MOD-1

Many solids exhibit magnetic order even if no external magnetic field applied.

- Fe: ferromagnetic (spins parallel)
- MnO: anti-ferromagnetic (spins on Mn atoms alternate ↑/↓)
- La_2CuO_4 and other cuprates: spins on Cu atoms alternate up/down
- iron-arsenide superconductors: parallel in 1 direction, antiparallel in other

↑ ↑ ↑ ↑ ↑
↓ ↓ ↓ ↓ ↓
↑ ↑ ↑ ↑ ↑

These phenomena all occur because spins interact with each other and influence each other to coordinate the directions they point.

Solid State physicists write down "models" to see under what circumstances (what types of interactions, temperatures, geometries,) such coordination is possible.

The simplest models address only qualitative issues: how does dimension affect ordering? Is lower dim better or worse?

More complex models can make quantitative predictions about specific solids. ~~These~~

~~In both cases~~,

Even "simple" models often need numerical solutions.

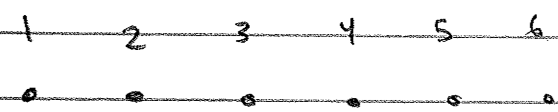
Simplest model is due to Onsager who assigned it to his student Ising. Now called Ising model. Ising solved it in $d=1$ in his PhD thesis.

Ising model:

* Lattice of sites i
* on each site a "spin" variable $S_i = \pm 1$
* Energy $E = -J \sum_{\langle ij \rangle} S_i S_j$

neighboring sites

for example: 6 site linear lattice



$$E = -J\,(S_1 S_2 + S_2 S_3 + S_3 S_4 + S_4 S_5 + S_5 S_6 + S_6 S_1)$$

pbc term

MOD -4

Ordered spins have lowest energy

$+ + + + + +$ $\quad E = -6J$

other configurations have higher energy

$+ + - + + +$ $\quad E = -2J$

$+ - - + + +$ $\quad E = -2J$

$+ - + - + +$ $\quad E = +2J$

Note if we change sign out front $E = +J \sum S_i S_j$

we favor antiferromagnetism : $+ - + - + -$ is lowest E

How many configurations? $2^6 = 64$.

Crude picture of phase transitions

2 perfectly ordered states of all spins same.

Lower in energy by 4J than all others. These are

favored by $e^{-\beta E}$.

But 62 "disordered" states favored by entropy

minimize $F = E - TS$

$\uparrow$ low T — minimize E wins $\Rightarrow$ order

high T — maximize S wins $\Rightarrow$ disorder

Surprise is that there is an <u>abrupt</u> transition

between order and disorder. A phase transition

Methods to solve Ising model

Numerics : Enumerate all states , $N=6$ just 64 of them

HW problem! 4×4 lattice $2^{16} \approx 64000$ (use $2^{10} \sim 1000$)

also easy! CPU estimate :

Compute E : 32 terms $\approx$ 100 operations per config
for 4×4
64000 configurations

$$\frac{64000 \cdot 100}{10^9} \sim 0.1 \text{ sec } !!$$

10^9 ← Gflop

Now 6×6 lattice $2^{36} \approx 64 \cdot 10^9$

Compute E : 72 terms ~ 100 ops
for 6×6

$$\frac{64 \cdot 10^9 \cdot 100}{10^9} \sim 6400 \text{ sec} \approx 2 \text{ hours}$$

8×8 $2^{64} \sim 16 \cdot 10^{18}$

$$\frac{16 \cdot 10^{18}\, 100}{10^9} \sim 10^{12} \text{ sec} \sim 10^7 \text{ days}$$

$\sim$ 3000 years.

$\boxed{\text{Exponential Growth}}$

MOD 7

Another numerical method : Monte Carlo.

Can easily do 10^8 spins! But not for this course

* TRANSFER MATRIX $d=1$ Ising Model

$$Z = \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} e^{-\beta E}$$

$$e^{\beta J (s_1 s_2 + s_2 s_3 + \ldots)}$$

$$e^{\beta J s_1 s_2} e^{\beta J s_2 s_3} e^{\beta J s_3 s_4}$$

Define matrix M $\quad \underbrace{M(s_1 s_2)}_{\text{components of } M} = e^{\beta J s_1 s_2}$

2x2 $\quad s_1 = +/-$
$s_2 = +-$

$$\begin{array}{ccc} & s_2=+ & s_2=- \\ s_1=+ & \multicolumn{2}{c}{\multirow{2}{*}{}} \\ s_1=- & & \end{array} \qquad \begin{pmatrix} e^{\beta J} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} \end{pmatrix} = M$$

MOD 8

$$Z = \sum_{s_1} \sum_{s_2} \sum_{s_3} \ldots \sum_{s_N} M(s_1 s_2) M(s_2 s_3) M(s_3 s_4) \ldots M(s_N s_1)$$

What is this?

Matrix product $M^2(s_1, s_3)$

ie s_1, s_3 element of M^2

Then $\sum_{s_3} M^2(s_1 s_3) M(s_3 s_4) = M^3(s_1 s_4)$

clearly continue process

length of chain

$$\underbrace{Z = \sum_{s_1} M^N(s_1 s_1)}_{\text{What is this? Trace}}$$

What is this? <u>Trace</u>

$$Z = \text{trace } M^N$$

To get $\text{tr } M^N$ just diagonalize M

$$\text{tr } M^N = \lambda_1^N + \lambda_2^N$$

$$0 = \begin{vmatrix} e^{\beta J} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J} - \lambda \end{vmatrix} = (e^{\beta J} - \lambda)^2 - e^{-2\beta J}$$

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

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

$$\lambda_1 = 2\cosh\beta J$$

$$\lambda_2 = 2\sinh\beta J$$

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

Check for $N=4$! (HW)

We have solved $d=1$ Ising Model Exactly!

But it has no phase transition

Another $d=1$ Ising Model soln:

* HIGH T EXPANSION

$$Z = \sum_{S_1} \sum_{S_2} \cdots \sum_{S_N} e^{\beta J S_1 S_2} e^{\beta J S_2 S_3} \cdots$$

Identity $\quad e^{ax} = \cosh a + x \sinh x$

if $x = \pm 1$ only

check by looking at 2 cases

$x = 1 \quad e^{a} \stackrel{?}{=} \cosh a + \sinh a$ ✓

$x = -1 \quad e^{-a} \stackrel{?}{=} \cosh a - \sinh a$ ✓

so $\quad e^{\beta J S_1 S_2} = \cosh \beta J + S_1 S_2 \sinh \beta J$

high T $\rightarrow$ small β

$\rightarrow \cosh \beta J \approx 1$

$\sinh \beta J \approx$ small

MOD-11

$c \equiv \cosh\beta J \qquad \not{s} \equiv \sinh\beta J$

$$Z = \sum_{S_1}\sum_{S_2}\cdots\sum_{S_N}(c + S_1S_2\not{s})(c + S_2S_3\not{s})\cdots(c + S_NS_1\not{s})$$

In this big product, largest term

is obtained by selecting c from each factor

$$Z = \sum_{S_1}\sum_{S_2}\cdots\sum_{S_N} c^N = 2^N c^N = (2c)^N$$

indep of S_1 S_2 ..

Look familiar?

Consider term like

$\underbrace{c\not{s}}S_2S_3\,cc\ldots c$

choose $\not{s}S_2S_3$ from second factor

$$\sum_{S_1}\sum_{S_2}\cdots\sum_{S_N} c^{N-1}\not{s}\,S_2S_3$$

but $\sum_{S_2} S_2 = 1 + (-1) = 0$

This term vanishes!

MOD-12

Could prevent $\sum_{S_2} S_2 = 0$

by also selecting $\theta S_2 S_3$ term

$$c\,\theta S_1 S_2\, \theta S_2 S_3\, c\, c \ldots c$$

get $(S_2)^2$

and $\sum_{S_2} (S_2)^2 = 1 + 1 = 2$

But still $\sum_{S_1} S_1 = 0$ and $\sum_{S_3} S_3 = 0$.

Only way to avoid $\emptyset$ is choose all θ terms

$$\sum_{S_1} \sum_{S_2} \ldots \sum_{S_N} \theta S_1 S_2\, \theta S_2 S_3\, \theta S_3 S_4 \ldots \theta S_N S_1$$

$$= \theta^N 2^N = (2\theta)^N$$

So all together

$$Z = (2c)^N + (2\theta)^N$$

Same as transfer matrix!

Bonus: can get Z for open b_c: $Z = (2c)^N$

MOD-13

High T Expansion for $d=2$ Ising model is cool!

Same starting approach

$$Z = \sum_{S_1} \sum_{S_2} \dots \sum_{S_N} (c + S_1 S_2 a)(c + S_2 S_3 a) \dots$$

Difference is pairs of sites are in 2D

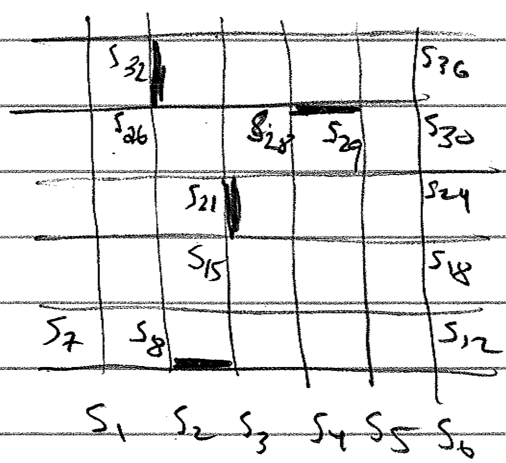
Pictorial Representation:

If you choose $S_i S_j a$ term from the factor

$$(c + S_i S_j a)$$

then "color in" the associated link

6x6 lattice



$$\Longleftrightarrow c^{32} a^{4} S_2 S_3 S_{15} S_{21} S_{26} S_{32} S_{29} S_{29}$$

pretty clearly this vanishes when we do the sum $\sum_{S_1} \sum_{S_2} \dots \sum_{S_{36}}$

Clearly to get non zero term cannot have any

s_i^1 ← first power since $\sum s_i = 0$

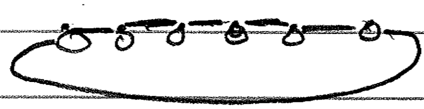
In $d=1$ only two ways to avoid s_i^1

↑

two "diagrams"

← choose all c

and no $s_i s_j \lambda$

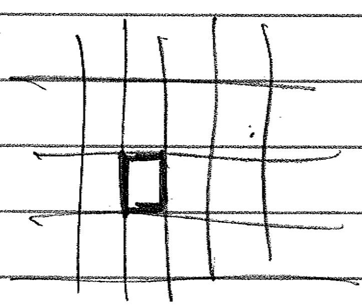


← choose all $s_i s_j \lambda$

then each s_i appears twice

$$\Rightarrow \quad Z = (2c)^N + (2\lambda)^N$$

What about 2D ??



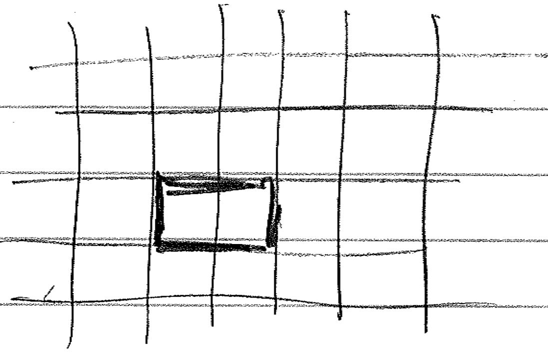
$$Z = (2c)^N + N(2c)^{N-4}\lambda^4$$

↑

N locations

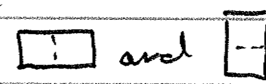
$N = \#$ sites

MoD-15

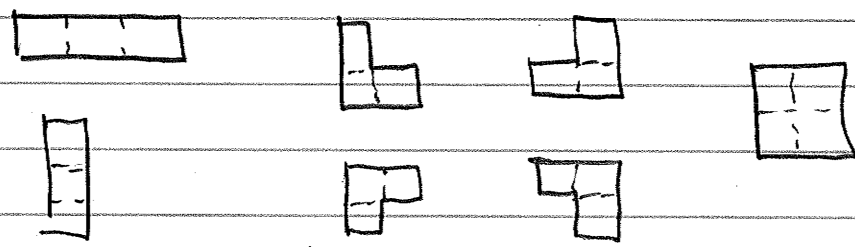


$$Z = (2c)^N \{ 1 + N t^4 + 2N t^6$$

$t = \tanh \beta J$

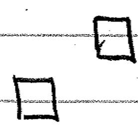


t^8 starts to get tricky!



$\leftarrow 7N t^8$

But also "disconnected"



$\frac{N(N-5)}{2} t^8$

why?!

$\frac{N(N-5)}{2} + 7N$

$= \frac{1}{2} N(N+9)$

MOD-16

$$Z = (2c)^{2N}\{1 + Nt^4 + 2Nt^6 + \tfrac{1}{2}N(N+9)t^8 + \dots\}$$

worrisome?
Expect physics
$\sim N$
not N^2

$$\langle E \rangle = -\frac{\partial}{\partial\beta}\ln Z$$

$$\ln Z = 2N\ln(2c) + \ln\{1 + Nt^4 + 2Nt^6 + \dots\}$$

$$\ln(1+x) = x - \tfrac{1}{2}x^2$$

$$Nt^4 + 2Nt^6 + \tfrac{1}{2}N(N+9)t^8 \quad - \tfrac{1}{2}(Nt^4 + \dots)^2$$

kills of N^2 term!

$$\ln Z = 2N\ln(2c) + Nt^4 + 2Nt^6 + \tfrac{9}{2}Nt^8$$

$$\langle E \rangle = -\frac{\partial}{\partial\beta}\ln Z$$

$$= -2N\frac{1}{2c}2\ell - (4Nt^3 + 12Nt^5 + 36Nt^7)\,\mathrm{sech}^2\beta J$$

$$\frac{1}{N}\langle E \rangle = -2\tanh\beta J - 4(\tanh^3\beta J + 3\tanh^5\beta J$$

$$+ 12\tanh^7\beta J)\,\mathrm{sech}^2\beta J.$$