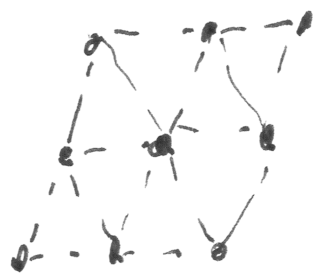
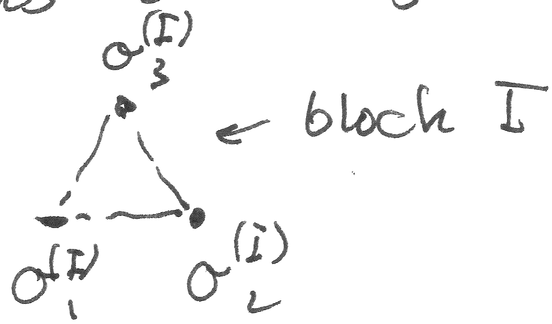
RG application: triangular lattice ①

Hamiltonian: $H = -K \sum_{\langle ij \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i$



blocks → triangular



associate spin with block S_I

rule to determine S_I: majority rule

$\sigma_1^{(I)}$	$\sigma_2^{(I)}$	$\sigma_3^{(I)}$	→	S_I	$\sigma_1^{(I)}$	$\sigma_2^{(I)}$	$\sigma_3^{(I)}$	→	S_I
1	1	1	→	1	−1	−1	−1	→	−1
1	1	−1	→	1	−1	−1	1	→	−1
1	−1	+1	→	1	−1	1	−1	→	−1
−1	1	1	→	1	1	−1	−1	→	−1

* based on this blocking scheme it is possible to carry out an approximate renormalization calculation
* here it will be done up to 1^{st} order which is not a major improvement over mean-field theory → but the purpose is to demonstrate how to do calculation
* 2^{nd} order result → major improvement over MFT

Hamiltonians: ②

blocked $\Rightarrow$ $H' = -K' \sum_{\langle I,J \rangle} S_I S_J - B' \sum_I S_I$

(should have this form)

unblocked $\Rightarrow$ $H = -K \sum_{\langle i,j \rangle} \sigma_i \sigma_j - B \sum_i \sigma_i$

equate partition functions:

$$Z(K', B'; N/3) = Z(K, B; N)$$

$$\sum_{S_1} \cdots \sum_{S_{N/3}} \exp[-H'] = \sum_{\sigma_1} \cdots \sum_{\sigma_N} \exp[-H]$$

$$= \sum_{S_1} \cdots \sum_{S_{N/3}} \left[\sum^{S_1}_{\sigma_1^{(1)} \sigma_2^{(1)} \sigma_3^{(1)}} \cdots \sum^{S_N}_{\sigma_1^{(N/3)} \sigma_2^{(N/3)} \sigma_3^{(N/3)}} \exp[-H] \right]$$

$$\Downarrow$$

$$\exp[-H'] = \sum^{S_1}_{\sigma_1^{(1)} \sigma_2^{(1)} \sigma_3^{(1)}} \cdots \sum^{S_{N/3}}_{\sigma_1^{(N/3)} \sigma_2^{(N/3)} \sigma_3^{(N/3)}} \exp[-H]$$

or more specifically

$$\exp[-H'(S_1 \ldots S_{N/3})] = \sum^{S_1}_{\sigma_1^{(1)} \sigma_2^{(1)} \sigma_3^{(1)}} \cdots \sum^{S_{N/3}}_{\sigma_1^{(N/3)} \sigma_2^{(N/3)} \sigma_3^{(N/3)}} \exp[-H(\sigma_1 \ldots \sigma_N)]$$

function of blocked spins

on RHS blocked spins S_I fix possible configurations of unblocked spins for example: if $S_1 = +1$ then the sums $\sum_{\sigma_1^{(1)}}^{S_1} \sum_{\sigma_2^{(1)}}^{S_1} \sum_{\sigma_3^{(1)}}^{S_1}$ → are over configurations

$\{\sigma_1^{(1)}, \sigma_2^{(1)}, \sigma_3^{(1)}\} = \{1,1,1\}, \{1,1,-1\}, \{1,-1,1\}, \{-1,1,1\}$

- write unblocked Hamiltonian as

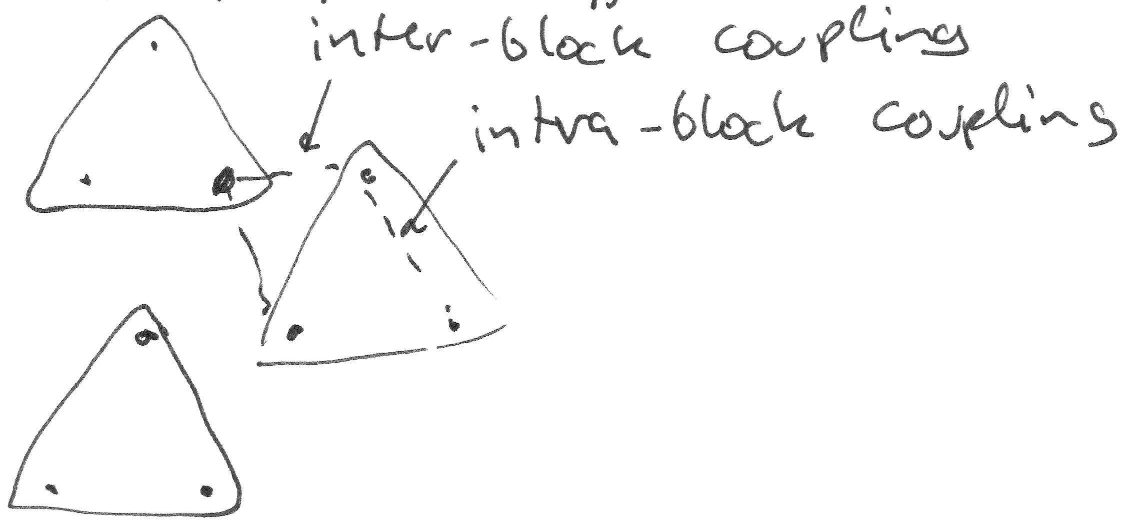
$$H(K, B; \sigma_1 \dots \sigma_\nu) = H_0 + V$$

H_0 → includes only <u>intra-block</u> couplings

V → includes only <u>inter-block</u> couplings + field term

$$H_0(K, B; \sigma_1 \dots \sigma_\nu) = -K \sum_{\langle i,j \rangle}^{(\text{intra})} \sigma_i \sigma_j$$

$$V(K, B; \sigma_1 \dots \sigma_\nu) = -K \sum_{\langle i,j \rangle}^{(\text{inter})} \sigma_i \sigma_j - B \sum_i \sigma_i$$



can write as

$$H_0 = -K \sum_I \sum_{i \in I} \sum_{j \in I} \sigma_i \sigma_j$$

$$V = -K \sum_I \sum_{i \in I} \sum_{\substack{J \\ I \neq J}} \sum_{j \in J} \sigma_i \sigma_j - B \sum_i \sigma_i$$

write partition function as 4

$$\cancel{\exp[K_0 + V]}$$

$$\exp[-H'(K', D'; S_1 \ldots S_{N/3})]$$

$$= \sum_{\sigma_1\sigma_2\sigma_3}^{S_1} \cdots \sum_{\sigma_1\sigma_2\sigma_3}^{S_{N/3}} \underbrace{\exp[-H_0 - V]}_{\exp[-H_0]\exp[-V]}$$

can define $\exp[-H']$ in terms of expectation values $\Rightarrow$

$$\exp[-H'] = \left[\frac{\sum \ldots \sum \exp[-H_0 - V]}{\sum \ldots \sum \exp[-H_0]}\right]\left[\sum \ldots \sum \exp[-H_0]\right]$$

$$= \frac{\sum \ldots \sum \exp[-H_0 - V]}{\sum \ldots \sum \exp[-H_0]}\left[\sum \ldots \sum \exp[-H_0]\right]$$

$$= \langle \exp[-V] \rangle_{H_0} \left[\sum \ldots \sum \exp[-H_0]\right]$$

$$\left[\sum_{\sigma\sigma\sigma}^{S_1} \ldots \sum_{\sigma\sigma}^{S_{N/3}} \exp[-H_0]\right] \Rightarrow \left(\sum_{\sigma_1^{(1)}}^{S_1}\sum_{\sigma_2^{(1)}}^{S_1}\sum_{\sigma_3^{(1)}}^{S_1} \exp[-H_0]\right) \times$$

$$\times \ldots \times \left(\sum_{\sigma_1^{(N/3)}}^{S_{N/3}}\sum_{\sigma_2^{(N/3)}}^{S_{N/3}}\sum_{\sigma_3^{(N/3)}}^{S_{N/3}} \exp[-H_0]\right)$$

$\Uparrow$

independent contributions

evaluate: $S_1 = +1 \to$ 1 1 1, 1 1 -1, 1 -1 1, -1 1 1 $\Rightarrow \sum_{\sigma_1\sigma_2\sigma_3} \exp K(\sigma_1\sigma_2 + \sigma_1\sigma_3 + \sigma_2\sigma_3)$

$$= \exp(3K) + 3\exp(-K)$$

$S_1 = -1 \to$ -1 -1 -1, -1 -1 1, -1 1 -1 $\Rightarrow \exp(3K) + 3\exp(-K)$

$\rightarrow \Rightarrow \exp[-H'] = \langle \exp(-V) \rangle_{H_0} (Z_0(S))^{N/3}$

$$Z_0(S) = \sum_{\sigma_1}^{S} \sum_{\sigma_2}^{S} \sum_{\sigma_3}^{S} \exp[+K(\sigma_1\sigma_2 + \sigma_1\sigma_3 + \sigma_2\sigma_3)]$$

$\rightarrow S = +1$

$$Z_0(S) = \exp(3K) + 3\exp(-K)$$

(independent of S)

$\langle \exp(-V) \rangle_{H_0}$ → approximate this via cumulant expansion → here we stop at 1st order

⇓

$$\langle \exp(-V) \rangle_{H_0} = \exp(-\langle V \rangle_{H_0})$$

(other terms would be ⇒ $\langle \exp(-V) \rangle_{H_0} =$

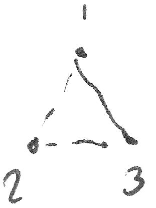
$$= \exp\left[-\langle V \rangle_{H_0} - \frac{1}{2}\left(\langle V^2 \rangle_{H_0} - \langle V \rangle_{H_0}^2\right)\right])$$

$$\langle \exp(-V) \rangle_{H_0} = \exp(-\langle V \rangle_{H_0})$$

need ⇒
$$\langle V \rangle_{H_0} = -K \sum_{\substack{i \in I \\ I \neq J}} \sum_{j \in J} \langle \sigma_i \rangle_I \langle \sigma_j \rangle_J - B \sum_I \sum_{i \in I} \langle \sigma_i \rangle_I$$

→ need $\langle \sigma_i \rangle_I$ →

$\langle \sigma_i \rangle_I \rightarrow$ average $\langle \sigma_i \rangle$ as a function of the spin S_I



$\rightarrow$ $\langle \sigma_1 \rangle$ under constraint $S_I = 1$

$S_I = 1 \Rightarrow$

σ_1	σ_2	σ_3
1	1	1
1	1	-1
1	-1	1
-1	1	1

$$\langle \sigma_1 \rangle_{S_I = 1} = \frac{e^{3K} + 2e^{-K} - e^{-K}}{e^{3K} + 3e^{-K}} = \frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}}$$

$$\langle \sigma_1 \rangle_{S_I = -1} = -\left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \right)$$

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in detail: $\sum_{\sigma_1} \sum_{\sigma_2} \sum_{\sigma_3} e^{+K(\sigma_1\sigma_2 + \sigma_1\sigma_3 + \sigma_2\sigma_3)} \sigma_1$

over configurations $S = 1 \Rightarrow 111, 11{-1}, 1{-1}1, {-1}11$

$$\Rightarrow e^{3K} + 2e^{-K} - e^{-K} \rightarrow e^{3K} + e^{-K}$$

for $S = -1$

average is over configurations

${-1}{-1}{-1}, {-1}{-1}1, {-1}1{-1}, 1{-1}{-1}$

$$-e^{3K} - 2e^{-K} + e^{-K} \rightarrow -e^{3K} - e^{-K}$$

$$\Rightarrow \boxed{\langle \sigma \rangle_S = \left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \right) S}$$

$$\langle V \rangle_{H_0} = -K \sum_{\substack{i\in I \\ I\neq J}} \sum_{j\in J} \langle \sigma_i \rangle_I \langle \sigma_j \rangle_J - B \sum_I \sum_{i\in I} \langle \sigma_i \rangle$$

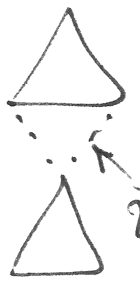
$$= -K \sum_{\substack{i\in I \\ I\neq J}} \sum_{j\in J} \left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \right)^2 S_I S_J$$

$$- B \sum_I \sum_{i\in I} \left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \right) S_I$$

two bonds between neighbour blocks

$$= -2K \left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \right)^2 \sum_I \sum_J S_I S_J$$

$$-3B \left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \right) \sum_I S_I$$



2 such bonds

So under the approximation scheme above:

$$H'[K', B'; S_1 \dots S_{N_3}] = -2K \left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \right)^2 \sum_{I,J} S_I S_J$$

$$-3B \left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \right) \sum_I S_J$$

$$= -K' \sum_{\langle I,J \rangle} S_I S_J - B' \sum_I S_I$$

$$\Rightarrow \boxed{\begin{aligned} K' &= 2K\left(\frac{e^{3K}+e^{-K}}{e^{3K}+3e^{-K}}\right)^2 \\ B' &= 3B\left(\frac{e^{3K}+e^{-K}}{e^{3K}+3e^{-K}}\right) \end{aligned}}$$

→ this is an example of a renormalisation group transformation

equation for fixed point $K = K'$, $B = B'$

$$\left(\frac{e^{3K^*}+e^{-K^*}}{e^{3K^*}+3e^{-K^*}}\right)^2 = \frac{1}{2} \Rightarrow (K^*, B^*) \text{ (critical fixed point)}$$

$$B^* = 0$$

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can construct matrix $\begin{pmatrix} \frac{\partial K'}{\partial K} & \frac{\partial K'}{\partial B} \\ \frac{\partial B'}{\partial K} & \frac{\partial B'}{\partial B} \end{pmatrix}$ at K^*, B^*

diagonalize $\Rightarrow \lambda_K, \lambda_B$ → obtain critical exponents

Eventually for the 1^{st} order approximation

$\alpha = -0.77 \quad \beta = 0.72 \quad \gamma = 0.83 \quad \delta = 2.2$

~~there are~~ better results obtained from higher-order approximations