The Potts model

"Spins" $\{\sigma_i\}_{1 \leq i \leq N}$ which can take q values ($\sigma_i \in [\![1,q]\!]$), interacting such that they tend to have the same value (Ising-like):

$$H = -\sum_{i,j=1}^{N} J_{ij}\,\delta_{\sigma_i,\sigma_j} - \sum_{i=1}^{N} h_{\sigma_i}$$

J_{ij}: Coupling constant between two spins, indep. of spin values

h_{σ_i}: "magnetic fields" $h_1, \dots, h_q$ acting on the q different values of a spin

Limiting cases, order parameter, connection to Ising model

1) For large T behavior, we except that the spins decouple ($k_B T \gg J_{ij}$) so effectively, $H \simeq -\sum_i h_{\sigma_i}$. If morever $k_B T \gg h$, then the spins are evenly distributed randomly in $[\![1,q]\!]$ ($\mathbb{P}[\sigma_i = \mu] = 1/q$).

2) Except if spins do not interact (graph of interactions J_{ij} not fully connected) a ground state must be when all spins are aligned ($\sigma_i = \mu\ \forall i$)

→ When all fields $h_\mu = 0$, there are q different ground states $\{\sigma_i = \mu\}_i$ for $\mu = 1, \dots, q$ (just as for the Ising model)

3) → When all fields $h_\mu \neq 0$ and are different, there is a single ground state $\{\sigma_i = \mu\}_i$, for $\mu = \operatorname{argmax}_\mu h_\mu$ (all spins align with the strongest field)

4) If only $h_1 > 0$ and other fields vanish, the ground state is $\{\sigma_i = 1\}_i$ so the ordered situations are when most spins are in state 1, and the disordered situations are when spins distribute evenly ($\mathbb{P}[\sigma_i = \mu] = 1/q$), i.e. when $1/q$ th of spins are in the state 1.

So $m = \dfrac{q\langle x\rangle - 1}{q-1}$ (where $\langle x\rangle$ is the mean fraction of spins in state 1)

goes from $m = 1$ in the ordered situation ($\langle x\rangle = 1$) to $m = 0$ in the disordered situation ($\langle x\rangle = 1/q$).

5) Link with the Ising model : for $q=2$

if we map $\sigma_i = 1 \longrightarrow \sigma_i^{(I)} = -1$, $\sigma_i^{(I)}$ is the usual Ising spin
$\sigma_i = 2 \longrightarrow \sigma_i^{(I)} = +1$

and $$2\delta_{\sigma_i\sigma_j} - 1 = \begin{Bmatrix} 1 \text{ if } \sigma_i = \sigma_j \\ -1 \text{ if } \sigma_i \neq \sigma_j \end{Bmatrix} = \sigma_i^{(I)} \cdot \sigma_j^{(I)}$$

so that $$\sum_{i,j=1}^{N} J_{ij}\,\delta_{\sigma_i\sigma_j} = \sum_{i,j=1}^{N} J_{ij}\,\frac{1+\sigma_i^{(I)}\sigma_j^{(I)}}{2} = cst + \sum_{i,j=1}^{N} J_{ij}^{(I)}\sigma_i^{(I)}\sigma_j^{(I)}$$
with $\boxed{J_{ij}^{(I)} = \frac{J_{ij}}{2}}$

and $$\frac{h_2+h_1}{2} + \frac{h_2-h_1}{2}\sigma_i^{(I)} = \begin{Bmatrix} h_2 \text{ if } \sigma_i^{(I)} = +1 \\ h_1 \text{ if } \sigma_i^{(I)} = -1 \end{Bmatrix} = h_{\sigma_i}$$

So that $$\sum_{i=1}^{N} h_{\sigma_i} = \underbrace{N\frac{h_2+h_1}{2}}_{cst} + h^{(I)}\sum_{i=1}^{N}\sigma_i^{(I)}$$ with $\boxed{h^{(I)} = \frac{h_2-h_1}{2}}$

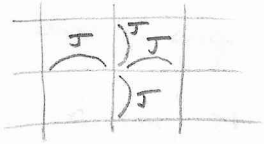
$$\Rightarrow H_{Potts}^{q=2}(\sigma_1,\dots,\sigma_N) = cst - \sum_{i,j=1}^{N} J_{ij}^{(I)}\sigma_i^{(I)}\sigma_j^{(I)} - h^{(I)}\sum_{i=1}^{N}\sigma_i^{(I)}$$ <u>Ising model</u>

6) Thus, for $q=2$, we expect (at the thermodynamic limit)

- a 2nd order phase transition if $h_1 = h_2$ and if the interactions J_{ij} does not form a 1D graph
- a 1st order phase transition if $h_1 \neq h_2$ and if not 1D
- no phase transition if the interactions form a 1D graph

The Curie-Weis approach

- on a cubic lattice of dimension d, with nearest neighbor interaction only



$d=2$

$$J_{ij} = \begin{cases} J \geq 0 & \text{with } i,j \text{ nearest neighbors} \\ 0 & \text{elsewhere} \end{cases}$$

7) A given spin has $2d$ neighbors (coordinance)

8) Case $J=0$, h_1 possibly $\neq h_2 = h_3 = \dots = h_q$:

$$H = -\sum_{i=1}^{N} h_{\sigma_i} = -\underbrace{N_1}_{\substack{\#\text{ spins such that}\\ \sigma_i = 1}} h_1 - h_2 \underbrace{(N - N_1)}_{\substack{\#\text{ of spins such}\\ \text{that } \sigma_i \neq 1}}$$

$N_1 = Nx$ with x the fractio[n] of spins in state 1

this hamiltonian is non-interacting so $Z = z^N$ with $z = \sum_{\sigma=1}^{q} e^{+\beta h_\sigma}$ the one-particle partition function

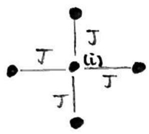
and $\langle N_1 \rangle = N \langle x \rangle_1$ so $\langle x \rangle = \langle x \rangle_1$

one-spin system

$$= \frac{1}{z} \sum_{\sigma=1}^{q} \delta_{\sigma,1} e^{+\beta h_\sigma} = \frac{1}{z} e^{+\beta h_1}$$

now, $z = \sum_{\sigma=1}^{q} e^{+\beta h_\sigma} = e^{+\beta h_1} + (q-1) e^{+\beta h_2}$ so $\boxed{\langle x \rangle = \dfrac{e^{\beta h_1}}{e^{\beta h_1} + (q-1) e^{\beta h_2}}}$ (3)

9) Now, in the $J \neq 0$ case, we will re-express the interactions in such a way that it looks like an external field $h_\mu^{(i)}$ acting on each spin σ_i



$\longrightarrow$ $\bullet^{(i)}$ in a $\underbrace{\text{field } h_\mu^{(i)} \text{ which depends on } \sigma_j \text{ neighbors}}$

called the molecular field because it is "created by its neighbors"

In the Curie-Weiss spirit / mean-field approach,

$h_\mu^{(i)}$ is replaced by its mean $h_\mu^{\text{Weiss}} = \langle h_\mu^{(i)} \rangle$ independant of the spin, so the hamiltonian becomes effectively non-interacting

10) $$H = -J \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j} \quad (\text{nearest neighbors, } h_\mu = 0 \ \forall \mu)$$

$$= -J \sum_{i=1}^{N} \sum_{j \in \text{Nbr}(i)} \delta_{\sigma_i, \sigma_j} \qquad \text{Nbr}(i) \text{ neighbors of } i$$

$$= -\sum_{i=1}^{N} h_{\sigma_i}^{(i)} \quad \text{with} \quad h_\mu^{(i)} = \sum_{j \in \text{Nbr}(i)} J \delta_{\sigma_j, \mu}$$

$\mathbb{P}[\sigma_j = 1] = \langle x \rangle$ by homogeneity

Now, $\boxed{H_{\text{Weiss}} = -J \sum_{i=1}^{N} h_{\sigma_i}^{\text{Weiss}}}$ with $h_1^{\text{Weiss}} = \left\langle \sum_{j \in \text{Nbr}(i)} J \delta_{\sigma_j 1} \right\rangle = J \underbrace{\sum_{j \in \text{Nbr}(i)}}_{=2d} \underbrace{\langle \delta_{\sigma_j 1} \rangle}_{=\langle x \rangle}$

$= 2dJ \langle x \rangle$

and $h_{\mu \neq 1}^{\text{Weiss}} = \left\langle \sum_{j \in \text{Nbr}} J \delta_{\sigma_j \mu} \right\rangle = J \sum_{j \in \text{Nbr}(i)} \langle \delta_{\sigma_j \mu} \rangle$ $\Rightarrow \boxed{h_1^{\text{Weiss}} = 2dJ \langle x \rangle}$

Preuve complète sans utiliser la séparabilité :

$$H = \overbrace{(h_2 - h_1)}^{\delta h} N_1 - N h_2 \qquad N_1 = \sum_{i=1}^{N} \delta_{\sigma_i = 1}$$

donc $$Z = \sum_{(\sigma_i)_{1\leq i\leq N}} e^{-\beta H} = e^{+\beta N h_2} \underbrace{\sum_{(\sigma_i)_{1\leq i\leq N} \in [\![1,q]\!]^N} e^{-\beta \delta h N_1}}$$

$$= \sum_{(\sigma_i)_i} \prod_{i=1}^{N} e^{-\beta \delta h \delta_{\sigma_i=1}} = \prod_{i=1}^{N} \underbrace{\sum_{\sigma=1}^{q} e^{-\beta \delta h \delta_{\sigma=1}}}_{= 1\cdot(q-1) + e^{-\beta\delta h}}$$

$$= \left(e^{-\beta \delta h} + (q-1)\right)^N$$

$$\frac{1}{Z}\frac{\partial Z}{\partial \delta h} = \frac{1}{Z} e^{\beta N h_2} \sum_{(\sigma_i)_i} -\beta N_1 e^{-\beta \delta h N_1}$$

$$= -\beta \langle N_1 \rangle$$

$$\Downarrow$$

$$\left\langle \frac{N_1}{N} \right\rangle = \frac{-1}{\beta N} \frac{\partial \ln Z}{\partial \delta h}$$

ou encore $$\sum_{(\sigma_i)_i} e^{-\beta \delta h N_1} = \sum_{N_1 = 1}^{N} \underbrace{\sum_{\substack{(\sigma_i)_i \text{ tq} \\ N_1((\sigma_i)_i) = N_1}} e^{-\beta \delta h N_1}}$$

$$= \sum_{N_1=1}^{N} \binom{N_1}{N} e^{-\beta \delta h N_1} (q-1)^{N-N_1}$$

- $N_1 = 0$: $(q-1)^N$ possibilités
- $N_1 = 1$: $N(q-1)^{N-1}$
- $N_2 = 2$: $\frac{N(N-1)}{2}(q-1)^{N-2}$

$\vdots$

$$= \binom{N_1}{N} (q-1)^{N-N_1} \, p$$

$$= \left(e^{-\beta \delta h} + q - 1\right)^N \checkmark$$

$$\Downarrow$$

$$\ln Z = N \ln\left(e^{-\beta \delta h} + q - 1\right)$$

$$\Downarrow$$

$$-\beta N \left\langle \frac{N_1}{N} \right\rangle = \frac{\partial \ln Z}{\partial \delta h} = N \frac{\partial \ln(\ldots)}{\partial \delta h} = N \frac{\frac{\partial}{\partial \delta h} e^{-\beta \delta h}}{e^{-\beta \delta h} + q - 1} = -\beta N \frac{e^{-\beta \delta h}}{e^{-\beta \delta h} + q - 1}$$

$$\Rightarrow \left\langle \frac{N_1}{N} \right\rangle = \frac{e^{-\beta \delta h}}{e^{-\beta \delta h} + q - 1} = \frac{e^{-\beta h_2} e^{\beta h_1}}{e^{-\beta h_2} e^{\beta h_1} + q - 1} = \frac{e^{\beta h_1}}{e^{\beta h_1} + (q-1) e^{\beta h_2}}$$

Now, to express $h^{\text{Weiss}}_{\mu\neq 1}$ as a function of $\langle x\rangle$ only, we make the approximation

$$\langle \delta_{\sigma_j=\mu}\rangle = \mathbb{P}[\sigma_j=\mu] \approx \frac{\mathbb{P}[\sigma_j\neq 1]}{q-1} \quad \text{(equiprobability among } \sigma\neq 1 \text{ spins)}$$

$$\underset{\text{homogeneity}}{=} \frac{1-\langle x\rangle}{q-1} \Rightarrow \boxed{h^{\text{Weiss}}_{\mu\neq 1} = 2dJ\,\frac{1-\langle x\rangle}{q-1}}$$

(only valid if spins of value $\sigma=1$ dominates over all other values)

11) Now, we are in the case of q8) with $H \to H_{\text{Weiss}}$
$h_\mu \to h^{\text{Weiss}}_\mu$

So we use (3) :

$$\langle x\rangle_{\text{Weiss}} = \frac{1}{1+(q-1)e^{\beta(h_2^{\text{Weiss}}-h_1^{\text{Weiss}})}} = \frac{1}{1+(q-1)\,e^{2dJ\beta(1-q\langle x\rangle)/(q-1)}}$$

$\parallel$

$\langle x\rangle$

mean field
<u>Self-consistency</u>

$$\underbrace{h_2^{\text{Weiss}}-h_1^{\text{Weiss}}}_{=2dJ\left(\frac{1-\langle x\rangle}{q-1}-\langle x\rangle\right) = 2dJ\,\frac{1-q\langle x\rangle}{q-1}} < 0 \text{ if } \langle x\rangle > \frac{1}{q}$$

12) $$\langle x\rangle\big|_{\text{disordered}} = \langle x\rangle_{\beta=0} = \frac{1}{1+q-1} = \frac{1}{q} \quad \text{as expected}$$

(and $\frac{1-q\langle x\rangle}{q-1} = 0$ reassuringly)

$$\langle x\rangle_{\beta=\infty} = \frac{1}{1+(q-1)e^{-\infty}} = 1 \quad \text{as expected}$$

So if we write $\left[\, m = \frac{\langle x\rangle - \langle x\rangle_{\text{disor}}}{\langle x\rangle_{\beta=\infty} - \langle x\rangle_{\text{disor}}}\right.$ such that $\begin{cases} m=0 & \text{if disordered} \\ m=1 & \text{if ordered}\end{cases}$

$$= \frac{\langle x\rangle - 1/q}{1-1/q} = \boxed{\frac{q\langle x\rangle - 1}{q-1}} \quad \text{(just like q4)}$$

then $$\langle x\rangle = \frac{1}{1+(q-1)e^{2dJ\beta(-m)}}$$

$$\Rightarrow m = \frac{\frac{q}{1+(q-1)e^{\cdots}}-1}{q-1} = \frac{1}{q-1}\,\frac{q-(1+(q-1)e^{\cdots})}{1+(q-1)e^{\cdots}} = \frac{1-e^{-2dJ\beta m}}{1+(q-1)e^{-2dJ\beta m}}$$

$$\Rightarrow \boxed{m = \frac{e^{2dJ\beta m}-1}{e^{2dJ\beta m}+q-1}} \quad \text{Self-consistency equation (4)}$$

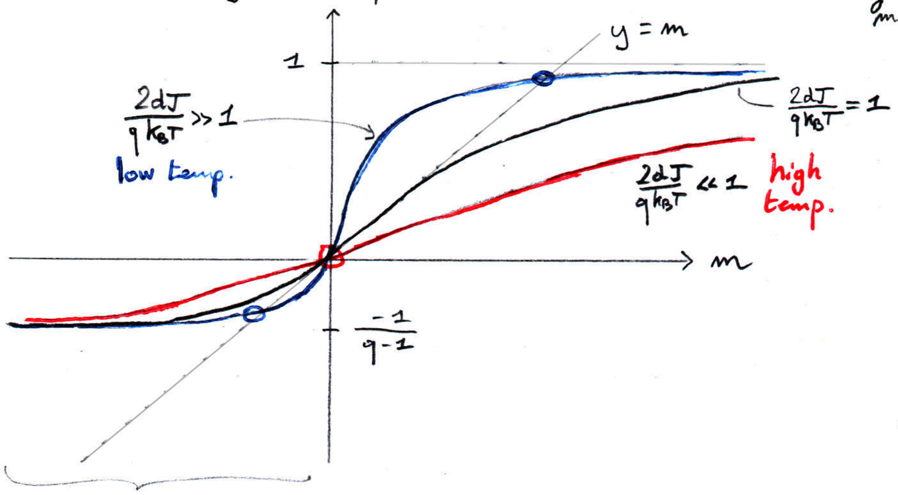
13) $y = \frac{e^{Km}-1}{e^{Km}+q-1}$ with $K = \frac{2dJ}{k_BT}$

$$\partial_m y = \frac{Ke^{Km}(e^{Km}+q-1) - Ke^{Km}(e^{Km}-1)}{(e^{Km}+q-1)^2} = \frac{qKe^{Km}}{(e^{Km}+q-1)^2}$$

$\Downarrow$

$$\partial_m y\big|_{m=0} = \frac{qK}{q^2} = \frac{2dJ}{qk_BT}$$

tangent at the origin



not realistic because our assumption "$\sigma = 1$" dominates is not valid here

$\Rightarrow$ we restrict to $m \geq 0$

$\Rightarrow$ @ high temp $k_BT \gg \frac{2dJ}{q}$, the only solution is $m = 0$

$\longrightarrow$ disordered

@ low temp $k_BT < \frac{2dJ}{q}$, there are 3 solutions, including $m > 0$

$\longrightarrow$ probably ordered

14) Taylor expansion :

$$m = \underbrace{y(0)}_{=0} + m \cdot \underbrace{\partial_m y(0)}_{=\frac{2dJ}{qk_BT}} + m^2 \underbrace{\frac{\partial_m^2 y(0)}{2}}_{=\frac{q^2K^2(q-2)}{2q^4} = \frac{1}{2}\left(\frac{K}{q}\right)^2(q-2)} + \mathcal{C}_3 m^3 + \mathcal{O}(m^4)$$

$$\Rightarrow \boxed{m = \frac{T^*}{T} m + \mathcal{C}_2 (q-2) m^2 + \mathcal{C}_3 m^3 + \mathcal{O}(m^4) \quad \text{with } k_BT^* = \frac{2dJ}{q} \text{ and } \mathcal{C}_2 = \frac{1}{2}\left(\frac{2dJ}{qk_BT}\right)^2}$$

15) $\hookrightarrow \quad 0 = \overbrace{\left(1 - \frac{T^*}{T}\right)}^{\simeq \frac{T-T^*}{T^*}} m - \mathcal{C}_2 (q-2) m^2 - \mathcal{C}_3 m^3 + \mathcal{O}(m^4)$

If we have a Landau free energy

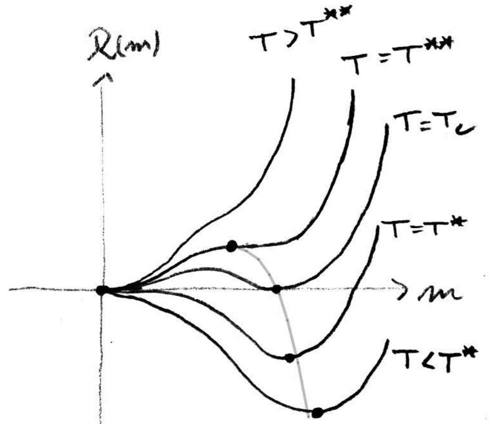
$$\mathcal{R}(m) = \frac{a_2}{2} m^2 + \frac{a_3}{3} m^3 + \frac{a_4}{4} m^4 + \mathcal{O}(m^5)$$

then m should be a minimum of $\mathcal{R}$, i.e. $\frac{\partial \mathcal{R}}{\partial m} = 0$

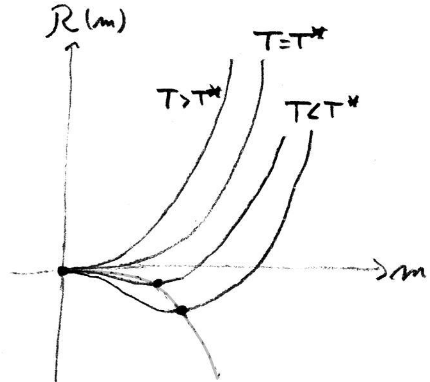
$$\Leftrightarrow \quad 0 = a_2 m + a_3 m^2 + a_4 m^3 + \mathcal{O}(m^4)$$

$$\begin{cases} a_2 = 1 - \frac{T^*}{T} \underset{T \simeq T^*}{\simeq} \frac{1}{T^*}(T - T^*) \\ a_3 = -\mathcal{C}_2 \cdot (q-2) \\ a_4 = -\mathcal{C}_3 \end{cases}$$

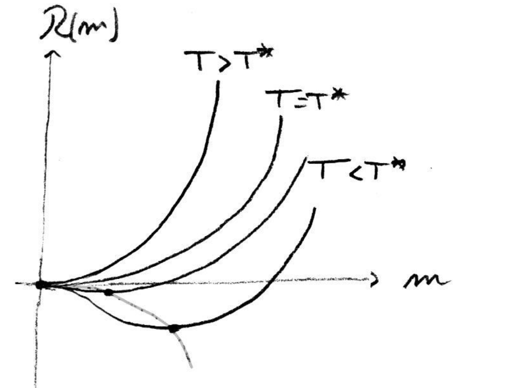
16)



$a_3 < 0 \iff \boxed{q>2}$

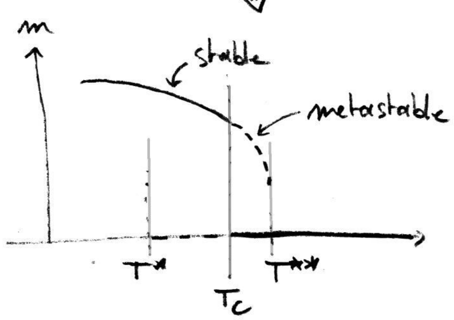


$a_3 = 0 \iff \boxed{q=2}$
(Ising)



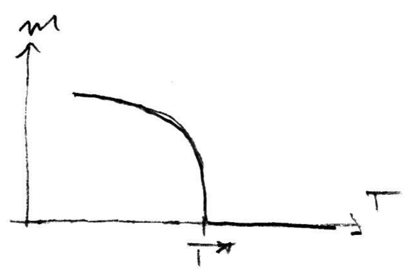
$a_3 > 0 \iff \boxed{q<2}$

$\Downarrow$



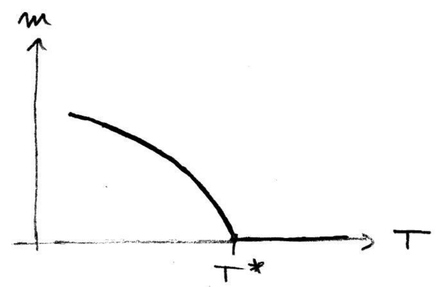
m is discontinuous at T_c
$\Rightarrow$ 1st-order phase transition

$\Downarrow$



2nd-order phase transition at T^*

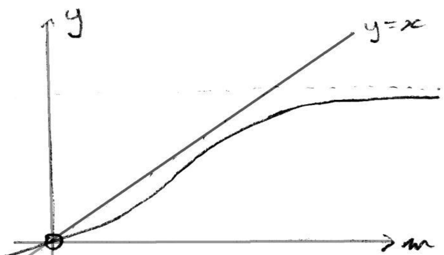
$\Downarrow$



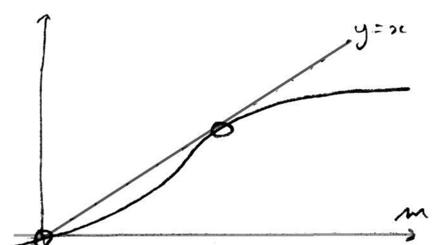
2nd-order phase transition at T^*

17) Consistent with the Ising model only for $q=2$ (without magnetic field)

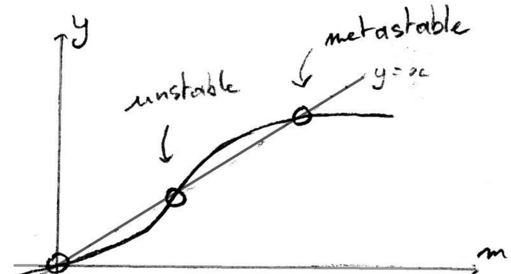
For $q>2$, the 1st order of the phase transition is consistent with the fact that the self-consistent graph looks like



$T > T^{**}$



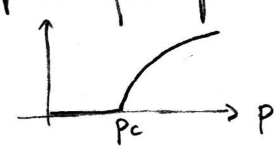
$T = T^{**}$



$T < T^{**}$

(fig. 1: $\frac{2dJ}{k_B T^{**}} \simeq 4.22$ for $q=8$)

18) If we accept that the Potts model can be "continualized" to real q, and that the limit $q \to 1$ describes percolation,
we expect for percolation a 2nd-order phase transition which looks like



(finite derivative at p_c), which is indeed the case.

The 1D setting : transfer matrix and renormalization

↳ N spins on a chain with periodic boundary conditions ($\sigma_1 = \sigma_{N+1}$) :

$$H = -J \sum_{i=1}^{N} \delta_{\sigma_i, \sigma_{i+1}}$$

19) $$Z = \sum_{(\sigma_i)_{1\le i\le N} \in [\![1,q]\!]^N} e^{-\beta H(\sigma_i)_i} = \sum_{(\sigma_i)_{1\le i\le N}} \exp\left(\beta J \sum_{i=1}^{N} \delta_{\sigma_i \sigma_{i+1}}\right)$$

20) $$= \sum_{(\sigma_i)_{1\le i\le N}} \prod_{i=1}^{N} \underbrace{e^{\beta J \delta_{\sigma_i, \sigma_{i+1}}}}_{=: T_{\sigma_i, \sigma_{i+1}}}$$ with $\boxed{T_{\sigma\mu} = e^{\beta J \delta_{\sigma\mu}}}$ $q\times q$ transfer matrix

$$= \sum_{1\le\sigma_1\le q} \sum_{1\le\sigma_2\le q} \sum_{1\le\sigma_3\le q} \cdots \sum_{1\le\sigma_N\le q} T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3} T_{\sigma_3\sigma_4} \cdots T_{\sigma_N\sigma_1}$$

$= T^2_{\sigma_1\sigma_3}$ (def° of matrix mul)

do the same for σ_3, then σ_4 ... all the way up to N

$$= \circ\circ\circ = \sum_{1\le\sigma_1\le q} T^N_{\sigma_1\sigma_1} = \operatorname{tr}(T^N) \Rightarrow \boxed{Z = \operatorname{tr}(T^N)}$$

using periodic boundary conditions

21) For $q=3$, the transfer matrix reads

$$T = \begin{bmatrix} e^{\beta J} & 1 & 1 \\ 1 & e^{\beta J} & 1 \\ 1 & 1 & e^{\beta J} \end{bmatrix}$$

which admits a simple eigenvector $v_+ = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$: $T v_+ = \begin{bmatrix} 2+e^{\beta J} \\ 2+e^{\beta J} \\ 2+e^{\beta J} \end{bmatrix} = (2+e^{\beta J}) v_+$

of eigenvalue $\boxed{\lambda_+ = 2 + e^{\beta J}} > 0$

Admitting the other eigenvalue λ_- is degenerate,

$$\operatorname{tr}(T) = 2\lambda_- + \lambda_+ = 2\lambda_- + 2 e^{\beta J} \iff \lambda_- + 1 = e^{\beta J} \iff \boxed{\lambda_- = e^{\beta J} - 1}$$

$\operatorname{tr}(T) = 3e^{\beta J}$

$< \lambda_+$

> 0

Associated eigenvectors : $v_{-,1} = \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix}$, $v_{-,2} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$

22) $$T^N = A \begin{bmatrix} \lambda_+ & & \\ & \lambda_- & \\ & & \lambda_- \end{bmatrix}^N A^{-1}$$ so $$Z = \operatorname{tr}(T^N) = \operatorname{tr}\left(\cancel{AA^{-1}} \begin{bmatrix} \lambda_+^N & & \\ & \lambda_-^N & \\ & & \lambda_-^N \end{bmatrix}\right) = \lambda_+^N + \lambda_-^N + \lambda_-^N$$

$$\Rightarrow \boxed{Z_{q=3} = (2+e^{\beta J})^N + 2(e^{\beta J}-1)^N}$$

Because $0 < \lambda_- < \lambda_+$, in the thermodynamic limit we have

$$Z \underset{N\to\infty}{\simeq} \lambda_+^N = (2+e^{\beta J})^N,$$ which is an analytic function of T,

so there is no phase transition in 1D

23) In this limit, the free energy reads $F = -\frac{1}{\beta}\ln Z \underset{N\to\infty}{\simeq} -\frac{N}{\beta}\ln(2+e^{\beta J})$

so the free energy per spin is $\boxed{f(\beta) = -\frac{1}{\beta}\ln(2+e^{\beta J})}$

24) For an arbitrary $q \in \mathbb{N}^+$, T is still a positive real matrix,
so by the Perron-Frobenius theorem, $\exists!\ \lambda_+$ unique largest eigenvalue,

thus $Z = tr(T^N) = \lambda_+^N + \sum \lambda^N$ strictly smaller eigenvalue

$$\underset{N\to\infty}{\simeq} \lambda_+^N \quad \Rightarrow \quad f(\beta) = -\frac{1}{\beta}\ln(\lambda_+(\beta))$$ analytic function of β

(clearly here $\lambda_+ = e^{\beta J} + q - 1$) $\Rightarrow$ no phase transition

Renormalization treatement :

we have $\sum_{1\leq\sigma'\leq q} e^{K\delta_{\sigma\sigma'} + K\delta_{\sigma'\sigma''}} = A e^{K'\delta_{\sigma\sigma''}}$ (8) with some A and K' depending on $K := \beta J$

$$e^{K'} = \frac{e^{2K}+q-1}{pe^K+q-2} \quad (10)$$
with some p

25) Thus, we can decimate every even-numbered spin :

$$Z = \sum_{\sigma_1,\sigma_3,\dots} \underbrace{\sum_{\sigma_2,\sigma_4,\dots} e^{K(\delta_{\sigma_1\sigma_2}+\delta_{\sigma_2\sigma_3})}}_{\text{apply (8)}} \underbrace{e^{K(\delta_{\sigma_3\sigma_4}+\delta_{\sigma_4\sigma_5})}}_{\text{apply (8)}} \dots$$

$$= \sum_{\sigma_1,\sigma_3,\dots} \overbrace{A e^{K'\delta_{\sigma_1\sigma_3}}}^{A^{N/2}}$$ which is the partition function of a 1D Potts chain with $N' = N/2$ spins and coupling constant K'

$$\Rightarrow \boxed{Z(N,a,K) = A^{N'} Z(N',b,K') \text{ with } N' = N/2,\ b = 2a} \quad (9)$$

26) We mapped the system onto the same system but dezoomed and with an other temperature given by K'. Thus, at infinite temperature $(K=0)$, it is clear that the dezoomed system is also at infinite temperature $(K'=0)$, and in this case (10) reads

$$e^0 = 1 = \frac{\cancel{e^0} + q \cancel{-1}}{p\cancel{e^0} + q - 2}, \text{ which can be true only if } \underline{p=2.} \quad (*)$$

i.e. $Z(K=0,N,a) = A^{N/2}\, Z(K=0, N/2, 2a)$ totally decoupled system

(can be easily checked explicitely : $Z(K=0,N) = q^N = q^{N/2}\, Z(K=0, N/2)$)

Fixed points $\underset{[0,+\infty]}{K^* \in}$: $e^{K^*} = \dfrac{e^{2K^*} + q - 1}{2e^{K^*} + q - 2} \iff x(2x+q-2) = x^2 + q - 1$ with $x = e^{K^*} \in [1, +\infty]$

$\iff$ $\boxed{K^* = \infty}$, which is unstable because for large K, $e^{K'} \simeq \dfrac{e^{2K}}{2e^K} = \dfrac{e^K}{2}$

So $K' < K$, so K decrease under renormalization

$x(2x+q-2) = x^2+q-1$ with $x = e^{K^*} > 1$

$\iff x^2 + (q-2)x - (q-1) = 0 \qquad \Delta = (q-2)^2 + 4(q-1) = q^2$

$\iff x = \dfrac{-q+2 \pm \sqrt{q^2}}{2} = \begin{cases} 1 \\ 1-q \leftarrow \text{impossible because } \leq 1 \end{cases}$

$\iff$ $\boxed{K^* = 0}$, which is stable because

$$\left| \frac{d}{dx} \frac{x^2+q-1}{2x+q-2} \right|_{x=1} = \left| \frac{2x^2 + 2x(q-2) - 2q - 2}{(2x+q-2)^2} \right|_{x=1} = 0 < 1$$

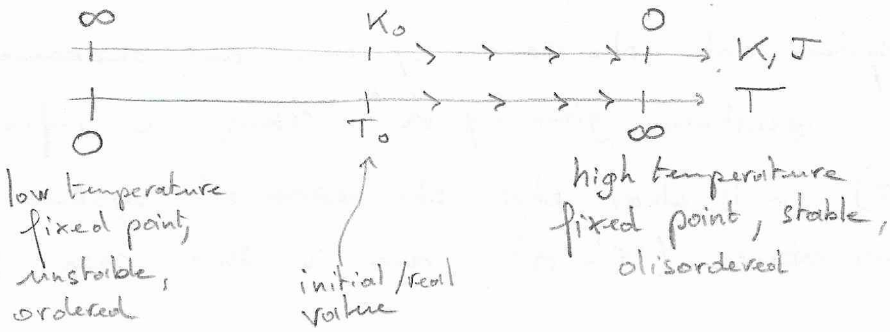
(*) Could also be derived directly from (8) :

- for $\sigma = 1, \sigma'' = 2$, $\displaystyle\sum_{\sigma'=1}^{q} \underbrace{e^{K\delta_{\sigma'1} + K\delta_{\sigma'2}}}_{\substack{= e^K \text{ if } \sigma' = 1,2 \\ = 1 \text{ else}}} = 2e^K + (q-2) = A e^{K'\delta_{12}} = A$

- for $\sigma = 1, \sigma'' = 1$, $\displaystyle\sum_{\sigma'=1}^{q} \underbrace{e^{K\delta_{\sigma'1} + K\delta_{\sigma'1}}}_{\substack{= e^{2K} \text{ if } \sigma' = 1 \\ = 1 \text{ else}}} = e^{2K} + (q-1) = A e^{K'\delta_{11}} = A e^{K'}$

$$\left.\begin{aligned} A &= 2e^K + q - 2 \\ e^{K'} &= \frac{e^{2K} + q - 1}{2e^K + q - 2} \end{aligned}\right\}$$

27)



When we re-normalize / dezoom, the system looks more and more like a disordered system, i.e. spins decorrelate at large distances, whatever its temperature (except for $T=0$ exactly)

28) There is no finite-T fixed point trough renormalization, so no scale invariance at finite temperature, so no finite-T critical point, so no phase transition in a 1D Potts model, as expected (cf. transition matrix treatement)

29) Computation of the correlation length $\xi(K)$:

if we define $\tilde{\xi} = \xi/a$ its dimensionless counterpart, we have after decimating half the spins, $\boxed{\tilde{\xi}(K') = \frac{\xi(K)}{b} = \frac{\xi(K)}{2a} = \frac{1}{2}\tilde{\xi}(K)}$

30)
$$\frac{e^{K'}+q-1}{e^{K'}-1} = \frac{\frac{e^{2K}+q-1}{2e^K+q-2}+q-1}{\frac{e^{2K}+q-1}{2e^K+q-2}-1} = \frac{e^{2K}+(q-1)(2e^K+q-1)}{e^{2K}\cancel{+q}-1-2e^K\cancel{-q}+2} \quad \begin{matrix} = (e^K+q-1)^2 \\ = (e^K-1)^2 \end{matrix}$$
$$= \left(\frac{e^K+q-1}{e^K-1}\right)^2$$

So $\boxed{f(K') = f(K)^2 \quad \text{if} \quad f(K) = \frac{e^K+q-1}{e^K-1} = 1 + \frac{q}{e^K-1}}$

$\Rightarrow$ if we write $\tilde{\xi}$ as a function of $x = \ln f(K)$, we have $x' = \ln f(K')$
$= \ln f^2(K) = 2x$

So $\tilde{\xi}(2x) = \tilde{\xi}(x') = \frac{1}{2}\tilde{\xi}(x)$

$\Leftrightarrow \tilde{\xi}^{-1}(2x) = 2\tilde{\xi}^{-1}(x)$, which is a well known functional equation of solution $\tilde{\xi}^{-1}(x) = cst \cdot x$

Thus $\tilde{\xi} \propto \frac{1}{x} = \frac{1}{\ln f(K)}$ $\Rightarrow$ $\boxed{\tilde{\xi}(K) \propto \frac{1}{\ln\left(1+\frac{q}{e^K-1}\right)}}$

For $q=2$, we get $f(K) = \frac{e^K+1}{e^K-1} = \frac{1}{\tanh(K/2)}$, so

$\tilde{\xi}(K) \propto \frac{-1}{\ln(\tanh(K/2))}$, which is exactly the result for the 1D Ising chain,

$\tilde{\xi}(K) \propto \frac{1}{\ln(\tanh K^{(I)})}$ with $K^{(I)} = \beta J^{(I)} = \beta \frac{J}{2} = K/2$

Mean-field analysis

⚠ Here, $E_{ground} = -\frac{J}{N} \cdot N^2 = -NJ$ while on a square grid, $E_{ground} = -\frac{zN}{2} J$ with pairs $\langle ij \rangle$ counted only once and $E_{ground} = -zNJ$ in section B (pairs counted twice)

31) We take $\boxed{J_{ij} = \frac{J}{N}}$ $\forall i,j$ $\longrightarrow$ a spin is coupled to every other spin in the system, but in a weak manner ($\propto 1/N \ll 1$).

This could model the fact that a spin may (weakly) influence an other spin at large distance, even if the interactions are local in reality. Moreover, because here a spin is only weakly coupled to its neighbors, fluctuations are drowned among the coupling to all other spins $\longrightarrow$ this approach has a "mean-field" flavor.

Let's rewrite the hamiltonian as a function of populations in spin values σ only:

$$H = -\frac{J}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \delta_{\sigma_i,\sigma_j} - \sum_{i=1}^{N} h_{\sigma_i}$$

$$= -\frac{J}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{\sigma=1}^{q} \delta_{\sigma\sigma_i} \delta_{\sigma\sigma_j} - \sum_{i=1}^{N} \sum_{\sigma=1}^{q} h_\sigma \delta_{\sigma\sigma_i}$$

$$= -\frac{J}{N} \sum_{\sigma=1}^{q} N_\sigma \cdot N_\sigma - \sum_{\sigma=1}^{q} h_\sigma N_\sigma$$ where $N_\sigma = \sum_{i=1}^{N} \delta_{\sigma\sigma_i}$ is the number of spins with value σ

$$= -NJ \sum_{\sigma=1}^{q} x_\sigma^2 - N \sum_{\sigma=1}^{q} h_\sigma x_\sigma$$ with $\boxed{x_\sigma = \frac{N_\sigma}{N} \text{ the fraction of spins with value } \sigma \in [\![1,q]\!]}$

x_σ can take values in $\frac{1}{N}[\![0,N]\!]$ $(0, \frac{1}{N}, \frac{2}{N}, \dots, 1)$ and are such that $\sum_\sigma x_\sigma = 1$

$$\Rightarrow \boxed{H(\sigma_i)_{1\le i\le N} = N e(x_1,\dots,x_q) \text{ with } e = -J\sum_{\sigma=1}^{q} x_\sigma^2 - \sum_{\sigma=1}^{q} h_\sigma x_\sigma}$$

one-spin hamiltonian

only depends on $x_1,\dots,x_q$

$$\Rightarrow \boxed{Z = \sum_{(\sigma_i)_{1\le i\le N} \in [\![1,q]\!]^N} e^{-\beta H} = \sum_{\substack{x_1,\dots,x_q \in \frac{1}{N}[\![0,N]\!] \\ \text{such that } \sum_\sigma x_\sigma = 1}} \mathcal{N}^{(N)}_{x_1,\dots,x_q} e^{-N\beta e(x_\sigma)}}$$

$\mathcal{N}^{(N)}_{x_1,\dots,x_q}$: number of configurations such that $\forall \sigma$, $N_\sigma(\sigma_i)_{1\le i\le N} = N x_\sigma$

Computation of the number of configurations with given $\{N_\sigma\}$:

- choose N_1 spins among N to have $\sigma = 1$ value : $\binom{N}{N_1}$ ways
- then choose N_2 spins among the $N - N_1$ remaining spins : $\binom{N-N_1}{N_2}$ ways
- ...

$$\Rightarrow \mathcal{N}^{(N)}_{x_1,\dots,x_q} = \binom{N}{N_1}\binom{N-N_1}{N_2}\binom{N-N_1-N_2}{N_3}\cdots\binom{\overbrace{0}^{= N - \sum_{\sigma=1}^{q} N_\sigma \text{ using the constraint}}}{N_q}$$

$$= \frac{N!}{N_1!\,\cancel{(N-N_1)!}}\cdot\frac{\cancel{(N-N_1)!}}{N_2!\,\cancel{(N-N_1-N_2)!}}\cdot\frac{\cancel{(N-N_1-N_2)!}}{N_3!\,(N-N_1-N_2-N_3)!}\cdots\frac{0!}{N_q!\,\cancel{0!}}$$

$$\boxed{\mathcal{N}^{(N)}_{x_1,\dots,x_q} = \frac{N!}{N_1!\,N_2!\cdots N_q!} = \binom{N}{N_1, N_2, \dots, N_q} \text{ multinomial coefficient}}$$

(we check that $\sum_{N_1+N_2+\dots+N_q=N} \binom{N}{N_1,\dots,N_q} = q^N$, the total number of configs)

32) Using Stirling's formula $n! \simeq e^{n(\ln n - 1)}\sqrt{2\pi n}$
in the thermodynamic limit we have

$$\mathcal{N}^{(N)}_{x_1,\dots,x_q} \underset{N\to\infty}{\simeq} C\, e^{N(\ln N - 1)} \prod_{\sigma=1}^{q} e^{-N_\sigma(\ln N_\sigma - 1)}$$

$$= C \exp\Big(\Big(\sum_\sigma N_\sigma\Big)(\cancel{\ln N}\cancel{-1}) - \sum_\sigma N_\sigma(\overbrace{\ln N_\sigma}^{=\ln N + \ln x_\sigma}\cancel{-1})\Big) = \exp\Big(-N\sum_\sigma x_\sigma \ln x_\sigma\Big)C$$

$$=: e^{N s(x_1,\dots,x_q)/k_B}\, \underbrace{C^{(N)}_{x_1,\dots,x_q}}_{\text{at most polynomial in } N}$$

thus
$$Z \simeq \sum_{x_1,\dots,x_q} C^{(N)}_{(x_\sigma)} e^{Ns/k_B} e^{-N\beta e}$$

$$= \sum_{x_1,\dots,x_q} C^{(N)}_{(x_\sigma)} e^{-N\beta(e - Ts)} \underset{N\gg 1}{\simeq} C^{(N)} \cdot e^{-N\beta \inf_{(x_\sigma)_\sigma}(e - Ts)}$$

only one term dominates in the sum, the one with smallest $e-Ts$

$$\Rightarrow \frac{1}{N}\ln Z \underset{N\gg 1}{\simeq} -\beta \inf_{\substack{(x_\sigma)_\sigma \in \frac{1}{N}[\![0,N]\!]^q \\ \text{s.t. } \sum x_\sigma = 1}} (e - Ts) + \frac{\ln C^{(N)}}{N} \xrightarrow[N\to\infty]{} -\beta \inf_{(x_\sigma)_\sigma \in \mathcal{D}_q} (e - Ts)$$

indep. of N — non-extensive term

$$\Rightarrow \boxed{f(\beta) = -\frac{1}{\beta}\lim_{N\to\infty}\frac{\ln Z}{N} = \inf_{(x_\sigma)_\sigma \in \mathcal{D}_q} \hat{f}(x_1,\dots,x_q,\beta)} \quad \text{where } \mathcal{D}_q = \left\{ (x_\sigma)_\sigma \in [0,1]^q \text{ such that } \sum_{\sigma=1}^{q} x_\sigma = 1 \right\}$$

with
$$\boxed{\hat{f}((x_\sigma)_\sigma, T) = e((x_\sigma)_\sigma) - T s((x_\sigma)_\sigma)} = \sum_{\sigma=1}^{q} \left(-J x_\sigma^2 - h_\sigma x_\sigma + k_B T x_\sigma \ln x_\sigma\right)$$

$s(x_1,\dots,x_q)$ is the Shannon entropy associated to the population distribution $(x_1,\dots,x_q)$

33) We could have found this free energy directly from the Bragg-Wiliams free energy

$$F_{BW} = \langle H \rangle_{\text{decoupled spins}} - TS$$

← Shannon entropy

More specifically, $\langle H \rangle_{decoupled} = \left\langle -\frac{J}{N}\sum_{i,j}\delta_{\sigma_i\sigma_j} - \sum_i h_{\sigma_i}\right\rangle_{decoupled}$

$$= -\frac{J}{N}\sum_{i,j}\langle\delta_{\sigma_i\sigma_j}\rangle_{decoupled} - \sum_i \langle h_{\sigma_i}\rangle_{decoupled}$$

$$= -\frac{J}{N}\sum_{i,j}\sum_{\mu=1}^{q}\underbrace{\langle\delta_{\sigma_i\mu}\delta_{\sigma_j\mu}\rangle_{decoupled}}_{\substack{=\langle\delta_{\sigma_i\mu}\rangle\langle\delta_{\sigma_j\mu}\rangle \\ = x_\mu\cdot x_\mu}} - \sum_i\sum_{\mu=1}^{q} h_\mu \underbrace{\langle\delta_{\sigma_i\mu}\rangle}_{=x_\mu}$$

$$\langle H\rangle_{decoupled} = N\cdot\sum_{\mu=1}^{q} -Jx_\mu^2 - h_\mu x_\mu$$

And $S/k_B = \sum_i S^{spin\, i}/k_B$ (independant spins $\Rightarrow$ entropy additivity)

$$= \sum_i\left(-\sum_{\mu=1}^{q}\mathbb{P}[\sigma_i=\mu]\ln\mathbb{P}[\sigma_i=\mu]\right) = -N\sum_{\mu=1}^{q}x_\mu\ln x_\mu$$

34) At <u>high temperatures</u>, entropy dominates : $\hat{f} = e - Ts \simeq -Ts$

so we must maximize entropy $s \propto -\sum_{\sigma=1}^{q}x_\sigma\ln x_\sigma$ on $\mathcal{D}_q$.

It is well known that then all x_σ's must be equal, and to respect the constraint $\mathcal{D}_q$, we must have

$\boxed{x_\sigma^*(T=\infty) = \frac{1}{q}}$ $\longrightarrow$ <u>disordered phase</u> $\left(m = \frac{q\langle x_1\rangle - 1}{q-1} = \frac{q/q - 1}{q-1} = 0\right)$

This can't be proven by usual variational minimization (including a Lagrange multiplier for the $\sum x_\sigma = 1$ constraint) because $[0,1]^q$ is <u>not an open domain</u> (we can have exteremums on the boundary, just like for q35).

By convexity of $x\ln x$, $\sum_{\sigma=1}^{q}\frac{1}{q}x_\sigma\ln x_\sigma \geq \left(\sum_\sigma\frac{x_\sigma}{q}\right)\ln\left(\sum_\sigma\frac{x_\sigma}{q}\right) \underset{\uparrow \\ \sum_\sigma x_\sigma = 1}{=} \frac{1}{q}\ln\frac{1}{q}$ (Jensen inequality)

but $x_\sigma^* = \frac{1}{q}$ gives indeed $\sum_{\sigma=1}^{q}\frac{1}{q}\cdot\frac{1}{q}\ln\frac{1}{q} = \frac{1}{q}\ln\frac{1}{q}$

So it is a minimum of $\sum_{\sigma=1}^{q}x_\sigma\ln x_\sigma$, so a maximum of entropy. (and it is unique)

35) If $h_\sigma = 0\ \forall\sigma$ and $J > 0$, at <u>vanishing temperature</u>,

$\hat{f} = e - \cancel{Ts}$ $\rightarrow$ the energy only has to be minimized

$= -J\sum_{\sigma=1}^{q}x_\sigma^2$ $\Rightarrow$ $\sum_{\sigma=1}^{q}x_\sigma^2$ has to be maximized

Now, $\boxed{\forall\mu\in[\![1,q]\!],\quad (x_\sigma^*)_\sigma = (\delta_{\sigma\mu})_\sigma} = (\text{—}0\text{—}, \overset{\mu}{1}, \text{—}0\text{—})$ is a maximum of

$\sum_{\sigma=1}^{q}x_\sigma^2$ because $\sum_{\sigma=1}^{q}x_\sigma^{*2} = \sum_{\sigma=1}^{q}\delta_{\sigma\mu} = 1$ and because $\sum_{\sigma=1}^{q}x_\sigma^2 \underset{x_\sigma\in[0,1]}{\leq} \sum_{\sigma=1}^{q}x_\sigma = 1$

And these are the only maxima. Indeed,

$$\begin{cases}\sum_\sigma x_\sigma^2 = 1\\ \sum_\sigma x_\sigma = 1\end{cases} \Rightarrow \sum_\sigma x_\sigma^2 = \sum_\sigma x_\sigma \Rightarrow \sum_\sigma \overbrace{x_\sigma}^{\geq 0}\overbrace{(x_\sigma - 1)}^{\geq 0} = 0 \Rightarrow \forall \sigma,\ \underline{x_\sigma^* = 0 \text{ or } 1}$$

$\Rightarrow$ The ground state is q-degenerate. (q "directions" for all spins to align).

↳ to study the low $T \leftrightarrow$ high T transition, we assume that the low T symmetry breaking occurs in the $\sigma = 1$ direction.

36) $\Rightarrow$ $x_1 = x$ and $x_2 = \cdots = x_q = \dfrac{1-x}{q-1}$ (we assume that there is no symmetry breaking between $\sigma = 2, \ldots, q$ directions)

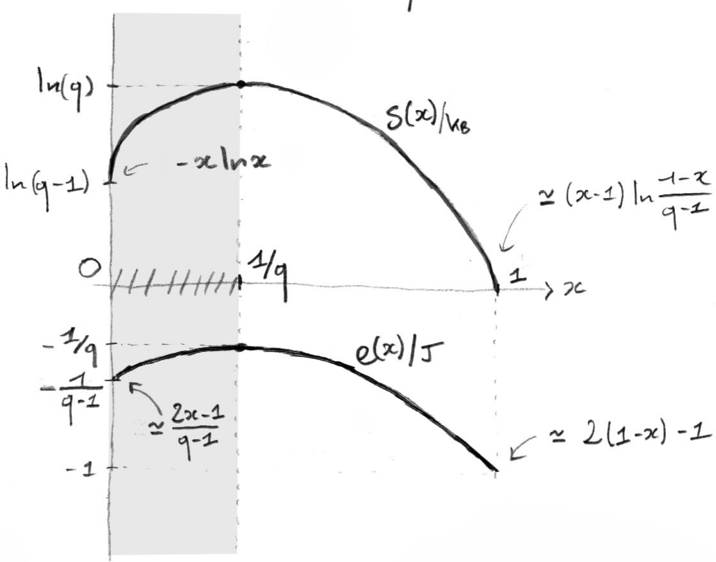
↳ $\sum_{\sigma=1}^{q} x_\sigma$ satisfied

Then,
$$\boxed{e(x) = \sum_{\sigma=1}^{q} -Jx_\sigma^2 \cancel{- h_\sigma x_\sigma}}$$
$$= -Jx^2 + (q-1)\left(-J\left(\frac{1-x}{q-1}\right)^2\right) = \boxed{-J\left(x^2 + \frac{(1-x)^2}{q-1}\right)}$$

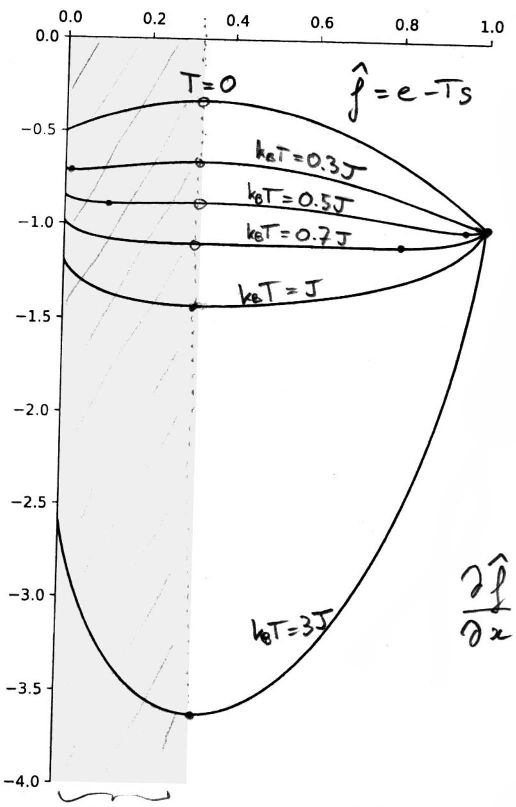
and
$$\boxed{\frac{S(x)}{k_B} = \sum_{\sigma=1}^{q} -x_\sigma \ln x_\sigma} = -x\ln x - (q-1)\frac{1-x}{q-1}\ln\frac{1-x}{q-1}$$
$$= \boxed{-x\ln x - (1-x)\ln\frac{1-x}{q-1}}$$

$$\Rightarrow f(T) = \inf_{x\in[0,1]} \underbrace{\left(e(x) - Ts(x)\right)}_{\hat{f}(x,T)}$$

37) Example for $q = 3$:



⇙



assumption "$\sigma=1$" dominates incorrect here ("$m<0$") $\Rightarrow$ we restrict to $x \geq 1/q$

38) Let's look for the local minima of $\hat{f}(x,T)$:

$$\frac{\partial \hat{f}}{\partial x} = -J\left(2x + \frac{-2}{q-1}(1-x)\right) + k_BT\left(\overbrace{\frac{\partial}{\partial x} x\ln x}^{= \ln x + 1} + \underbrace{\frac{\partial \overbrace{(1-x)}^{x'}}{\partial x}}_{=-1} \underbrace{\frac{\partial}{\partial x'} x' \ln\frac{x'}{q-1}}_{= \ln\frac{1-x}{q-1} + 1}\right)$$

$$= \frac{2J}{q-1}(1-qx) + k_BT\left(\ln x - \ln(1-x) + \ln(q-1)\right)$$

We see that $\boxed{x_0 = \frac{1}{q}}$ is always an extremum of $\hat{f}(x,T)$

because $\partial_x \hat{f}(x_0,T) = \frac{2J}{q-1}\left(\cancel{1-q\frac{1}{q}}\right) + k_B T\left(\ln\frac{1}{q} - \ln\underbrace{\left(1-\frac{1}{q}\right)}_{=\frac{q-1}{q}} + \ln(q-1)\right) = 0$

Moreover, this is the only one at high T:

$$\partial_x \hat{f}(x,T) \underset{k_BT \gg J}{\simeq} k_B T \ln\frac{(q-1)x}{1-x} = 0 \iff \frac{(q-1)x}{1-x} = 1 \iff (q\cancel{-1+1})x = 1 \iff x = \frac{1}{q}$$

To see when it is a minimum,

$$\partial_x^2 \hat{f}(x,T) = -\frac{2Jq}{q-1} + k_B T\left(\frac{1}{x} + \frac{1}{1-x}\right) = -\frac{2Jq}{q-1} + k_B T\frac{1}{x(1-x)} \quad (16)$$

and at x_0, $\partial_x^2 \hat{f}(x_0,T) = -\frac{2Jq}{q-1} + k_B T\frac{q^2}{q-1} \propto -2J + k_B T q > 0$

$\iff \boxed{k_B T q > 2J}$ where $x_0 = \frac{1}{q}$ is a local minimum

$$\boxed{k_B T_c^{(2)} = \frac{2J}{q}}$$

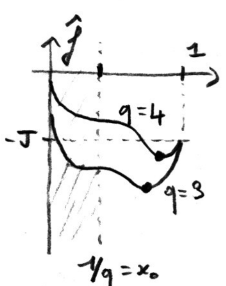
39) Expansion around $x = x_0$ @ $T_c^{(2)}$:

$$\hat{f}(x,T_c^{(2)}) \simeq \hat{f}(x_0,T_c^{(2)}) + (x-x_0)\underbrace{\partial_x \hat{f}(x_0,T_c^{(2)})}_{=0} + \frac{1}{2}(x-x_0)^2\partial_x^2 \hat{f}(x_0,T_c^{(2)}) + \frac{1}{6}(x-x_0)^3\partial_x^3 \hat{f}(x_0,T_c^{(2)})$$

$$= \underbrace{e(x_0) - T_c^{(2)} s(x_0)}_{-J\frac{1}{q} - \frac{2J}{q}\ln q = -\frac{J}{q}(1+2\ln q)} + \frac{1}{2}(x-x_0)^2 \underbrace{\left(-\frac{2Jq}{q-1} + \frac{2J}{q}\frac{q^2}{q-1}\right)}_{=0} + \frac{1}{6}(x-x_0)^3$$

$$\partial_x^3 \hat{f}(x_0,T_c^{(2)}) = k_B T_c^{(2)} \frac{2x_0 - 1}{x_0^2(1-x_0)^2} = \frac{2Jq^2(2-q)}{(q-1)^2}$$

$$\Rightarrow \boxed{\hat{f}(x,T_c^{(2)}) \underset{x=x_0}{\simeq} -\frac{J(1+2\ln q)}{q} + \underbrace{\frac{Jq^2(2-q)}{3(q-1)^2}}_{<0 \text{ for } q>2}(x-x_0)^3 + \mathcal{O}(x-x_0)^4}$$

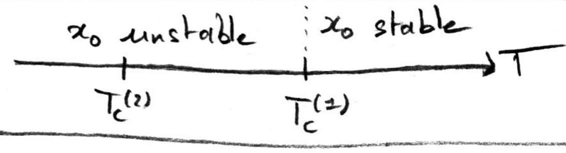


$\Downarrow$ necessarily, $\hat{f}(x,T_c^{(2)})$ decrease with $x > x_0$ so there exist an other (global) minimum

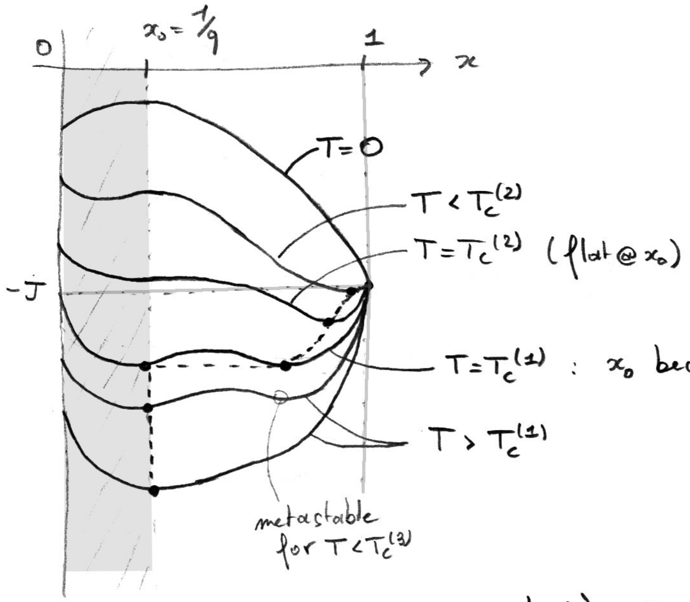
$\Rightarrow$ $x = x_0 = \frac{1}{q}$ is not stable @ $T_c^{(2)}$ with $q > 2$

But for $k_B T \gg J$, we know that $x = x_0$ is the global minimum,

so necessarily $\exists\, T_c^{(1)} > T_c^{(2)}$ such that



40)



: x_0 becomes global minimum $\Rightarrow$ phase transition (1st order)

41) Condition : $\boxed{\exists x^{(1)} \neq x_0 \; : \; \hat{f}(x_0, T_c^{(1)}) = \hat{f}(x^{(1)}, T_c^{(1)})}$

Looking at the curve on a computer, it is clear that

$\boxed{x^{(1)} = 1 - \frac{1}{q}}$ because the curve is symmetrical at $T_c^{(1)}$.

Then, it is just a matter of computing $\hat{f}(x^{(1)}, T) = -J\frac{(q-3)q-3}{q(q-1)} + \frac{k_B T}{q}\left(\ln\frac{1}{q(q-1)} + (q-1)\ln\frac{q-1}{q}\right)$

and equilizing with $\hat{f}(x_0, T) = -J\frac{1}{q} + k_B T \ln\frac{1}{q}$ and solving for T :

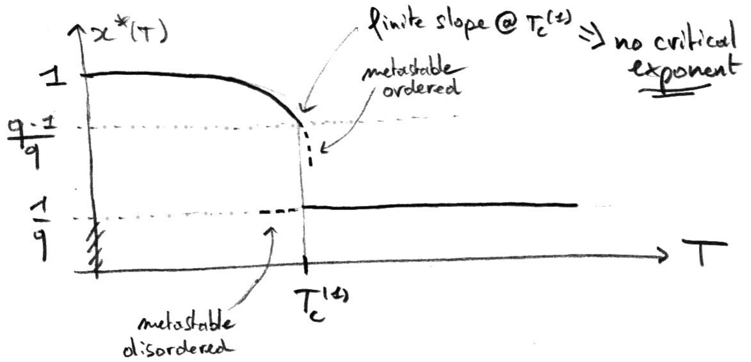
$$\frac{k_B T}{J} = \frac{(q-2)^2}{q-1} \frac{1}{\underbrace{\ln\frac{1}{q(q-1)} + (q-1)\ln\frac{q-1}{q} + q\ln q}_{= -2\ln(q-1) + q\ln(q-1) = (q-2)\ln(q-1)}} \Rightarrow \boxed{\frac{k_B T_c^{(1)}}{J} = \frac{q-2}{(q-1)\ln(q-1)}}$$

We indeed check that $x^{(1)} = 1 - \frac{1}{q} = \frac{q-1}{q}$ is a local extremum :

$$\partial_x \hat{f}(x^{(1)}, T_c^{(1)}) = \frac{2J}{q-1}\underbrace{\left(1 - \cancel{q}\frac{q-1}{\cancel{q}}\right)}_{= 2-q} + J\frac{q-2}{(q-1)\ln(q-1)}\underbrace{\left(\ln\frac{q-1}{\cancel{q}} - \ln\frac{1}{\cancel{q}} + \ln(q-1)\right)}_{= 2\ln(q-1)}$$

$$= \frac{2}{q-1}\left(2(2-q) + (q-2)\frac{2\cancel{\ln(q-1)}}{\cancel{\ln(q-1)}}\right) = 0 \; \checkmark$$

42) <u>For $q > 2$</u> : as shown above, $x^*(T)$ looks like

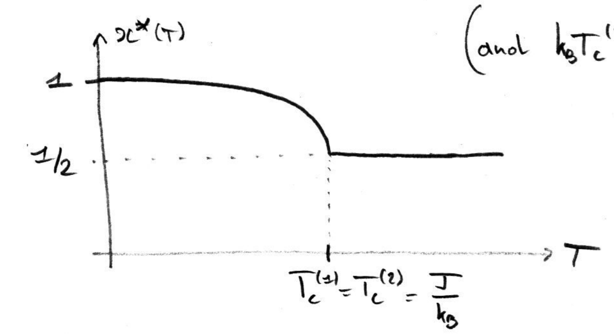


discontinuity in $x^*(T)$
$\Rightarrow$ <u>1st order phase transition</u>

Order parameter : as usual,

$m := \frac{q x^* - 1}{q - 1}$ goes from 0 (disordered, $x^* = x_0$) to 1 (ordered, $x^* = 1$)

For $q=2$ $\quad x_0 = x^{(1)} = \frac{1}{2}$ so there is no discontinuity of $x^*(T)$:



$\left(\text{and } k_B T_c^{(2)} = J \text{ and } k_B T_c^{(1)} = J \dfrac{q-2}{(q-1)\underbrace{\ln(q-1)}_{\simeq (q-1)-1 = q-2}} = J \text{ at } q=2 \right)$

$\Rightarrow$ 2nd order phase transition

$m = 2x^* - 1$

Critical exponent : it is Ising mean-field, so we expect $\boxed{\beta = \frac{1}{2}}$.

Let's derive it : $\tau := \frac{T - T_c}{T_c} \Leftrightarrow k_B T = J\cdot(1+\tau)$ so

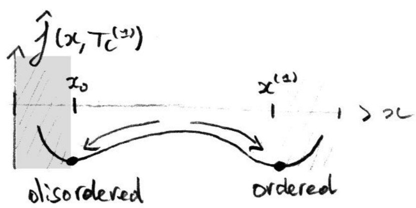
$$
\begin{aligned}
0 = \frac{\partial \hat{f}}{\partial x} &= -2J(1-2x) + J(1+\tau)\left(\ln x - \ln(1-x)\right) \\
&= J\cdot\left(-2m + (1+\tau)\left(\ln\frac{1+m}{2} - \ln\frac{1-m}{2}\right)\right) \\
&\underset{m\to 0}{\simeq} J\left(-2m + (1+\tau)\left(m - \cancel{\frac{m^2}{2}} + \frac{m^3}{3} - \left(-m - \cancel{\frac{m^2}{2}} - \frac{m^3}{3}\right)\right)\right) = 2mJ\tau + J(1+\tau)\frac{2}{3}m^3
\end{aligned}
$$

$$
\Leftrightarrow 2mJ\left(\tau + \underbrace{(1+\tau)}_{\simeq 1 \text{ near critical point}}\frac{m^2}{3}\right) = 0 \Leftrightarrow m = 0 \text{ or } \tau + \frac{m^2}{3} = 0
$$

$$
\Updownarrow
$$

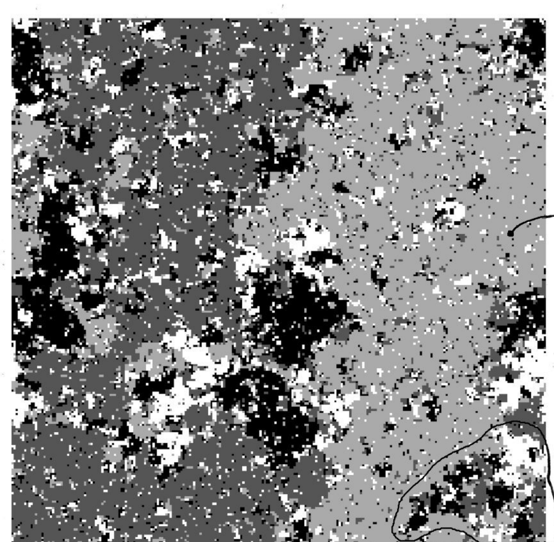
$$
m^2 = -3\tau \Leftrightarrow \boxed{m = \sqrt{-3\tau}} \Rightarrow \beta = \frac{1}{2}
$$

43) At $T = T_c^{(1)}$ (if we impose $\frac{1}{q} \leq x_1 \leq \frac{q-1}{q}$ so that $\sigma = 1$ is the chosen direction), the (Landau) free energy landscape looks like this :



$\Rightarrow$ the system will choose $x_* = x_0$ if $x_{\text{initial}} < \frac{1}{2}$ (mostly disordered)

and $x_* = x^{(1)}$ if $x_{\text{initial}} > \frac{1}{2}$ (mostly ordered).



MC simulation of the $q=4$ Potts model at T_c (exact)

Now for a real macroscopic system, there are fluctuations so that

- locally (or for a small system) the phase switches / fluctuates between x_0 and x_1
- if x_{initial} is close to $1/2$, there is the formation of "domains" $\rightarrow$ ordered zones ($x^{(1)}$) ; disordered zones with mixed values of spins (x_0)
- if we vary the temperature $\rightarrow$ hysteresis cycle with metastability

Some exact results

On a square lattice, we can map the Potts model onto itself :

$$\underbrace{Z(K) = Z(\tilde{K})}_{\text{"duality transformation"}} \left(\frac{1}{q} (e^K - 1)^2 \right)^N \quad \text{with} \quad (e^{\tilde{K}} - 1)(e^K - 1) = q \qquad (48)$$

$$(K = \beta J)$$

44) To look for a critical temperature, we look for finite fixed points of the map $K \mapsto \tilde{K}$:

$$(e^{K^*} - 1)(e^{K^*} - 1) = q \iff e^{K^*} - 1 = \pm\sqrt{q}$$

$$\iff e^{K^*} = 1 \pm \sqrt{q} \iff K^* = \ln(\underbrace{1 \pm \sqrt{q}}_{})$$

only defined for + when $q \geq 1$

$$\longrightarrow K^* = \ln(1 + q) \Rightarrow \boxed{k_B T_c = \frac{J}{\ln(1 + \sqrt{q})}}$$

For $q = 2$, we recover Onsager's exact solution $k_B T_c = \dfrac{J^{\text{Potts}}}{\ln(1+\sqrt{2})} = \dfrac{2 J^{\text{Ising}}}{\ln(1+\sqrt{2})}$.

45)
46) To study the properties of the critical point, we start from the critical line AB which is in the $\Delta = -\infty$ plane (Potts without vacancies). Upon renormalisation, we go out of the plane, and then

- if $q \leq 4$, we land on the EF critical line (stable fixed point), which is finite T and finite Δ : there are some vacancies (i.e. "disordered" domains) and thermal fluctuations

  $\Rightarrow$ it looks like the transition is continuous between the ordered and disordered phase $\Rightarrow$ <u>2nd order phase transition</u>

- if $q > 4$, we land at $T = 0$: the critical point looks ordered at large scale (no thermal fluctuations outside vacancies)

  $\Rightarrow$ it looks like the transition to the disordered phase will be dis<u>con</u>tinuous

  $\Rightarrow$ <u>1st order phase transition</u>

$q > 4$: the system looks ordered at large distance (one σ dominates) (and more and more with increasing q)

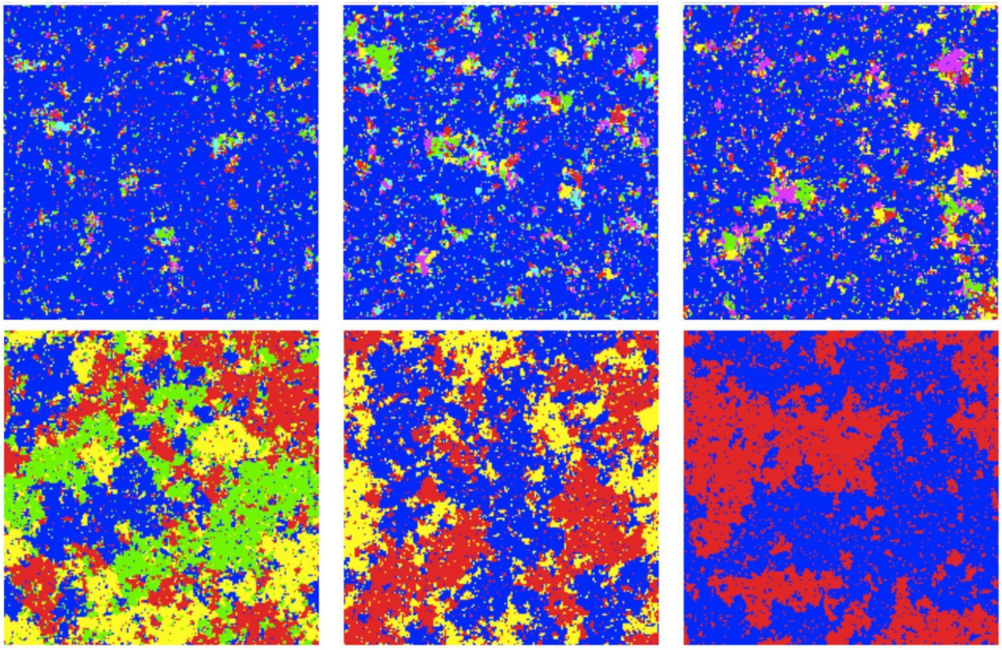
$\Rightarrow$ $T=0$ upon renormalization and the transition to the disordered phase will be discontinuous

($m \neq 0$ at T_c)

$q \leq 4$

each value of $\sigma \in [\![1,q]\!]$ is present at all scales

$\Rightarrow$ large scale fluctuations and $T \neq 0$ upon renormalization and we expect continuous behavior of m when crossing T_c ($m=0$ at T_c)



Simulations of the 2D Potts model with $q = 9, 6, 5$
at the critical temperature. $4, 3, 2$

$\Rightarrow$ $q=4$ is a critical value separating 1st and 2nd order phase transition behavior

which is not what the mean-field treatement predicted (1st order as soon as $q>2$)

$\downarrow$ again, mean field underestimates fluctuations so predicts too strong coupling.

47) Critical temperature in 2D :

$$\frac{k_B T_c^{MF}}{J} = 2\frac{q-2}{(q-1)\ln(q-1)} > \frac{1}{\ln(1+\sqrt{q})} = \frac{k_B T_c^{Exact}}{J}$$

$\Rightarrow$ mean-field overestimates critical temperature, as usual (overestimates coupling)

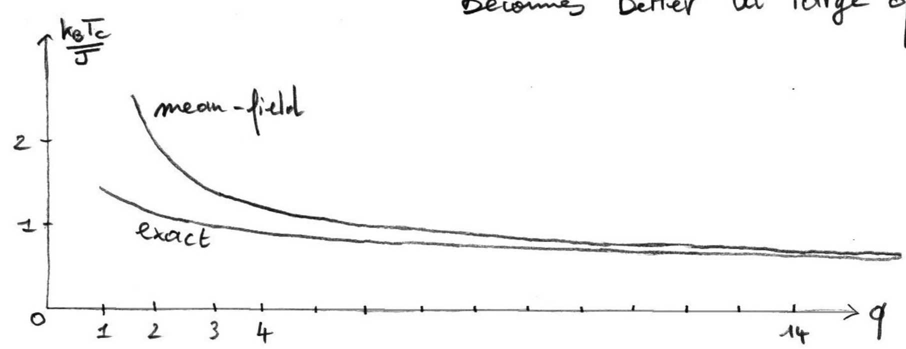
⚠ To compare critical temperatures, we must have the same J's :

- with $J\sum_{\langle i,j\rangle}$, $E_0 = -\frac{zN}{2}J = -2NJ$
- with $\frac{J'}{N}\sum_{i,j}$, $E_0 = -NJ'$

$J' = 2J$!

$\left(\text{in general } \frac{k_B T_c^{MF}}{J} = d\,\frac{q-2}{(q-1)\ln(q-1)}\right)$

both $\frac{k_B T_c}{J}$ tends to the same limit $\underset{q\to\infty}{\simeq} \frac{2}{\ln(q)}$, as expected (mean-field becomes better at large q)



48) We know that the upper critical dimension d_u is

- $d_u = 4$ for the Ising model $q=2$
- $d_u = 6$ when $q \to 1$ (percolation, well known)
- $d_u = 2$ for $q=4$ (litterature : cited review by F. Wu tel-00959733 p7)
- for $q=3$, mean-field is 1st order but in reality it is 2nd order in $d=2$ and 1st order in $d=3$ according to the litterature, so $d_u = 3$ maybe

q	1	2	3	≥ 4
d_u	6	4	3	2

But I fail to prove this.

- We could use the scaling relation $d\nu = 2-\alpha$, knowing $\nu = \frac{1}{2}$ and check for which dimension it works with $\alpha = \alpha_{\text{Mean-field}}$, but this gives always $d=4$ because $\alpha_{MF} = 0$ obviously.
- Ginzburg criterion : $E_G \propto k_B T \dfrac{\xi^{d-2}}{m_*^2}$ mean relative fluctuations in the sample at the critical point

  which should not diverge at $T=T_c$ for mean-field to be correct

$$E_G \underset{t}{\propto} \frac{(t^{\nu})^{d-2}}{t^{2\beta}} = t^{\nu(d-2)-2\beta} \quad \text{with } t = \frac{T-T_c}{T_c}$$

$$= \begin{cases} t^{\frac{d-4}{2}} \text{ for } q=2 \longrightarrow d_u = 4 \quad (\nu = \frac{1}{2}, \beta = \frac{1}{2} \text{ in mean field}) \\ t^{\frac{d-2}{2}} \text{ for } q>2 \longrightarrow \underline{d_u = 2} \quad (\nu = \frac{1}{2}, \beta = 0 \text{ in mean field}) \end{cases}$$

  which is wrong obviously for $q=3$.

- We could maybe compute corrections to mean-field due to fluctuations, or compute mean-field exponents and compare with the litterature for exact critical exponents.

refs: DOI 10.1103/PhysRevLett.48.1552 (main paper)
DOI 10.1063/1.5024027
Two dimensional cristals, Lyuksyutov, Naumovets, Pokrovsky, p178, p241

G. Application

The physisorption of Krypton atoms onto a graphite plane provides a possible realization of Potts model. In such a plane, carbon atoms are organized in a hexagonal structure, and Krypton preferentially adsorbs in the center of the hexagonal rings (shown by circles on figure 4-a)). For steric reasons, an adsorbed Krypton atom makes adsorption on nearest neighboring sites less likely, and we shall consider a 1/3 coverage (one site occupied on average out of three). In this case, a possible ground state is shown in Fig. 4-b). There thus exist three equivalent positions for the lattice of adsorbed Kr, and we admit that such a system can be described by a Potts model, where a site corresponds to a triplet of original adsorption sites (see figure 4-c)), and where the spin indicates which of the three original sites is occupied. We therefore exclude the possibility that Kr atoms desorb, which certainly happens at high T.

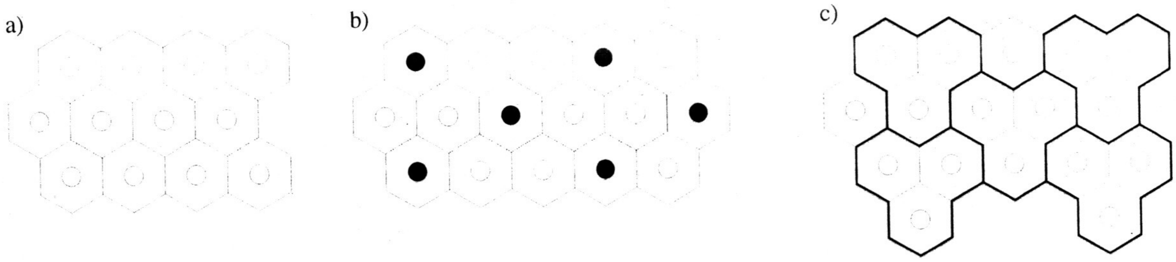
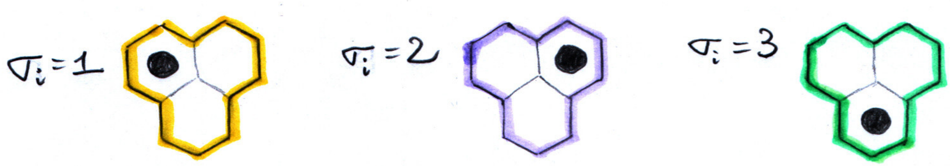


FIGURE 4 – a) Sketch of a graphite surface, where possible adsorption sites for Krypton atoms are represented by the circles. b) A possible ground state at filling fraction 1/3. The sites occupied by Krypton correspond to the black disks. c) Groups of triplets of adsorption sites, to define the sites considered in the Potts model (where a q-states spin lives). Five such groups are shown in panel c).

4g) The 1/3rd coverage adsorption is described by a $q=3$ state Potts model:



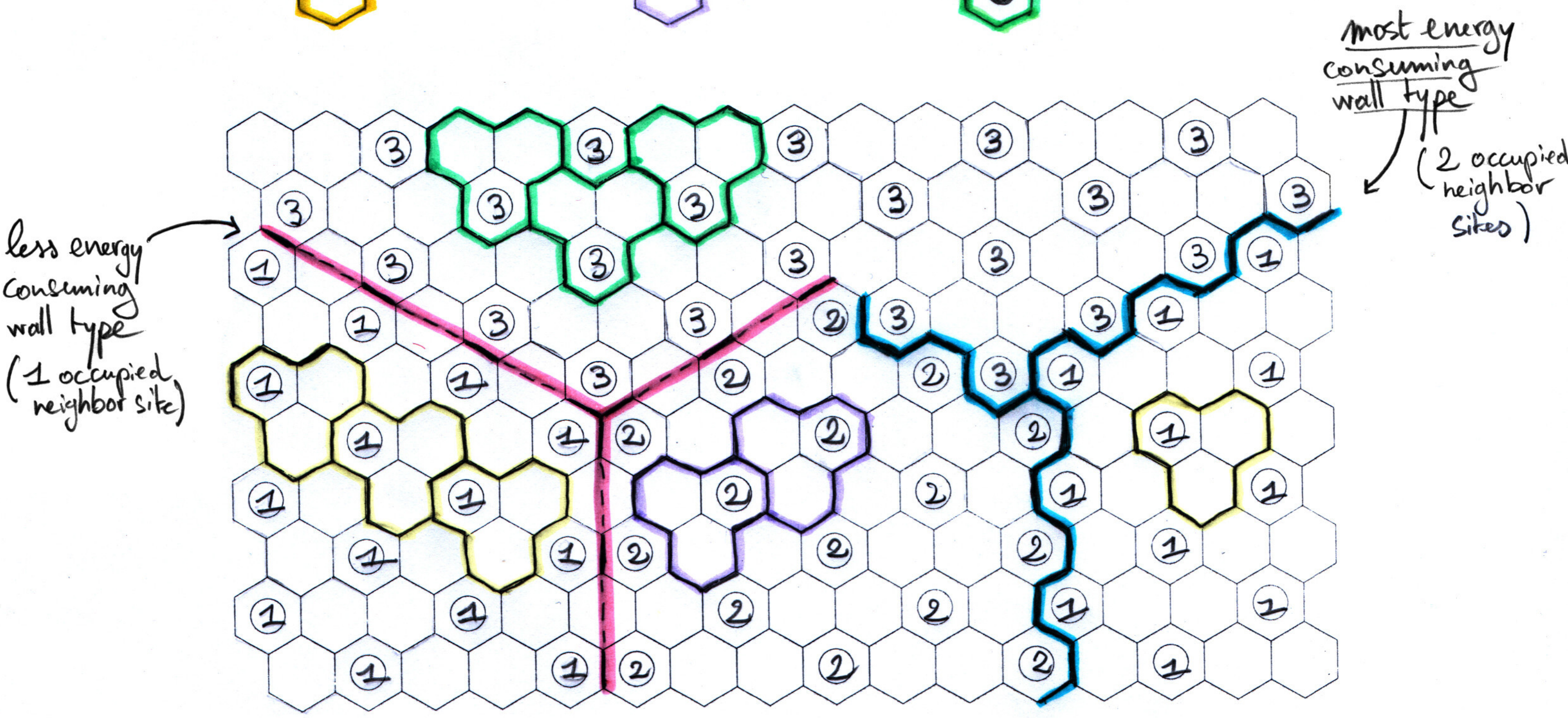
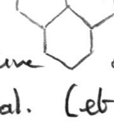


FIGURE 5 – An instantaneous configuration of adsorbed Kr atoms on graphite, at filling fraction 1/3; the question is to identify the different ground states coexisting, and the domain walls between them...

⚠ Ne pas essayer de parer une config avec des  contigus, ça ne peut pas fonctionner aux murs / dislocations. Le mapping d'une quelconque config sur un modèle de Potts n'est pas trivial. (cet peut être approximatif uniquement)