Critical Phenomena

1^{st} order phase transition: phases coexist, they have different values of thermodynamic quantities (entropy, specific volume) and these quantities change discontinuously around a phase transition

2^{nd} order phase transition: thermodynamic variables change continuously, no metastability

* cooperative phenomena: Hamiltonian describing the system has short-range interactions → around T_c correlations ~~diverge~~ are long range → at T_c correlations are infinite

because of infinite correlations, the microscopic details do not matter so much, and many models which are very different microscopically exhibit identical features around T_c → universality

* symmetry breaking: symmetry group of low temperature phase ($T<T_c$) is ~~lower~~ a subgroup of the symmetry group of Hamiltonian

example: Ising model $\mathbb{Z}_2$ symmetry

$\sigma_i \to -\sigma_i$ for all $i \Rightarrow H \to H$

but for low-T ordered state

$\sigma_i \to -\sigma_i$ for all i leads to a different ~~phase~~ state

Order parameter: sensitive to change in symmetry group $\Rightarrow$ zero in high-symmetry phase, finite in low-symmetry phase

(In Ising model: $M = \frac{1}{N} \sum_i \langle \sigma_i \rangle \Rightarrow \sigma_i \to -\sigma_i$
$M \to -M$ in low-symmetry phase but $M = 0$ $T > T_c$)

order parameter vanishes continuously at $T = T_c$

order parameter / symmetry breaking $\Rightarrow$ associated with continuous phase transitions – but may also occur in 1st order phase transitions

- ferro-electric transition in barium-titanate: symmetry breaks, but order parameter changes discontinuously
- Bose-Einstein condensation: pathological
- XY-model: continuous phase transition without order parameter or symmetry breaking

Ising model

$D=1 \rightarrow$ no phase transition

can show that for $D \geq 2$ ordering occurs

* thermodynamic limit exists:

$$f = \lim_{N\to\infty} \frac{1}{N} F_N = \lim_{N\to\infty} -\frac{kT \ln Z_N}{N}$$

if $B=0 \Rightarrow S_i \rightarrow -S_i$ means $M = \frac{1}{N}\sum_i \langle S_i \rangle$ even in the limit $N \to \infty$

to obtain order => impose particular boundary conditions, since it is impossible to obtain non-zero magnetization otherwise

- impose: all the spins along boundary must be up → for a lattice of N spins, boundary will have extent of $\sqrt{N}$
- at $T=0$ all spins up (ordered state) → take energy to be zero

* 1st give a handwaving argument for the existence of order for $D \geq 2$, and absence ~~for~~ of order for $D=1$

<u>$D=1$</u>

$T=0 \rightarrow$ all spins up (ground state)

1st excited state obtained by creating two kinks

kink 1 kink 2

$$\underbrace{\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow}$$

energy of 1st excited state: $4J$

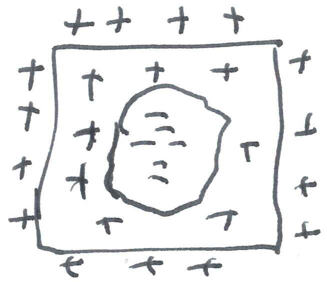
entropy of 1st excited state: kinks can be placed at $N(N-1)$

$$S = k\ln N(N-1) \sim k\ln N^2 = 2k\ln N$$

$$F = 4J - 2kT\ln N$$

- if $T>0$ $\quad F<0$ free energy smaller than ground state energy => <u>$T>0$ disordered for $D=1$</u>

* now consider $D=2$



1st excited state: "bubble" of '−' spins

- bubble enclosed by length of $\underline{b}$ (perimeter)

$$\Downarrow \qquad \Downarrow$$

energy cost: $2bJ$

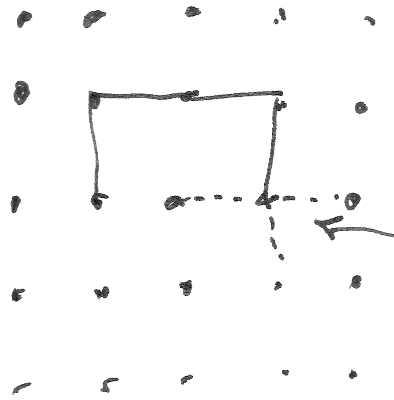
- entropy of configuration: $\nu(b)$ − number of configurations with perimeter $\underline{b}$

$$\nu(b) \le N\, 3^{b-1}$$

explanation: N → we can start a bubble anywhere

3^{b-1} → for square lattice one can construct bubble by starting at some site, and going in three possible directions at each step

⑤



3 possible directions at each step

→ self-avoiding random walk which returns to starting point

free energy: $F = 2bJ - kT \ln N 3^{b-1}$

$= 2bJ - kT \ln N - b kT \ln 3$

$F \leq 0 \rightarrow b \leq \dfrac{kT \ln N}{2J - kT \ln 3} = b_{max}$

if $2J > kT \ln 3$

for $b > b_{max}$ $F > 0$ → negligible probability

for $b < b_{max}$ ⇒ percentage of downspins

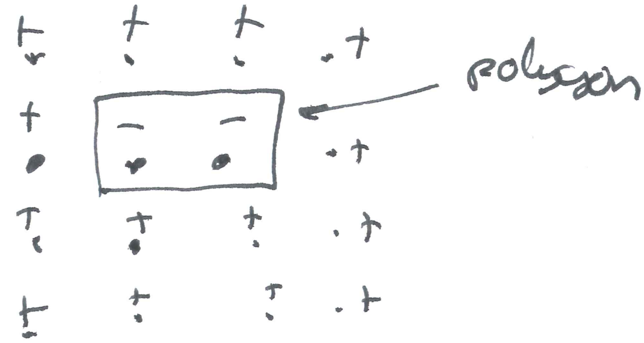
will be ⇒ $\dfrac{b_{max}^2}{N} \rightarrow \dfrac{(\ln N)^2}{N} \xrightarrow[N \to \infty]{} 0$

⇒ sponteneous magnetization can exist in $D = 2$

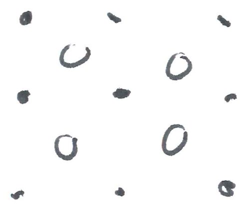
⇒ but this argument is handwaving, not rigorous

* rigorous Peierls argument: observe that there is a one-to-one correspondence between a spin configurations and a set of polygons

- justification:



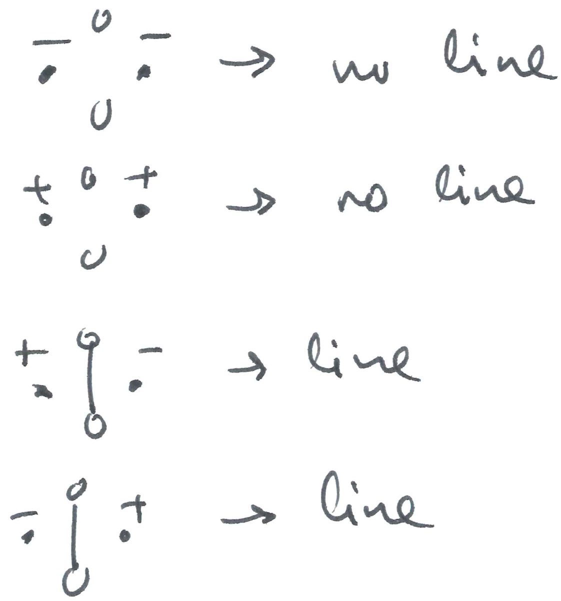
polygons are constructed using the dual lattice:

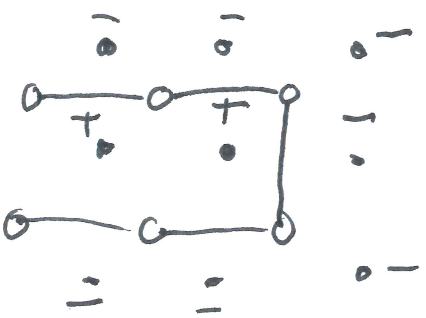


• – lattice (regular)

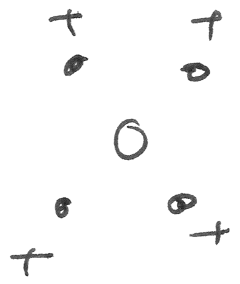
o – dual lattice

- for bonds on the regular lattice which connect + – or – + ⇒ draw a line which is perpendicular to the bond on the dual lattice

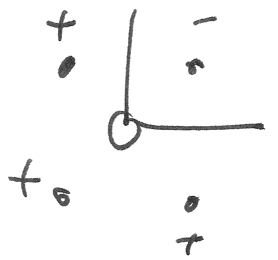


⇒ 

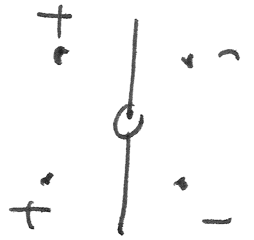
- under these conditions the number of lines going into a dual lattice site is always <u>even</u> =>



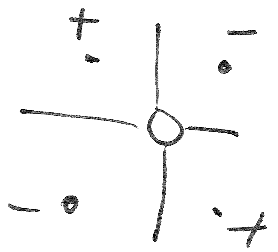
→ 0 lines



→ 2 lines

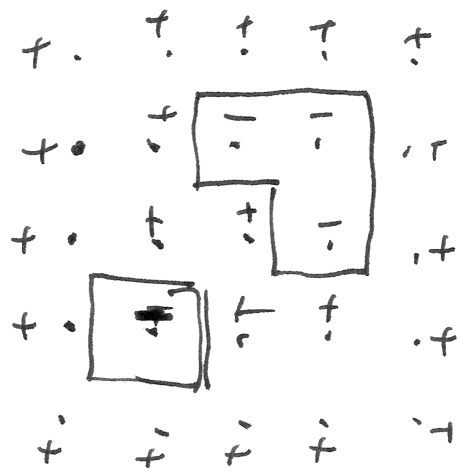


→ 2 lines



→ 4 lines

=> since each dual lattice points has an even number of lines going into it



any given spin configuration corresponds to a set of closed polygons

$C = \{ P_{b_1}^{(j_1)} \dots P_{b_n}^{(j_n)} \dots \}$ → polygon configuration

↑

one polygon → has perimeter b_1

→ has another index j_1

(there are many closed polygons with perimeter b_1)

we can say: $\sum_{\{C\}} = \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \dots \sum_{S_N=\pm 1}$

(replace the sum over configurations with a sum over closed polygons)

- let $N_b^{(j)}$ denote the number of sites within polygon $P_b^{(j)}$
- let $N_+(C) / N_-(C)$ denote the number of up spins / down spins of configuration C

$$M(C) = \frac{1}{N} [N_+(C) - N_-(C)] = 1 - \frac{2N_-(C)}{N}$$

→ strategy: prove that $\frac{N_-(C)}{N} < 1/2$ for low T

inequality: $N_-(C) \le \sum_b \sum_{1 \le j \le \nu(b)} \chi_b^{(j)} N_b^{(j)}$

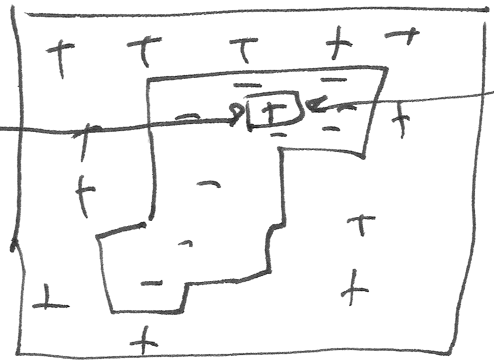
$\chi_b^{(j)}$ – characteristic function of polygon $P_b^{(j)}$ ⇒ $\chi_b^{(j)} = 1$ if $P_b^{(j)}$ present in config. C

0 otherwise

$N_b^{(j)}$ - number of sites within $P_b^{(j)}$ (9)

- if there are boxed polygons, ~~that~~ strict inequality holds

$$N_-(C) < \sum_b \sum_{1 \le j \le \nu(b)} \chi_b^{(j)} N_b^{(j)}$$

because  in this case some sites are +

equality if no boxed polygons

- also $\Rightarrow$ the maximum number of sites enclosed by a polygon occurs if polygon is a square

$$N_b^{(j)} \le \left(\frac{b}{4}\right)^2$$

$$\Downarrow \qquad \Downarrow$$

$$\langle N_-(C)\rangle \le \sum_b \sum_{1 \le j \le \nu(b)} \langle \chi_b^{(j)} \rangle \left(\frac{b}{4}\right)^2$$

- for $\langle \chi_b^{(j)} \rangle$ we can write

$$\langle \chi_b^{(j)} \rangle = \frac{1}{Z} \sum_{P_b^{(j)} \in C} e^{-\beta E(C)} = \frac{1}{Z} \sum_{\tilde{C}} e^{-\beta E(\tilde{C})}$$

$E(C) \to$ energy of configuration

$$Z = \sum_{C} e^{-\beta E(C)} \geq \sum_{P_b^{(j)} \in C} e^{-\beta E(C)}$$

consider flipping all spins within polygon $P_b^{(j)} \rightarrow$ in this case the energy will change by $2Jb$

- given a configuration $\tilde{C}$ which includes $P_b^{(j)}$

~~if we~~ $\Rightarrow$ energy $E(\tilde{C})$

- if all spins within $P_b^{(j)}$ are switched

then $E(\tilde{C}) \longrightarrow E(\tilde{C}^*)$

$\tilde{C}^*$ config. with $P_b^{(j)}$ all up-spins

$$E(\tilde{C}^*) = E(\tilde{C}) - 2bJ$$

$$Z = \sum_{C} e^{-\beta E(C)} \leq \sum_{\tilde{C}^*} e^{-\beta E(\tilde{C}^*)} = \sum_{\tilde{C}^*} e^{-\beta E(\tilde{C}) + \beta 2bJ}$$

but there is a one-to-one correspondence between $\tilde{C}$ and $\tilde{C}^*$

- we can write: $\langle \psi_b^{(j)} \rangle \leq \dfrac{\sum_{\tilde{C}} e^{-\beta E(\tilde{C})}}{\sum_{\tilde{C}^*} e^{-\beta E(\tilde{C}^*)}} =$

$$= \frac{\sum_{\tilde{C}} e^{-\beta E(\tilde{C})}}{\sum_{\tilde{C}^*} e^{-\beta E(\tilde{C}) + \beta 2bJ}} = e^{-2\beta bJ}$$

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$$\langle N_- \rangle \leq \sum_b \left(\frac{b}{4}\right)^2 \sum_j \langle \chi_b^{(j)} \rangle \leq \underbrace{\sum_b \left(\frac{b}{4}\right)^2 e^{-2\beta b J} \sum_{j=1}^{\nu(b)} 1}_{\sum_b \left(\frac{b}{4}\right)^2 e^{-2\beta b J} \nu(b)}$$

$$\nu(b) = N\, 3^{b-1}$$

$$\sum_b \left(\frac{b}{4}\right)^2 e^{-2\beta b J} N\, 3^{b-1}$$

$$\langle N_- \rangle \leq N \sum_b \left(\frac{b}{4}\right)^2 e^{-2\beta b J} 3^{b-1}$$

$$\Downarrow$$

$$\frac{\langle N_- \rangle}{N} \leq \underbrace{\sum_b \left(\frac{b}{4}\right)^2 e^{-2\beta b J} 3^{b-1}}$$

series is convergent if

$$3 e^{-2\beta J} < 1$$

can identify the critical temperature as

$$\sum_b \left(\frac{b}{4}\right)^2 e^{-2\beta_c b J} 3^{b-1} = 1/2$$

$\rightarrow$ ~~wen~~ for $T < T_c$ $\quad \beta > \beta_c$

$$\frac{\langle N_- \rangle}{N} \leq 1/2 \Rightarrow \boxed{M > 0}$$

finite magnetisation for $D = 2$

Lee-Yang theorem

modify Hamiltonian as

$$H' = -J\sum_{\langle i,j\rangle} S_i S_j - \mu B \sum_i (S_i - 1) = H_0 - \mu B \sum_i (S_i - 1)$$

let $z = e^{-2\beta\mu B}$

$$Z_N = \sum_C e^{-\beta H_0[S_i]} \prod_{i=1} e^{\beta\mu B(S_i - 1)}$$

$$\sum_i (S_i - 1) = -2n \qquad n = \text{number of down-spins}$$

$$Z_N = \sum_{n=0}^{N} z^n Q_n$$

Z_N - <u>analytic</u> function of z for <u>finite N</u>

finite N $\Rightarrow$ Z_N and all thermodynamic function are analytic

$\Downarrow$

phase transition can only occur in the thermodynamic limit

Lee Yang theorem states $Z = \lim_{N\to\infty} (Z_N)^{1/N}$

<u>Z may vanish only if $|z| = 1$</u>

$\Rightarrow$ only if $B = 0$

this can be calculated explicitly for many models for example 2D Ising