Basics for Ice Models

Basics for XY R - model

- two models each of which can be solved by Bethe ansatz

→ Ice models

- hydrogen bonds in ice: coordinated in a particular way
  - usually tetrahedral environment
  - four-fold coordinated Oxygens with hydrogen in between

  - here ● are oxygen atoms

- in a hydrogen bond typically the hydrogen bond is closer to one oxygen atom than the other:

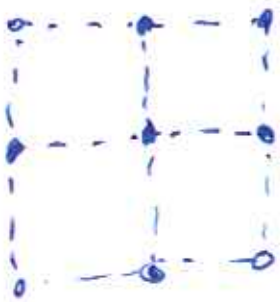
- in the four-fold coordinated case inside an ice crystal, considering the environment of <u>one</u> central oxygen atom, there are four hydrogen bonds

- the ice rule states that two of the bonding hydrogens are close to central oxygen, two are far

something like this =>

=> ice crystal consists of such tetrahedra put together

- in 3D difficult to solve (only possible in particular cases)
- the problem can be mapped into 2D
  - => square lattice - each site has four nearest neighbors
  - can place "hydrogens" on nearest neighbor bonds
  - introduce rule two close two far (ice rule)



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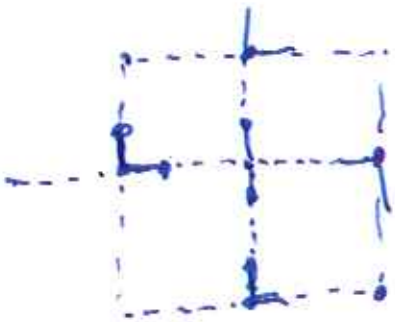


allowed

=> ~~not~~

!

not allowed

- each lattice site will be in one of the following configurations:

=> six $\left(\frac{4!}{2!2!}\right)$ configurations

can also be represented using arrows (arrow points toward direction of close hydrogen)

six arrow represented configurations:

lattice can only be put together so that arrows do not "contradict"

OK

not OK

- ice model: assign energies to each configuration

ε_1 ε_2 ε_3 ε_4 ε_5 ε_6

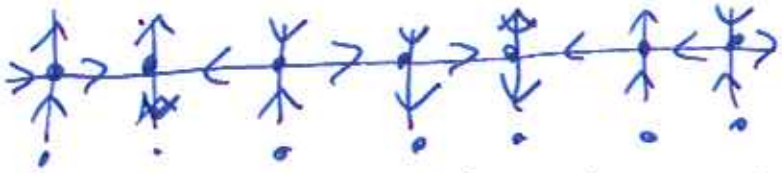
- a configuration will contain m_1 lattice sites in configuration with energy ε_1, m_2 with ε_2, etc.

☺

partition function: $Q = \sum_{m_1 m_2 \ldots m_6}' \ldots \exp(-m_1\varepsilon_1 - \ldots - m_6\varepsilon_6)$

sum over $m_1, m_2, \ldots$ are constrained by ice rules

- consider a lattice with periodic boundary conditions in both directions ↑→



consider one row of lattice sites (length N)

- bonds above: either up or down → 2^N configs.
- bonds below: either up or down → 2^N configs.

- can represent one row in terms of a transfer matrix

$V_{\sigma,\sigma'}$ $\quad \sigma \to 2^N$ dimensional

$\to 2^N \times 2^N$ dimensional matrix

- partition function

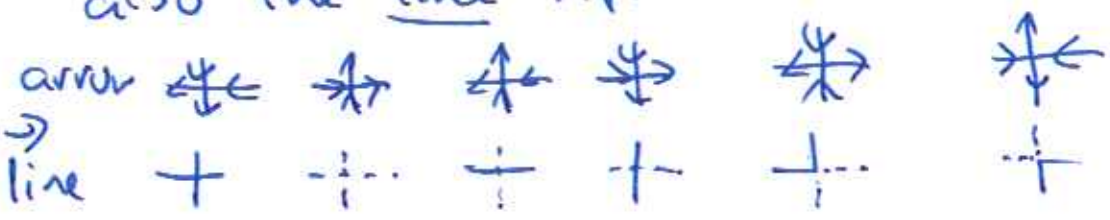
$\underline{Q = \mathrm{Tr}\, V^M}$; if there are M rows ~~with periodic boundary condition~~

→ for large M $\quad \to Q = \lambda_{max}^M$

- transfer matrix V is a row of lattice sites

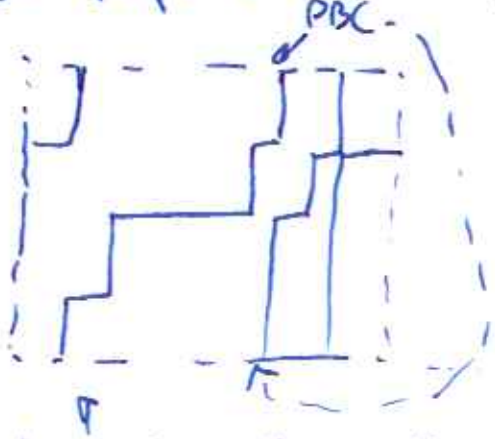
→ V - can also be represented as

- besides arrow representation there exists also the line representation



- ice rule for line representation means → solid line must continue
  - can put together: ✗ + | ⇒ |
  - can not put together: + | ⇒ +

- for an entire lattice it holds that ~~each~~ a configuration is only allowed if it can be represented by one line which returns to itself when periodic boundary conditions are considered



allowed configuration in line representation

- line which "leaves" lattice comes back on the opposite side for both directions

- when the line is drawn ⇒ it must come back to itself

‼ ☺ ☺

IMPORTANT CONSEQUENCE!!!

→ all transfer matrices will have an equal number of lines entering from below and leaving above

what does that mean?

- transfer matrix represents one row in the 2D lattice

⇒ 

- when drawn according to line representation example

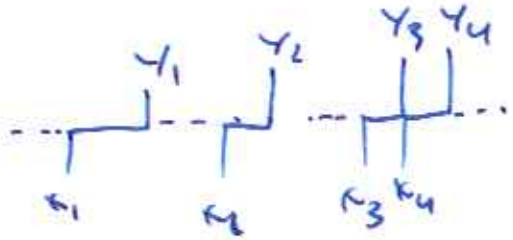
number of solid lines below = number of solid lines above

⇒ transfer matrix, as a result, is <u>block</u> diagonal

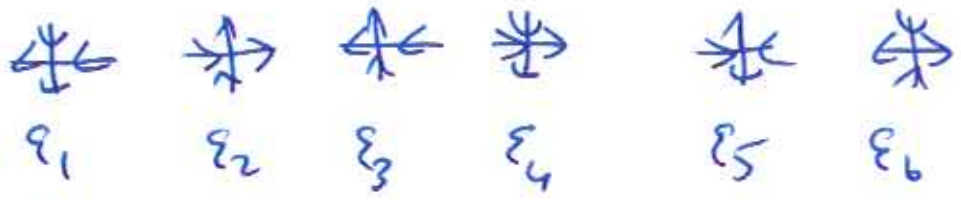
→ the number of lines entering from below, or leaving towards above can be considered a <u>quantum number</u> - let's call it n

$$V = \begin{bmatrix} V_0 & & & \\ & V_1 & & \\ & & V_2 & \\ & & & \ddots \end{bmatrix}$$

→ can represent a transfer matrix in terms of coordinates as



- to be more specific let's consider an ice model for which



$\varepsilon_1 = \varepsilon_2 \quad \varepsilon_3 = \varepsilon_4 \quad \varepsilon_5 = \varepsilon_6$

⇒ statistical weights can be represented as

$$e^{-\varepsilon_1} = e^{-\varepsilon_2} = a \qquad e^{-\varepsilon_3} = e^{-\varepsilon_4} = b \qquad e^{-\varepsilon_5} = e^{-\varepsilon_6} = c$$

let's construct transfer matrix for some fixed values of quantum number n

$n = 0$ ⇒ no lines cross the row represented by the transfer matrix vertically

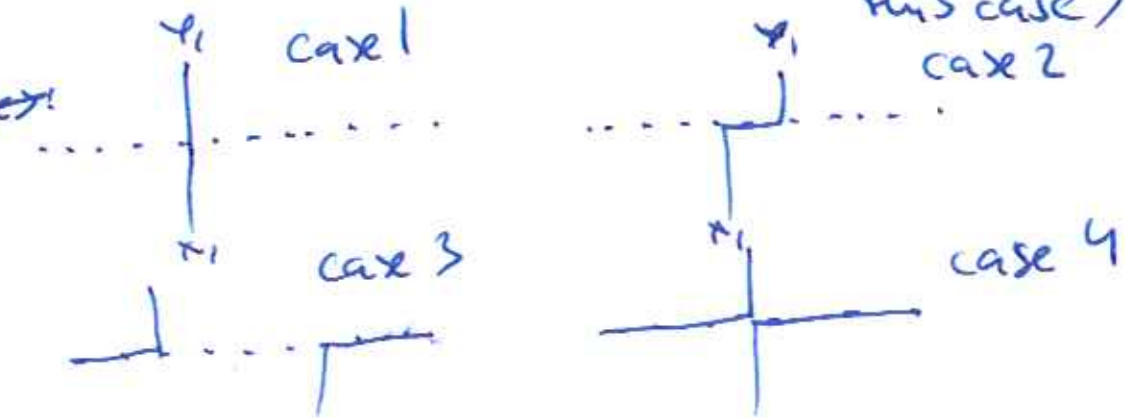
two possibilities

⇒ ..... or ———

a^N $\quad$ b^N

transfer matrix ⇒ $a^N + b^N$ (also eigenvalue in this case)

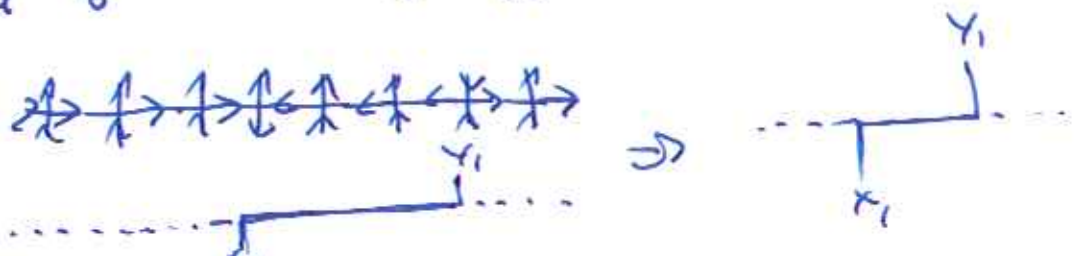
$n = 1$



case 1: all ⇉ (a) except one site, which is ⇊ (b)

$\rightarrow a^{N-1} b \qquad (x_1 = y_1)$

case 2:



$\rightarrow a^N \left(\frac{c}{a}\right)\left(\frac{b}{a}\right)^{y_1 - x - 1}\left(\frac{c}{a}\right)$

case 3:

$\rightarrow a^N \left(\frac{c}{a}\right)^2 \left(\frac{b}{a}\right)^{N - x_1}\left(\frac{b}{a}\right)^{y_1 - 1}$

case 4: $b^{N-1} a^1$

→ the matrix equation for the case $n = 1$ can be written as

$$\Lambda\, g(x) = \sum_y V(x,y)\, g(y)$$

$g(x)$ – eigenvector Λ – eigenvalue

→ putting together the 4-cases from above we have the equation:

$$\Lambda\, g(x) = \left(a^{N-1} b + b^{N-1} a\right) g(x) + \sum_{y=x+1}^{N} a^N \left(\frac{c}{a}\right)^2 \left(\frac{b}{a}\right)^{y-x-1} g(y) + \sum_{y=1}^{x-1} a^N \left(\frac{c}{a}\right)^2 \left(\frac{b}{a}\right)^{N-x} \left(\frac{b}{a}\right)^{y-1} g(y)$$

can be solved by taking $g(x) = * z^x$

$$1 z^x = (a^{N-1} b + b^{N-1} a) z^x + \sum_{y=x+1}^{N} a^{N-2} c^2 \left(\frac{b}{a}\right)^{-x-1} \left(\frac{bz}{a}\right)^y + \sum_{y=1}^{x-1} a^{N-2} c^2 \left(\frac{b}{a}\right)^N \left(\frac{b}{a}\right)^{-x-1} \left(\frac{bz}{a}\right)^y$$

can use formula for geometric series to obtain

$$1 z^x = (a^{N-1} b + b^{N-1} a) z^x + a^{N-2} c^2 \left(\frac{b}{a}\right)^{-x-1} \left[\frac{\left(\frac{bz}{a}\right)^{x+1} - \left(\frac{bz}{a}\right)^{N+1}}{1 - \frac{bz}{a}}\right] + a^{N-1} c^2 \left(\frac{b}{a}\right)^N \left(\frac{b}{a}\right)^{-x-1} \left[\frac{\left(\frac{bz}{a}\right) - \left(\frac{bz}{a}\right)^x}{1 - \frac{bz}{a}}\right]$$

to obtain a solution assume

$$z^N = 1$$

in this case: $$1 = (a^{N-1} b + b^{N-1} a) + \frac{(a^{N-2} c^2 z)}{1 - \frac{bz}{a}} + \frac{a^{N-2} c^2 \left(\frac{b}{a}\right)^{N-1}}{1 - \frac{bz}{a}}$$

vacuum state: $H|0\rangle = \frac{1}{2}JN|0\rangle$

$\Rightarrow$ eigenstate with eigenvalue $\frac{1}{2}JN$

- $n=1$ state

→ somewhere there is an up-spin, say at position m

state: $|m\rangle$

$$|\downarrow_1 \downarrow_2 \cdots \uparrow_m \cdots \downarrow_N\rangle$$

$$\sum_{i=1}^{N} J S_i^q S_{i+1}^q |m\rangle = \frac{1}{2}J(N-4)|m\rangle$$

$$\sum_{i=1}^{N} \frac{1}{2} S_i^+ S_{i+1}^- |m\rangle = \frac{1}{2}|m+1\rangle \quad \text{(only } i=m \text{ gives contribution)}$$

$$\sum_{i=1}^{N} \frac{1}{2} S_i^- S_{i+1}^+ |m\rangle = \frac{1}{2}|m+1\rangle \quad \text{(only } i=m \text{ gives contribution)}$$

$$\Rightarrow H|m\rangle = \frac{1}{2}\left[|m+1\rangle + |m-1\rangle + J(N-4)|m\rangle\right]$$

- take wavefunction in 1st quantized form

$$|\Psi\rangle = \sum_{m=1}^{N} a_m |m\rangle \Rightarrow \text{linear combination of all single particle states}$$

$H|\Psi\rangle = E|\Psi\rangle$ → looking for this! ($|\Psi\rangle$ and E)

$$H|\Psi\rangle = \sum_m \left[\frac{1}{2} a_m |m+1\rangle + \frac{1}{2} a_m |m-1\rangle + J(N-4) a_m |m\rangle\right]$$

since m goes from 1 to N $\Rightarrow$ can shift

$$\rightarrow \sum_m \left[\frac{1}{2} a_{m-1}|m\rangle + \frac{1}{2} a_{m+1}|m\rangle + J(N-4) a_m |m\rangle\right]$$

$$H \sum_m a_m |m\rangle = \sum_m \left[\frac{1}{2}(a_{m-1} + a_{m+1}) + J(N-4) a_m\right]|m\rangle$$

$n = 2 \Rightarrow$ homework exercise for case $a = b = c = 1$

XXZ (Heisenberg) model – Basics

Hamiltonian:

$$H = \sum_{i=1}^{N} \left[\left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) + J S_i^z S_{i+1}^z \right]$$

$$S_i^x = \frac{S_i^+ + S_i^-}{2} \qquad S_i^y = \frac{S_i^+ - S_i^-}{2i}$$

$$S_i^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_i^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad S_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$H = \sum_{i=1}^{N} \left[\frac{1}{2} \left\{ \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) + J S_i^z S_{i+1}^z \right] \right.$$

want to find ground state

$$H |\Psi\rangle = E |\Psi\rangle$$

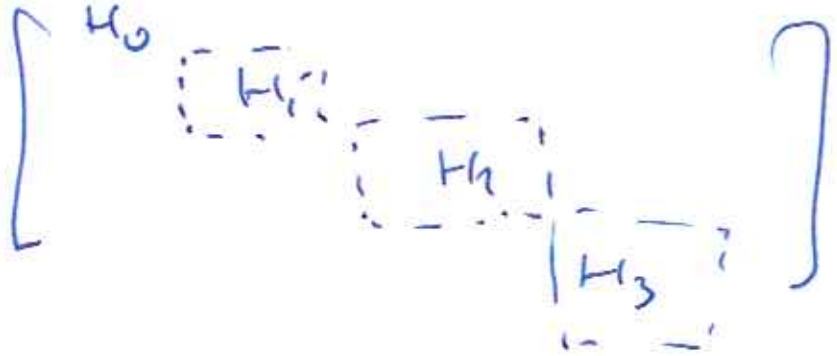
→ H conserves z-component of spin

→ take vacuum to be state with all down-spins

→ since H conserves z-component of total spin

S_z^{TOTAL} is a good quantum number

→ Hamiltonian is block-diagonal



$$\sum_m a_m \hat{H}|m\rangle = \sum_m \left[\frac{1}{2}(a_{m+1} + a_{m-1}) + J(N-u)\,a_m\right]|m\rangle$$

$\langle n| \rightarrow$

$$\sum_m H_{nm}\, a_m = \frac{1}{2}(a_{n+1} + a_{n-1}) + J(N-u)\,a_n = E\,a_n$$

$$H_{nm} \rightarrow \begin{bmatrix} J(N-u) & \frac{1}{2} & 0 \\ \frac{1}{2} & J(N-u) & \frac{1}{2} \\ 0 & \frac{1}{2} & \ddots \end{bmatrix}$$

- can diagonalize by choosing $a_m = e^{ikm}$

RHS becomes: $\underbrace{\left[\frac{1}{2}(e^{ik} + e^{-ik}) + J(N-u)\right] e^{ikm} = E\, e^{ikn}}_{\text{diagonal}}$

$$E = \cos k + J(N-u)$$

- next problem: number of up-spins equals two
  - this is a homework problem, but here are a few hints:

1.) state $|m_1, m_2\rangle \rightarrow$ basis

wavefunction $|\Psi\rangle = \sum_{m_1, m_2} a_{m_1, m_2} |m_1, m_2\rangle$

we are after

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

assume $m_1 \leq m_2$

2.) apply $\hat{H}|\Psi\rangle$, you know what it does

BUT treat two cases separately

case 1: $m_1, m_2 \Rightarrow$ not nearest neighbors

=> in this case $\hat{H}$ can take $|m_1, m_2\rangle$

to $|m_1+1, m_2\rangle$ $|m_1-1, m_2\rangle$, $|m_1, m_2+1\rangle$

and $|m_1, m_2-1\rangle$

case 2: m_1 and m_2 are nearest neighbors

$\Rightarrow m_1+1 = m_2$

=> in this case $\hat{H}$ can take $|m_1, m_2\rangle$

to $|m_1-1 m_2\rangle$ but not (m_1+1, m_2)

=> $\hat{H}$ can also take $|m_1, m_2\rangle$ to $|m_1, m_2+1\rangle$

but not $|m_1, m_2-1\rangle$

case 1 and case 2 give you two equations

case 1 => valid for $m_1 \leq m_2 - 1$

but not at $m_1 = m_2 - 1$

(it is not invalid there either!)

case 2 => valid for $m_1 = m_2 - 1$

=> subtracting one equation from the other gives a condition free of the energy E

=> assume $\psi_{m_1 m_2} = A_{12} e^{i(k_1 m_1 + k_2 m_2)} + A_{21} e^{i(k_1 m_2 + k_2 m_1)}$

-> can use condition to obtain relationship between A_{12} and A_{21}