cosh 2\beta J) + \frac{1}{2\pi}\int_0^{\pi} d\vartheta \ln\left\{\frac{1}{2}\left(1+\sqrt{1-K^2\sin^2\vartheta}\right)\right\}\right]$$

$\boxed{K \text{ depends on } \beta}$

$$e = -J\coth(2\beta J)\left(1 + \frac{2}{\pi}K' K_1(K)\right)$$

where $K' = 2\tanh^2(2\beta J) - 1$, $K^2 + (K')^2 = 1$

and $K_1(K) = \int_0^{\pi/2} \frac{d\vartheta}{\sqrt{1-K^2\sin^2\vartheta}}$

$$c = \frac{\partial e}{\partial T}$$

$$\boxed{\beta = \frac{1}{kT} \quad T = \frac{1}{\beta k}}$$

Specific heat per site

$$c = k\frac{2}{\pi}\left(\beta J\coth 2\beta J\right)^2\left\{2K_1(K) - 2E_1(K) - (1-K')\left(\frac{\pi}{2} + K' K_1(K)\right)\right\}$$

where $E_1(K) = \int_0^{\pi/2} d\vartheta\sqrt{1-K^2\sin^2\vartheta}$

Let us analyze & see if there is any source of singularity at some finite temp. — we'll analyse free energy & its derivatives

$\ln(2\cosh 2\beta J)$ (& its derivatives) doesn't have any singularity at exactly 0 & ∞

If $|K| < 1$, $\sqrt{1-K^2\sin^2\theta}$ is never zero & we never get any singularity for the 2nd term or its derivatives

There are no singularities in f or any of its derivatives if $K < 1$.

(we need to analyze functional dependence of K on T & see if $|K|$ can be 1 or more)

$$K = \frac{2}{\cosh 2\phi \coth 2\phi} = \frac{2\sinh 2\phi}{\cosh^2 2\phi}$$

$$= \frac{4\left(e^{2\beta J} - e^{-2\beta J}\right)}{\left(e^{2\beta J} + e^{-2\beta J}\right)^2}$$

$$= \frac{4(y - y^{-1})}{(y + y^{-1})^2}$$

$\boxed{\text{Put } y = e^{2\beta J} \quad \therefore 1 \le y < \infty}$

$\longrightarrow 0$ as $y \to 1$

$\longrightarrow 0$ as $y \to \infty$

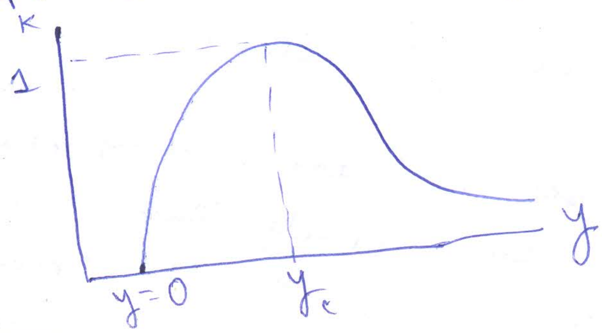
If $K > 1$, we will get an imaginary answer. $\because T(\sigma, \sigma')$ is a real sym. matrix, its eigvalues should be real & so we don't get an imaginary answers

Find the maximum of this function

Answer:- $y = \sqrt{\frac{\sqrt{2}+1}{\sqrt{2}-1}}$

At the maximum, the function $= 1$

Also you will find that there's a unique soln. for $y = 1$



Critical temp. T_c is given by:

$$e^{2\beta_c J} = \sqrt{\frac{\sqrt{2}+1}{\sqrt{2}-1}}$$

$K = 1$ at $T = T_c$

Q) How does K behave near $T = T_c$, i.e. near $y = y_c$?

Near $y = y_c$,

$$K \simeq 1 - \underbrace{A}_{\text{const} = -\frac{1}{2} \left.\frac{d^2K}{dy^2}\right|_{y=y_c}} (y - y_c)^2$$

$A > 0$ (bcos $K_{max} = 1$)

$$(1-K) \simeq A(y - y_c)^2$$

$$y = e^{2\beta J} = e^{2J/kT}$$

$$y - y_c \simeq e^{(2J/kT_c)} \left(-\frac{2J}{kT_c^2}\right)(T - T_c)$$

$$\Rightarrow \quad 1 - K \simeq \underbrace{B}_{\text{constant}} (T - T_c)^2$$

Also, $\because$ K has a max. as a fn. y, it'll also have a max. as a fn. of T

① f is non-singular.

② $E_1(K)$ is non-singular.

Cosh --- is never singular

$E_1(K)$ is never singular (even for $K=1$)

③ $K' = \sqrt{1 - K^2}$

$= \sqrt{1 - (1-\eta)^2} \simeq \sqrt{2\eta}$

$K = 1 - \eta$ ~~small~~ η small

④ $$K_1(K) = \int_0^{\pi/2} \frac{d\vartheta}{\sqrt{1 - (1 - 2\eta + \eta^2)\sin^2\vartheta}}$$

$\psi = \pi/2 - \vartheta$

$$= \int_0^{\pi/2} \frac{d\psi}{\sqrt{\sin^2\psi + (2\eta - \eta^2)\cos^2\psi}}$$

$$\sim \int^{\epsilon} \frac{d\psi}{\sqrt{\psi^2 + 2\eta - \eta^2}} \overset{\psi = t\sqrt{\eta}}{\sim} \int_0^{\epsilon/\sqrt{\eta}} \frac{dt}{\sqrt{t^2 + 2 - \eta}}$$

We noted that possible divergence comes from small ψ

trying to identify the divergent piece — so this drastic modification

(Divergence comes from large t region in terms of the t variable) — large contribution to the integral)

$$\sim \int_{1/\epsilon'}^{\epsilon/\sqrt{\eta}} \frac{dt}{t} \sim \ln \frac{\epsilon}{\epsilon'} + \ln \frac{1}{\sqrt{\eta}}$$

t near zero there is no divergence so we make large t approxmn. & take a cut-off

$$K_1(K) \simeq \ln \frac{1}{\sqrt{\eta}} + \text{finite} \quad \text{as } \eta \to 0.$$

$$K' K_1(K) \sim \sqrt{\eta} \ln \frac{1}{\sqrt{\eta}} \to 0 \text{ as } \eta \to 0$$

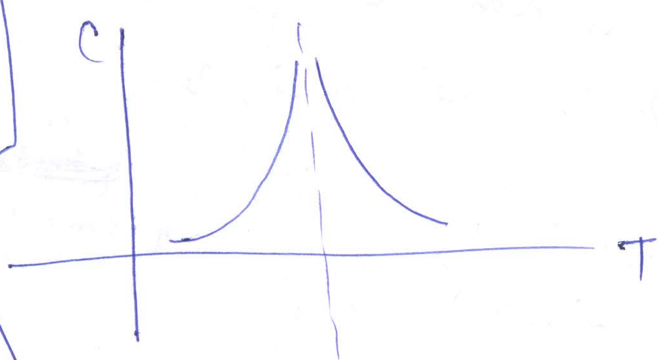
$\therefore$ e has no divergence as $K \to 1$.

$$C \simeq \frac{2k}{\pi} \left\{ \beta_c J \cosh(2\beta_c J) \right\}^2 2 \ln \frac{1}{\sqrt{\eta}} + \text{finite} \quad \text{as } \eta \to 0$$

$$\Rightarrow C \simeq \frac{2k}{\pi} \left\{ \beta_c J \cosh 2\beta_c J \right\}^2 2 \ln \frac{1}{|T - T_c|} + \text{finite}$$

$\because$ $\eta = 1 - K = B(T - T_c)^2$

This clearly is the signal that there is a phase transition (2nd order)



Here we have analysed thermal prop. & not the magnetic prop. of the system

At $B=0$, due to fluctuation of spins phase transition is taking place