

Interacting Systems and Phase Transitions

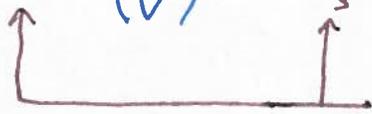
So far, we focused on non-interacting (ideal) systems / Gases.

include interactions \rightarrow new phenomena: Universality, phase transitions

I Interacting gas and Van der Waals equation

Consider a dilute, monoatomic gas:

$$\frac{P}{k_B T} = \frac{N}{V} + B_2(T) \left(\frac{N}{V}\right)^2 + B_3(T) \left(\frac{N}{V}\right)^3 + \dots$$



Virial coefficients: from QM on interactions.

\Rightarrow focus on classical gas, ideal gas law only ok at low density $\frac{N}{V}$.

Take:

$$\mathcal{H} = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i < j} U(r_{ij})$$

$$r_{ij} = |\vec{r}_i - \vec{r}_j|$$

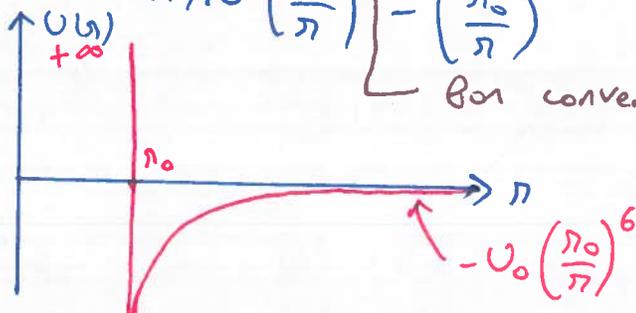
\uparrow Pairwise interaction

Main features of $U(r)$: • short range repulsion (from Pauli exclusion)

• attractive $\frac{1}{r^6}$ VdW: dipoles $\frac{p_1 p_2}{r^3}$ with $p_2 \sim E \sim \frac{p_1}{r^3}$ induced field

• popular choices: • Lennard-Jones: $U(r) \sim \left(\frac{r_0}{r}\right)^{12} - \left(\frac{r_0}{r}\right)^6$ for convenience

• Hard core:



General approach: Virial expansion. → focus on lowest order

$$Z = \frac{1}{\lambda^{3N} N!} \int \prod_i d\vec{r}_i e^{-\beta \sum_{j < k} U(r_{jk})}$$

$\uparrow \int d^3\vec{r}$ easy Hard! ($= V^N$ if $U=0$)

→ expansion? $U \rightarrow \infty$ as $r \rightarrow 0$!

Mayer function: $\beta(r) = e^{-\beta U(r)} - 1$

\nearrow $r \rightarrow 0$ \searrow $r \rightarrow \infty$
 "good" expansion parameter

$$\Rightarrow e^{-\beta \sum_{j < k} U(r_{jk})} = \prod_{j < k} (1 + \beta_{jk}) \quad \text{with } \beta_{jk} \equiv \beta(r_{jk})$$

Lowest order: $Z = \frac{1}{\lambda^{3N} N!} \int \prod_i d\vec{r}_i \left(1 + \sum_{j < k} \beta_{jk} + \dots \right)$

$$= \frac{1}{\lambda^{3N} N!} \left(V^N + \sum_{j < k} \underbrace{V^{N-2}}_{i \neq j, k} \int d\vec{r}_j d\vec{r}_k \beta_{jk} + \dots \right)$$

\nearrow $\frac{N(N-1)}{2}$ pairs $\vec{R}_{jk} = \frac{\vec{r}_j + \vec{r}_k}{2}$
 $\vec{r}_{jk} = \vec{r}_j - \vec{r}_k$

$$= \frac{1}{\lambda^{3N} N!} \left(V^N + \underbrace{\frac{N(N-1)}{2}}_{\approx N^2/2} V^{N-1} \int d\vec{r} \beta(r) + \dots \right)$$

$$\Rightarrow Z = Z_{\text{ideal}} \left[1 + \frac{N}{2V} \int d\vec{r} \beta(r) + \dots \right]^N$$

"trick" $(1 + \epsilon)^N \approx 1 + N\epsilon$

small for a dilute gas: $\int d\vec{r} \beta(r) \sim \rho_0^3$

$$\Rightarrow F = F_{\text{ideal}} - N k_B T \ln \left(1 + \frac{N}{2V} \int d\vec{r} \beta + \dots \right) \approx F_{\text{ideal}} - \frac{N^2 k_B T}{2V} \int d\vec{r} \beta + \dots$$

$\rho_0 \sim$ atom size

$$\Rightarrow P = - \left. \frac{\partial F}{\partial V} \right|_{T,N} = \frac{Nk_B T}{V} - \frac{N^2 k_B T}{2V^2} \int d^3 \beta + \dots$$

$$= \frac{Nk_B T}{V} \left(1 - \frac{N}{2V} \int d^3 \beta + \dots \right)$$

↑ gives $B_2(T)$

→ take hard core model: $\int d^3 \beta = \int_{\beta=0}^{\beta=\infty} (-1) d\beta + \int_{\beta=0}^{\infty} d\beta 4\pi \beta^2 \left[\frac{e^{\beta U_0 (\frac{\eta_0}{\beta})^6} - 1}{\beta U_0 (\frac{\eta_0}{\beta})^6} \right]$

assume $\frac{U_0}{k_B T} \ll 1$

$$\Rightarrow \int d^3 \beta = -\frac{4}{3} \pi \eta_0^3 + \beta \eta_0^6 U_0 4\pi \int_{\eta_0}^{\infty} \frac{d\eta}{\eta^4} = \frac{4}{3} \pi \eta_0^3 \left[\frac{U_0}{k_B T} - 1 \right]$$

This yields: $\frac{PV}{Nk_B T} = 1 - \frac{N}{V} \left(\frac{a}{k_B T} - b \right)$ with $a = \frac{2\pi \eta_0^3 U_0}{3}$

$$b = \frac{2\pi \eta_0^3}{3}$$

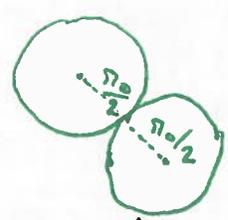
$$\Rightarrow P = - \left(\frac{N}{V} \right)^2 a + \frac{Nk_B T}{V} \left(1 + \frac{bN}{V} \right)$$

$$\approx \frac{1}{1 - \frac{bN}{V}}$$

$$B_2(T) = b - \frac{a}{k_B T}$$

2nd virial coeff.

$$\Rightarrow P = \frac{Nk_B T}{V - Nb} - \frac{N^2 a}{V^2}$$



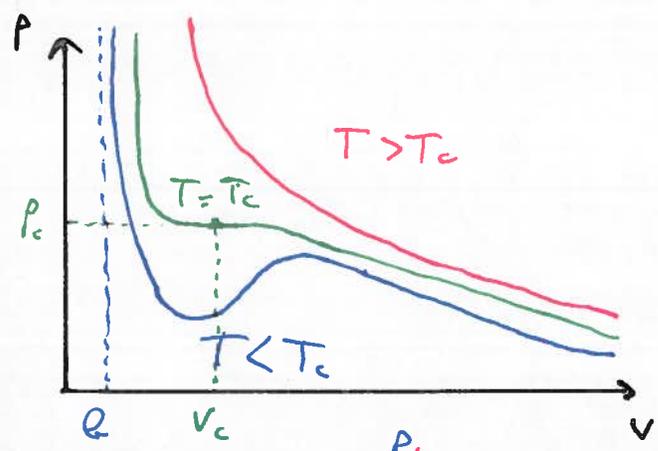
* Hard core repulsion: 1st atom has space V , 2nd: $V - \frac{4}{3} \pi \eta_0^3$
 \Rightarrow accessible volume $\prod_{i=0}^{N-1} (V - i \cdot 2b) \approx V^N \left(1 - \frac{N^2}{2} \frac{2b}{V} + \dots \right)$ $b \ll V$

(i with group $N-i-1$) $\times \frac{N}{2}$ times $\approx (V - Nb)^N$

* $\int d^3 \beta(\eta)$ convergent only if $U(\eta) \sim \eta^{-\alpha}$ with $\alpha > 3$
 \rightarrow short range interactions only

B) Liquid-gas transition

Starting point: VdW equation of state $p = \frac{k_B T}{v-b} - \frac{a}{v^2}$ with $v = \frac{V}{N}$

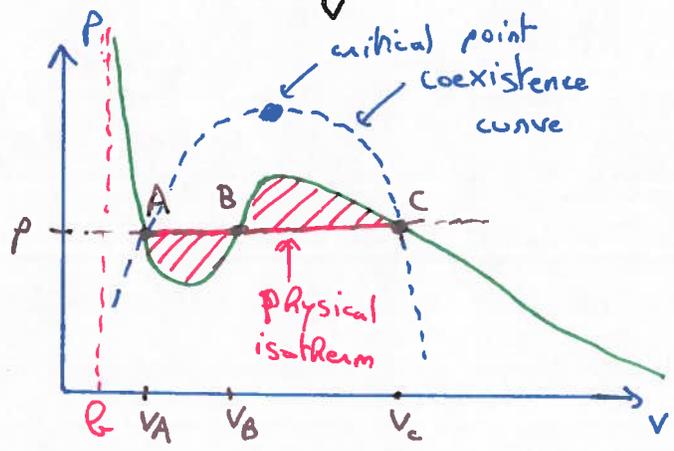


Inflexion point: $\frac{\partial p}{\partial v} = -\frac{k_B T}{(v-b)^2} + \frac{2a}{v^3} = 0$

$\frac{\partial^2 p}{\partial v^2} = \frac{2k_B T}{(v-b)^3} - \frac{6a}{v^4} = 0$

$\Rightarrow \frac{3}{v_c} = \frac{2}{v_c - b} \Rightarrow v_c = 3b$
 $k_B T_c = \frac{8a}{27b}$
 $p_c = \frac{a}{27b^2}$

For $T < T_c$:



(A) $v_A \gtrsim b$: liquid, atoms very close (contradicts assumptions to derive VdW but OK...)

(B): unstable (unphysical) $\frac{\partial p}{\partial v} \Big|_T > 0$ $p \uparrow$ $v \uparrow$!

(C) $v_c \gg b$: gas phase

\Rightarrow For a given p , what is v ? unphysical?

Maxwell construction: region between A and C corresponds to coexistence of liquid and vapor (gas). Equilibrium: $p_p = p_v$, $T_p = T_v$, $\mu_p = \mu_v$

$G = \mu N = F + pV \Rightarrow F_v - F_p = p(v_p - v_v)$

$\frac{\partial F}{\partial v} \Big|_{T,N} = -p$. Suppose we can integrate p from the VdW eq. of state

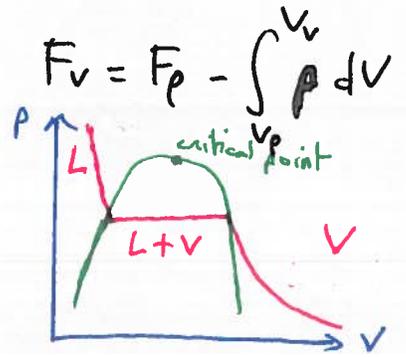
(very questionable: this region is unstable!!):

$$-\int_{v_p}^{v_v} p dv = p(v_p - v_v)$$

with $v_p = v_A N$
 $v_v = v_c N$

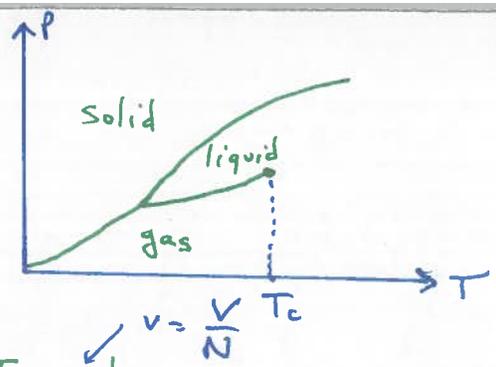
\uparrow gives physical isotherm

equal area condition



Clausius - Clapeyron equation

Coexistence curve in P, T space?



$$\mu_v = \mu_p \Rightarrow d\mu_v = d\mu_p \text{ along the curve}$$

Recall: Gibbs - Duhem relation $dp = -s dT + v dp$

$$\Rightarrow v_p dp - s_p dT = v_v dp - s_v dT \Rightarrow \Delta v dp = \Delta s dT$$

$s = \frac{S}{N}$

$$\left(\frac{dp}{dT}\right)_{\text{coex}} = \frac{S_{\text{vap}} - S_{\text{liq}}}{V_{\text{vap}} - V_{\text{liq}}} = \frac{R}{T(V_v - V_p)}$$

$$\text{with } R = (S_{\text{vap}} - S_{\text{liq}})T$$

Latent heat of vaporization per particle

• in practice: $V_{\text{vap}} \gg V_{\text{liq}}$ and $V_{\text{vap}} \approx \frac{k_B T}{p} \Rightarrow \frac{dp}{dT} \approx \frac{R p}{k_B T^2} \Rightarrow p \approx p_0 e^{-R/k_B T}$

• Def: n^{th} order phase transition = n^{th} derivative of thermodynamic potential (F or G) is discontinuous: "Ehrenfest classification" (outdated)

→ here, $V = \frac{\partial G}{\partial p}$ and $S = -\frac{\partial F}{\partial T}$ are discontinuous \Rightarrow liquid-gas transition is 1st order

→ critical point is 2nd order: much more interesting

→ Modern def: discontinuous ("1st order", latent heat) vs continuous ("2nd order", critical behavior)

• Universality: critical point given by $v_c = 3b$, $k_B T_c = \frac{8a}{27b}$, $p_c = \frac{a}{27b^2}$

$$\Rightarrow \frac{p_c v_c}{k_B T_c} = \frac{3}{8}$$

indep. from a, b; should hold for all gases (only rough agreement with experiments)

• rescaled variables: $\bar{T} = T/T_c$, $\bar{p} = p/p_c$, $\bar{v} = v/v_c \rightarrow$ universal coexistence curve for various gases in rescaled variables. Same curve regardless of chemical make up \Rightarrow "Universality"

↳ independent from microscopic details

Critical exponents: From the VdW equation of states, one can show that

near the critical point:

$$V_{vap} - V_{liq} \sim |T - T_c|^{1/2}$$

$$\kappa = -\frac{1}{V} \left. \frac{\partial V}{\partial P} \right|_T \sim \frac{1}{|T - T_c|}$$

(We'll compute similar exponents in the next section)

- $\kappa \rightarrow \infty$ as $T \rightarrow T_c$! Fluctuation-dissipation $\frac{(\Delta V)^2}{V} \sim \kappa$ (see HW #5) \Rightarrow large fluctuations!
- Only qualitative agreement with experiments (correct behavior, wrong exponents)

© Ferromagnetism and Ising Model

So far, we mostly discussed paramagnetism in class when it comes to magnetism. Recall: $H = -\vec{\mu} \cdot \vec{B}$ with $\mu = g\mu_B S$ spin angular momentum

Curie's law: $\chi = \lim_{B \rightarrow 0} \frac{\partial M}{\partial B} = \frac{N\mu_B^2}{k_B T} \sim \frac{1}{T}$ with M magnetization

Focus now on Ferromagnetism: spontaneous alignment of magnetic moments at low temperature.

\Rightarrow simple example of phase transition (heat up a magnet)

©.1 Ising Model: "Drosophila" of phase transition model!

spins $s_i = \pm 1$ on a lattice:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - B \sum_i s_i$$

⚠ not really a classical or quantum "Hamiltonian". No dynamics!!

Microstate: configuration $\{s_i\}$.

$J > 0$ favors aligned spins $\uparrow\uparrow, \downarrow\downarrow$

Magnetization: $M = \sum_i \langle s_i \rangle = \frac{1}{\beta} \frac{\partial \ln Z}{\partial B} = -\frac{\partial F}{\partial B} \Big|_T$

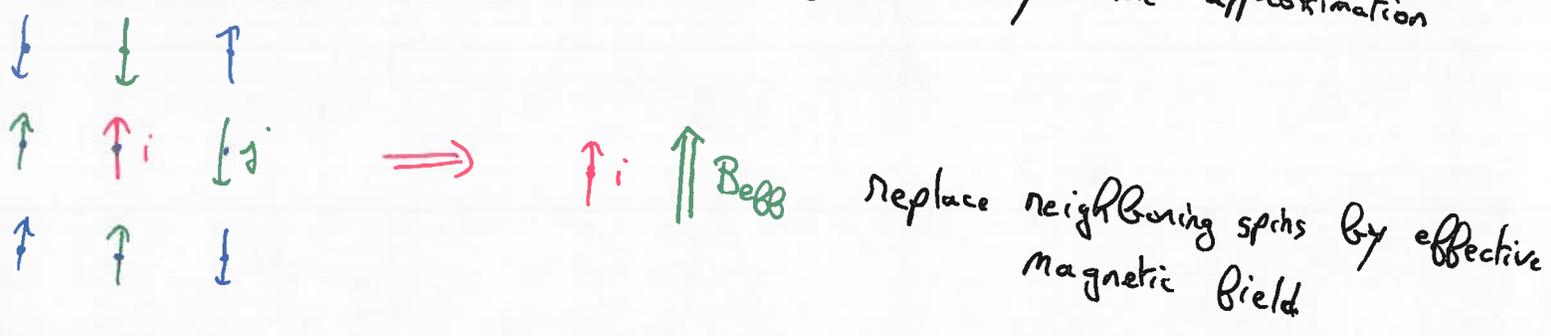
with

$$Z = \sum_{\{s_i\}} e^{-\beta \mathcal{H}(\{s_i\})}$$

- $d=1$: "easy" (see below)
- $d=2$: square lattice, solution due to Onsager 1944
- $d=3$: no exact solution

C.2 Mean field approximation

Computing Z is very hard in general: try some approximation



More precisely: neglect fluctuations $S_i = m + \underbrace{(S_i - m)}_{\delta S_i}$ with $m = \langle S_i \rangle = \frac{M}{N}$

$$-J \sum_{\langle i,j \rangle} S_i S_j = -J \sum_{\langle i,j \rangle} (m^2 + m(\delta S_i + \delta S_j) + \delta S_i \delta S_j)$$

and $\sum_{\langle i,j \rangle} = \frac{1}{2} \sum_i \sum_{j \sim i}$ $\rightarrow \frac{NZ}{2}$ terms with $Z = \# \text{ neighbors} = 2d$ (take square/cubic lattices)
otherwise, count pairs twice

$$\Rightarrow -J \sum_{\langle i,j \rangle} S_i S_j = + \frac{JNZ}{2} m^2 - J \sum_i m \left(\underbrace{\sum_{j \sim i} 1}_Z \right) S_i - J \sum_{\langle i,j \rangle} \delta S_i \delta S_j$$

neglect: "small"

*$\frac{1}{2} \times 2$: $\frac{1}{2}$ from $\sum_{\langle i,j \rangle} = \frac{1}{2} \sum_i \sum_{j \sim i}$
 2 from $m(S_i + S_j)$*

This yields:

$$\mathcal{H} \approx - \underbrace{(B + JmZ)}_{B_{\text{eff}}(m)} \sum_i S_i \quad \left(+ \frac{JNZ}{2} m^2 \right)$$

constant term unimportant

Paramagnet with effective field: m given by $m = \langle S_i \rangle = \frac{e^{+\beta B_{\text{eff}}} - e^{-\beta B_{\text{eff}}}}{e^{-\beta B_{\text{eff}}} + e^{+\beta B_{\text{eff}}}}$

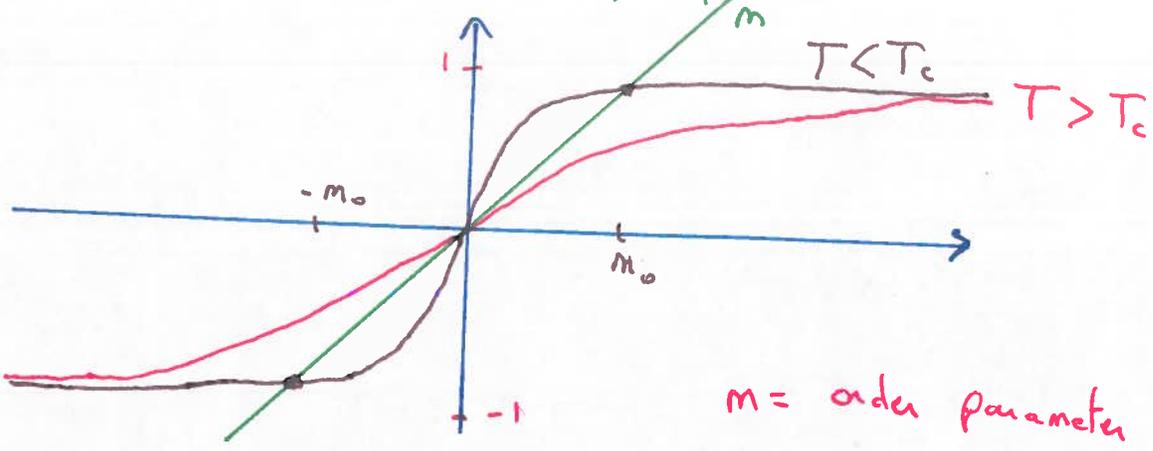
$$\Rightarrow m = \tanh(\beta(B + JZm))$$

self-consistency equation

We can also easily write down the partition function:

$$Z = e^{-\frac{1}{2} \beta J N z m^2} (2 \cosh[\beta B e z m])^N$$

with m given by the self-consistency equation



Let $B=0$: $\tanh x \approx x - \frac{x^3}{3} + \dots$

→ if $\beta J z < 1$: only solution $m = \langle S_i \rangle = 0$
paramagnetic phase

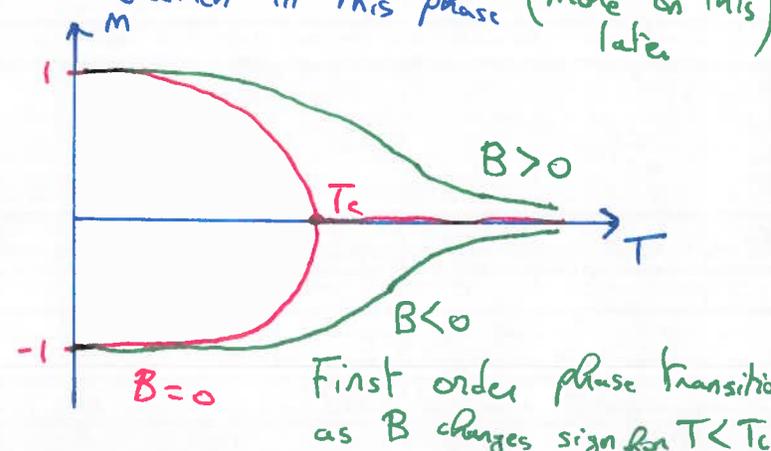
→ if $\beta J z > 1$: 3 solutions $m = 0, m = \pm m_0$ ← order

we'll show below that $m=0$ is unstable ($F[m_0] < F[m=0]$)

ferromagnetic phase: spins tend to align. $\uparrow\uparrow\uparrow$ or $\downarrow\downarrow\downarrow$
spontaneous symmetry breaking: symmetry $S_i \rightarrow -S_i$ in \mathcal{H}
broken in this phase (more on this later)

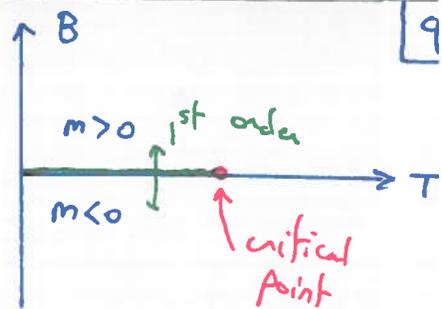
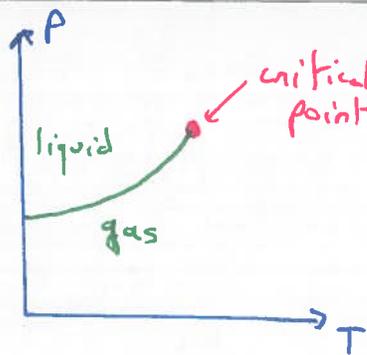
Critical temperature: $T_c = \frac{Jz}{k_B}$

if $B \neq 0$: no phase transition (will become clear when we study the free energy)



First order phase transition as B changes sign for $T < T_c$

Similar to liquid gas transition:



Critical exponents: $B=0$ $\tanh x = x - \frac{x^3}{3} + \dots \Rightarrow m \approx \frac{T_c}{T} m - \frac{1}{3} \left(\frac{T_c}{T}\right)^3 m^3 + \dots$

$$\Rightarrow m^2 = 3 \left(\frac{T}{T_c}\right)^3 \left[\frac{T_c - T}{T}\right]$$

expand in $T_c - T$:
($T < T_c$)

$$m_0 \sim \pm (T_c - T)^{1/2}$$

this exponent is called $\beta = 1/2$

now set $T = T_c$ and $B \neq 0$: $m = \tanh\left(\frac{B}{Jz} + m\right) \approx \frac{B}{Jz} + m - \frac{1}{3} m^3 + \mathcal{O}(B^2)$

$$\Rightarrow m \sim B^{1/3} \leftarrow 1/3 \text{ with } \delta = 3$$

small B and m

Keep only leading order in B

Susceptibility: $\chi = \frac{\partial M}{\partial B} \Big|_T = \frac{N\beta(1 + Jz \frac{\partial m}{\partial B})}{\cosh^2(\beta Jz m)}$

$T \rightarrow T_c^+$: set $m=0$

$$\Rightarrow \chi = \frac{N\beta}{1 - Jz\beta}$$

$$\Rightarrow \chi \sim \frac{1}{T - T_c} \leftarrow \gamma = 1$$

Validity of mean-field theory: turns out to be exact for $d = \infty$ (!)

For subtle reasons, mean-field theory predicts the correct exponents for $d \geq 4$ (this is known as the upper critical dimension)

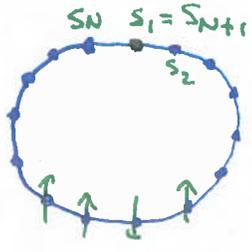
completely wrong in $d=1$: see below, we'll show that there's no phase transition

qualitatively OK for $d=2$ and $d=3$, but exponents wrong.

in $d=2$: $\beta = 1/8$, $\gamma = 7/4$ etc.

in $d=3$: $\beta \approx 0.32$, $\gamma \approx 1.2 \rightarrow$ same exponents as observed experimentally for the liquid gas transition **UNIVERSALITY!**

C.3 Exact solution in one dimension: transfer matrix



Use periodic boundary conditions: $s_{N+1} = s_N$

$$\mathcal{H}(\{s_i\}) = - \sum_{i=1}^N \left(J s_i s_{i+1} + \frac{B}{2} (s_i + s_{i+1}) \right)$$

and $Z = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \dots \sum_{s_N=\pm 1} e^{-\beta \mathcal{H}(\{s_i\})}$

Introduce a matrix: $T_{s_i s_{i+1}} = \langle s_i | T | s_{i+1} \rangle = e^{\beta J s_i s_{i+1} + \frac{\beta B}{2} (s_i + s_{i+1})}$

Then $Z = \sum_{s_1} \dots \sum_{s_N} T_{s_1 s_2} T_{s_2 s_3} \dots T_{s_{N-1} s_N} T_{s_N s_1} = \sum_{s_1} \langle s_1 | T^N | s_1 \rangle$

$\Rightarrow Z = \text{Tr } T^N$ with $T = \begin{pmatrix} e^{\beta J + \beta B} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta J - \beta B} \end{pmatrix}$

\hookrightarrow transfer matrix: "Guides" the system spin by spin.

Diagonalize T: $Z = \lambda_+^N + \lambda_-^N$ with $\lambda_+ > \lambda_-$ eigenvalues of T
 $\underset{N \rightarrow \infty}{\sim} \lambda_+^N$ for $N \rightarrow \infty$

This means that $F = -N k_B T \ln \lambda_+ \rightarrow$ just need to diagonalize this 2x2 matrix

$\text{Det} \begin{pmatrix} e^{\beta(J+B)} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)} - \lambda \end{pmatrix} = 0 \Rightarrow e^{-2\beta J} = \lambda^2 + e^{2\beta J} - \lambda e^{\beta J} 2 \cosh \beta B$
 $\Rightarrow \lambda^2 - e^{\beta J} 2 \cosh \beta B \lambda + 2 \sinh 2\beta J = 0$

$\Delta = e^{2\beta J} 4 \cosh^2 \beta B - 8 \sinh 2\beta J = 4 (e^{2\beta J} \sinh^2(\beta B) + e^{-2\beta J}) > 0$

$\lambda_{\pm} = e^{\beta J} \cosh \beta B \pm \sqrt{e^{2\beta J} \cosh^2 \beta B - 2 \sinh 2\beta J}$

$F = -N k_B T \ln \left[e^{\beta J} \cosh \beta B + \sqrt{e^{2\beta J} \cosh^2 \beta B - 2 \sinh 2\beta J} \right]$

magnetization: $m = -\frac{1}{N} \frac{\partial F}{\partial B} \Big|_T = -\frac{k_B T}{\lambda_+} \frac{\partial \lambda_+}{\partial B} \rightarrow 0 \text{ as } B \rightarrow 0$ $m = 0$

→ no phase transition / ordered phase in 1d! MF theory wrong.

D Landau theory

• Unified way to look at phase transitions in terms of symmetry-breaking

• Coarse-grained picture: Key ingredient = $F[m]$
 → $\frac{\partial F}{\partial m} = 0$ at equilibrium free energy order parameter
 with m small near transition

• \Leftrightarrow Mean-field, but useful starting point to include fluctuations (Ginzburg-Landau)

Ising model (MF): $F = \frac{1}{2} J N z m^2 - N k_B T \ln [2 \cosh(\beta J z m)]$

→ can be thought of as a function of m

$\frac{\partial F}{\partial m} = \cancel{J N z} m - \cancel{N k_B T} \beta \cancel{J z} \tanh(\beta J z m) = 0$

$\Rightarrow m = \tanh(\beta J z m) \rightarrow$ mean-field solution for m minimizes $F[m]$

• in general: $m =$ order parameter $\begin{pmatrix} m = 0 & \text{disordered phase} \\ m \neq 0 & \text{ordered phase} \end{pmatrix}$

eg: liquid gas: $m = V_{\text{gas}} - V_{\text{liquid}}$

D.1 Second order phase transitions

Consider a system with $m \rightarrow -m$ symmetry ($G = \mathbb{Z}_2$)

Near the transition, m is small: $F[m] = F_0(T) + a(T)m^2 + b(T)m^4 + \dots$ (1)

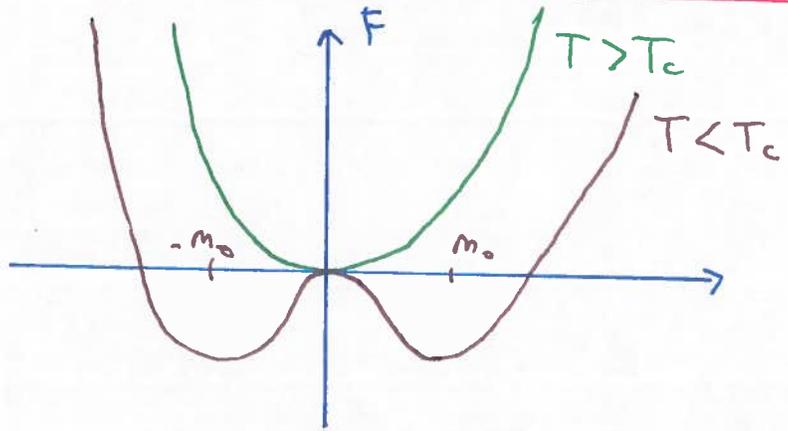
↑
even powers

e.g. Ising model: $F[m] = -NK_B T \ln 2 + \frac{NJz}{2} \left(1 - \frac{Jz}{k_B T}\right) m^2 + \frac{N\beta^3 J^4 z^4}{12} m^4$
 using $\cosh x \approx 1 + \frac{x^2}{2} + \frac{x^4}{24} + \dots$ and $\ln(1+x) \approx x - \frac{1}{2}x^2 + \dots \propto (T-T_c)$

Assume $b(T) > 0$ (otherwise we need higher order terms for stability)

minima changes for $a(T) \lesseqgtr 0$: Let $a(T) \approx a_0(T-T_c) + \dots$
 $b(T) \approx b_0 + \dots$ (regular at T_c)

so $F[m] = F_0 + a_0(T-T_c)m^2 + b_0 m^4$



$$\frac{\partial F}{\partial m} = 2a_0(T-T_c)m + 4b_0 m^3 = 0$$

$$m_0 \approx \pm \sqrt{\frac{a_0}{2b_0}} (T_c - T)^{1/2}$$

↑
mean-field exponent
spontaneously broken symmetry
for $T < T_c$

D.2 First order transitions: add a "field B " \Rightarrow breaks $m \rightarrow -m$ symmetry
 (more general than magnets!!)

$F[m] = F_0 - Bm + a_0(T-T_c)m^2 + c(B,T)m^3 + b_0 m^4 + \dots$

$\left. \frac{\partial F}{\partial B} \right|_T = -m$

not there if B field $\left\{ \begin{array}{l} \text{ignore for simplicity: can be} \\ \text{set to 0 by shifting } m \rightarrow m+m_0 \end{array} \right.$

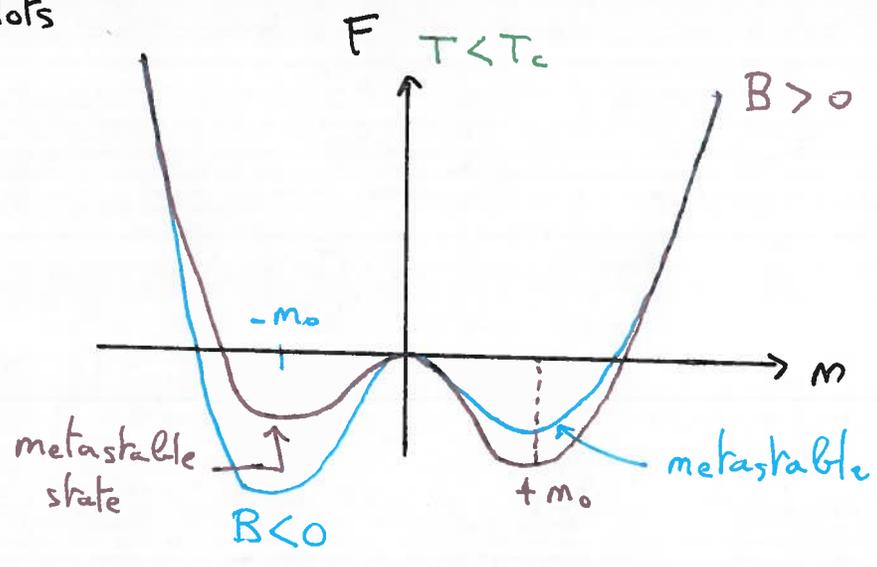
$$\frac{\partial F}{\partial m} = 0 = -B + 2a_0(T-T_c)m + 4b_0 m^3$$

\Rightarrow if $T = T_c$ $m \sim B^{1/3}$ ↑ $1/3$ with $\delta = 3$

$$\chi = \left. \frac{\partial m}{\partial B} \right|_{B=0} \Rightarrow 1 = 2a_0(T-T_c)\chi + 12b_0 m^2 \chi \Rightarrow \chi \sim \frac{1}{T-T_c}$$

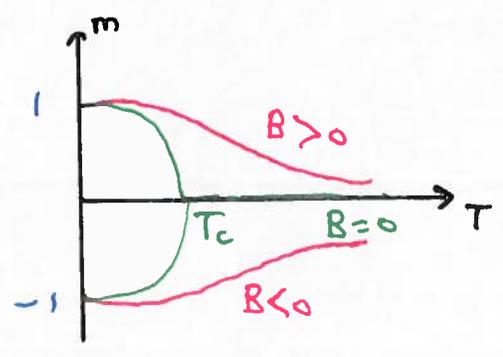
\Rightarrow mean field exponents follow from simple polynomial analysis.

Plots

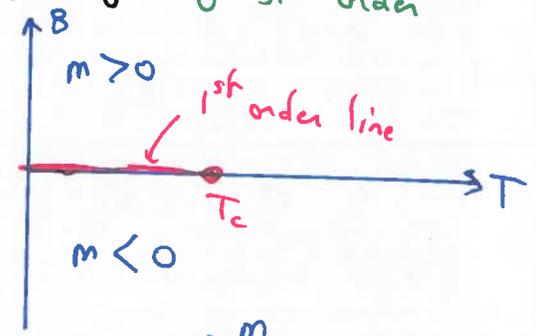


unique true minimum when $B \neq 0$, but there's another local minimum when $T < T_c$.
 "False vacuum" = metastable state

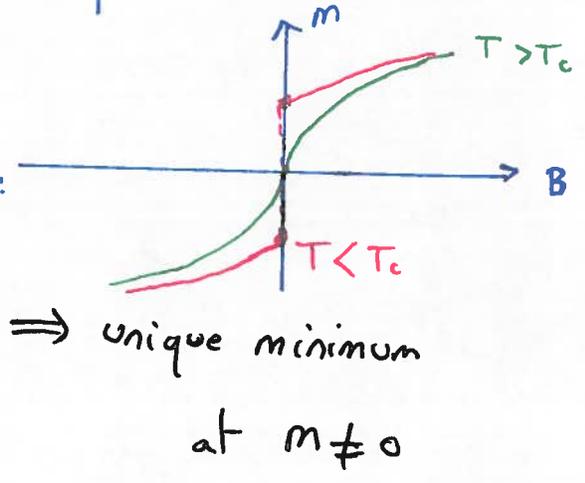
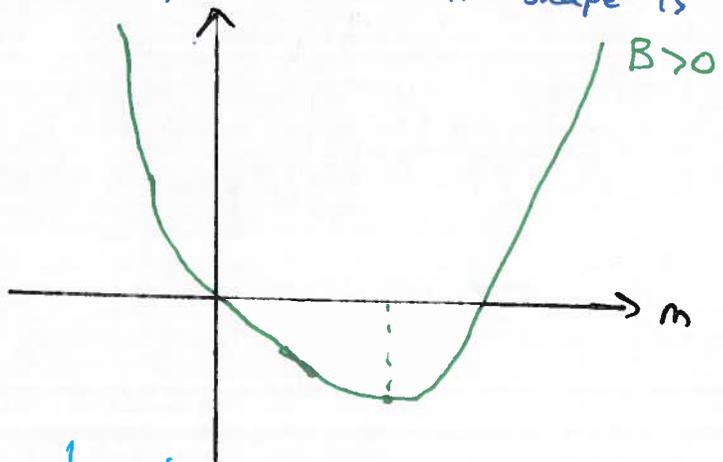
m jumps from $\pm m_0$ to $\mp m$ when B changes sign. first order



Phase diagram:



when $T > T_c$, double well shape is lost:

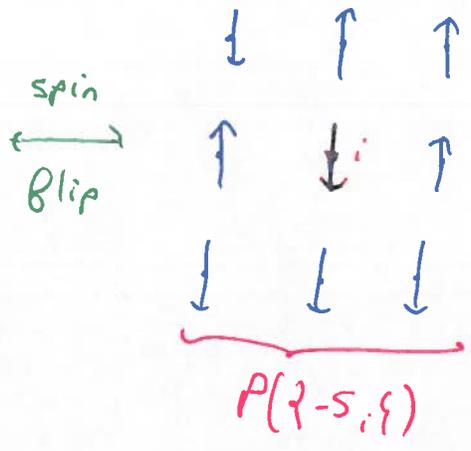
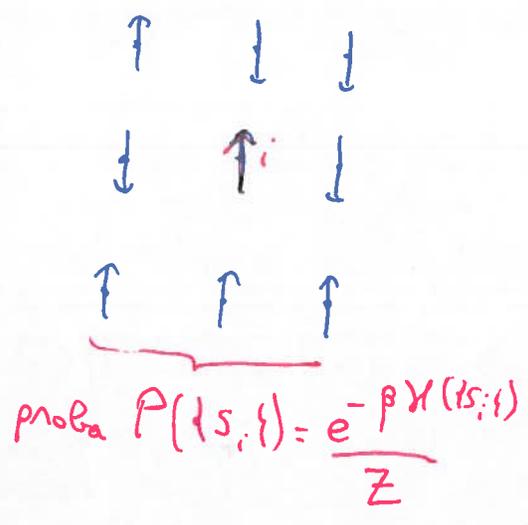


Remarks: Landau theory very general: could consider vector order parameter \vec{m} or some anisotropic tensors (liquid crystals).

Ginzburg Landau theory: $F[m] = \int d^d x [a_0(T-T_c)m^2 + \frac{K}{2}(\nabla m)^2 + G_0 m^4]$
 - ∇m : gradient expansion for $m(x)$ non-uniform
 - $\frac{K}{2}(\nabla m)^2$: energy cost of spatial variation

D.3 General remarks about Spontaneous Symmetry Breaking

$\mathcal{H}(\{s_i\}) = \mathcal{H}(\{-s_i\})$ for $B=0$



$P(\{s_i\}) = P(\{-s_i\})$
 $\Rightarrow \langle s_i \rangle = \sum_{\{s_i\}} s_i P(\{s_i\}) = 0!$
 by symmetry

How did we get $m = \langle s_i \rangle \neq 0$?

\Rightarrow introduce a very small field: GS energies $E_{\pm} = -\frac{NZJ}{2} \pm BN$ ^{all spins aligned}
 \hookrightarrow all spins + or -

now B splits the 2 states, in fact: $\frac{e^{-\beta E_-}}{e^{-\beta E_+}} = e^{-2\beta BN}$

\Rightarrow in the thermodynamic limit, only the $\{s_i = +1\}$ state contributes. $\xrightarrow{N \rightarrow \infty} 0$

Key point:

$\lim_{B \rightarrow 0} \lim_{N \rightarrow \infty} \langle s_i \rangle \neq \lim_{N \rightarrow \infty} \lim_{B \rightarrow 0} \langle s_i \rangle$

always = 0 by symmetry

Phase transitions occur only in the thermodynamic limit $N \rightarrow \infty$

That is also how we obtain non analyticities in $\beta = -\frac{k_B T}{N} \ln Z$
 ($e^{-\beta E_N}$ analytic function, so are Z and β if N finite!)

(E) Renormalization Group

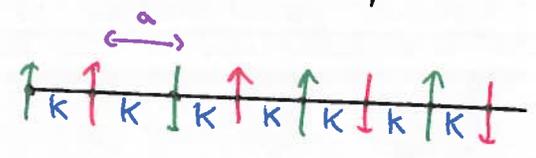
- Wilson 70's (Nobel prize '82): very important tool in particle physics, statistical physics, condensed matter (soft and quantum) etc...
- General set of ideas (not a single technique)
- Led to the so-called ϵ expansion with $d = 4 - \epsilon$
 - ↳ requires Quantum Field Theory, Feynman diagrams etc. ↑ MF works for $d \geq 4$
- Explains "universality"

→ Focus here on early work by Kadanoff and others ("real space" RG: will use uncontrolled approximations)

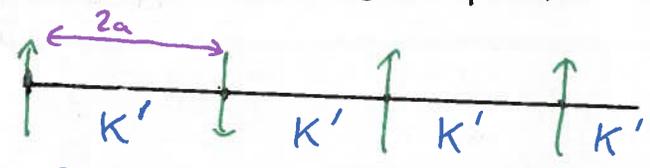
General idea: Coarse graining: sum over only some of the degrees of freedom and perform scale transformation. Find an effective stat. mech. model for the remaining degrees of freedom. Iterate and follow the "flow" of the effective coupling constants. Phase transition = RG fixed point (scale invariance)

(E.1) 1d Ising Model

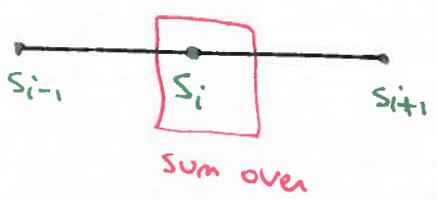
Sum over every other spin with $-\beta \mathcal{H} = K \sum_i s_i s_{i+1}$ ($K = \beta J$)



Sum over ("trace") red spins



Effective Ising model for remaining spins with coupling constant $K' = \beta(K)$



$$\sum_{s_i} e^{K(s_{i-1}s_i + s_i s_{i+1})} = e^{K(s_{i-1} + s_{i+1})} + e^{-K(s_{i-1} + s_{i+1})}$$

$$= C e^{K' s_{i-1} s_{i+1}}$$

$$\Rightarrow \begin{cases} 2 \cosh(2K) = C e^{K'} & (s_{i-1} = s_{i+1}) \\ 2 = C e^{-K'} & (s_{i-1} \neq s_{i+1}) \end{cases}$$

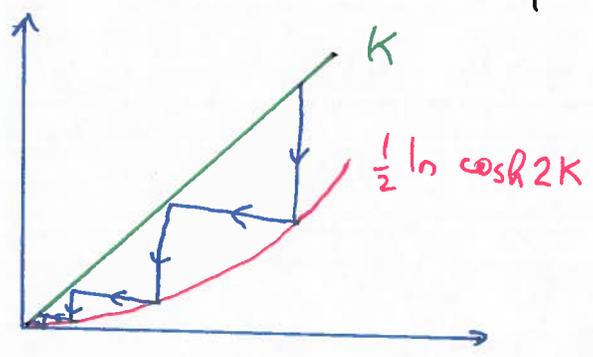
$$\Rightarrow \begin{cases} K' = \frac{1}{2} \ln \cosh(2K) & \leftarrow \beta(k) \\ C = 2 \sqrt{\cosh(2K)} & \leftarrow g(k) \end{cases}$$

we have

$$Z_N(K) = (g(K))^{N/2} Z_{N/2}(\beta(K))$$

renormalized Ising model with $N/2$ spins, lattice spacing $2a$

- $g(K)$ can be used to keep track of the free energy
- Here focus on "flow equation": $K' = \beta(K) = \frac{1}{2} \ln \cosh(2K)$

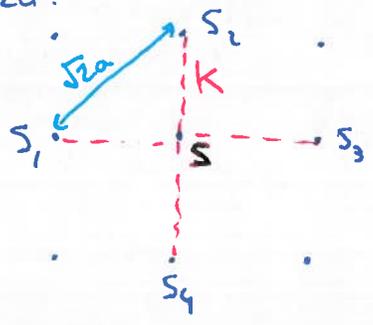


K flows to disordered (infinite T)
Fixed point $K^* = 0$. No phase transition!

System looks more and more disordered upon coarse graining

E.2 2d Ising model: Migdal-Kadanoff approximation

Try same in 2d:



$$\sum_{s_i} e^{K(s_1 + s_2 + s_3 + s_4)}$$

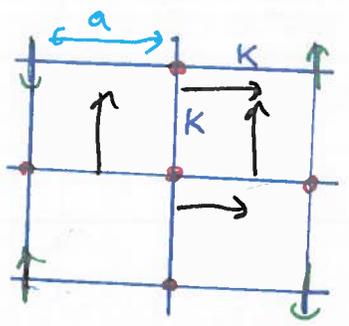
$$= C e^{K'(s_1 s_2 + s_2 s_3 + s_3 s_4 + s_4 s_1 + s_1 s_3 + s_2 s_4)}$$

$\sim e^{U s_1 s_2 s_3 s_4}$
 \uparrow 4-spin interaction

next nearest neighbor

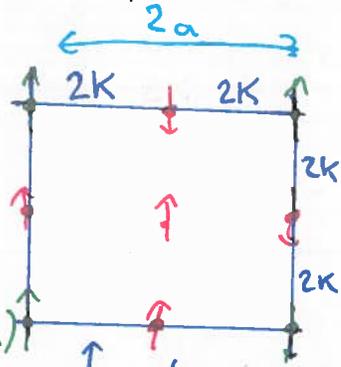
⇒ generate new interactions: need to keep track of all couplings!

Here: approximation (various non-equivalent methods)



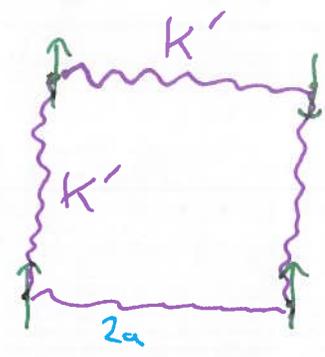
in red: spins to be summed over

move bonds (approximation)
black arrows



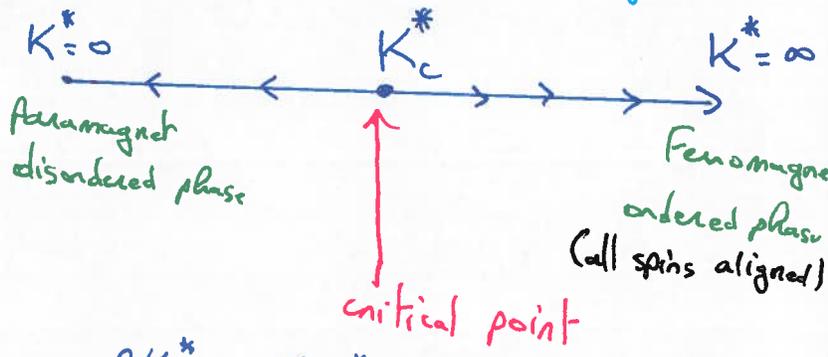
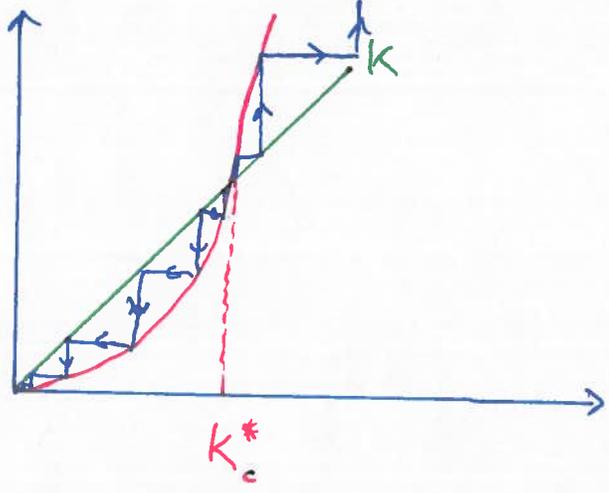
strengthened bonds = 2K (denoted $\beta = 2$)
scale factor = 2

decimate red spins



⊕ rescale $x \rightarrow x/\ell$ so that level spacing = a again

Eq. 1d: $K' = \frac{1}{2} \ln \cosh(4K)$



$$e^{2K_c^*} = \frac{e^{4K_c^*} + e^{-4K_c^*}}{2} \Rightarrow K_c^* \approx 0.305$$

vs exact: $K_c = \frac{1}{2} \ln(1 + \sqrt{2}) \approx 0.441...$

Critical exponents: linearize near K_c^* : $K' = K_c^* + \delta K'$
 $K = K_c^* + \delta K$

⇒ $\delta K' = \left. \frac{\partial K'}{\partial K} \right|_{K_c^*} \delta K$ with $\Lambda = \left. \frac{\partial K'}{\partial K} \right|_{K_c^*} = 2 \tanh 4K_c^* \approx 1.6786$

Free energy (density): $\beta(K) = A|K - K_c^*|^{2-\alpha}$ + regular and higher order terms

↳ α = specific heat exponent (see HW)

Rescaled volume smaller by factor ℓ^d : $\beta(K) = \frac{1}{\ell^d} \beta(K')$

of spins after decimation = $N/\ell^d = N/4$

$V\beta(K) = V'\beta(K')$

$x \rightarrow x/\ell$

⇒ $V|\delta K'|^{2-\alpha} = \ell^d V|\delta K|^{2-\alpha}$

this yields $\Lambda^{2-\alpha} = b^d \Rightarrow \alpha = 2 - d \frac{\ln b}{\ln \Lambda} \approx -0.6765$

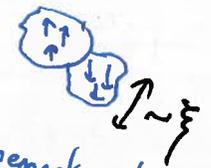
$d=2, b=2$ vs exact: $\alpha=0, c_v$ divergent

Correlation length: Diverging lengthscale at the transition

↳ measures distance over which fluctuations in the magnetization are correlated.

High T phase: size of domains with \sim aligned spins

Low T phase: size of misaligned regions (spontaneous alignment gets weaker and weaker as $T \rightarrow T_c$).



More precisely: need to observe the system over scales $L \gg \xi$ to know which phase the system is in.

Near the transition:

$$\xi \sim |T - T_c|^{-\nu} \sim |K - K_c|^{-\nu}$$

Under RG, we have

$$a \xi(K) = b a \xi(K')$$

(dimension full correlation length invariant)

↳ dimensionless correlation length

$$\Rightarrow |bK|^{-\nu} = b |bK'|^{-\nu} \Rightarrow \ln b = \nu \ln \Lambda \quad \text{so that} \quad \nu = \frac{\ln b}{\ln \Lambda} \approx 1.39$$

(exact: $\nu = 1$)

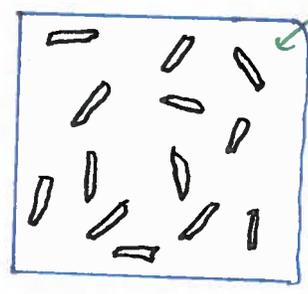
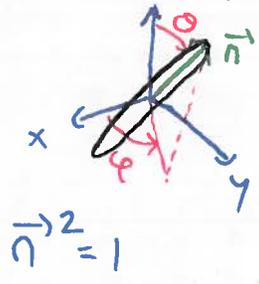
Note the relation: $\alpha = 2 - d\nu$

Hyperscaling

Exact "scaling relation" even if ν and α are approximate

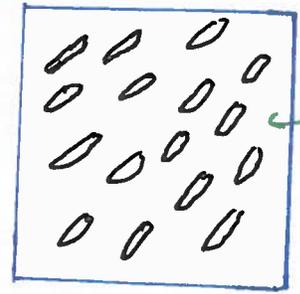
Appendix: Landau theory of liquid crystals

Rod like molecules



isotropic phase

High T: random orientations



nematic phase (no crystalline order)

Low T: molecules spontaneously align along a given axis

Ingredients: Order parameter + symmetry

Order parameter: guess: orientation $\langle \vec{n} \rangle$? No because \vec{n} and $-\vec{n}$ correspond to the same orientation. Need something invariant under $\vec{n} \rightarrow -\vec{n}$.

What about $\langle n_i(\vec{n}) n_j(\vec{n}) \rangle$? $\langle n_i n_j \rangle_{T=\infty} = \frac{1}{4\pi} \int_0^\pi d\theta \int_0^{2\pi} d\phi \sin\theta n_i n_j$

with $\vec{n} = \begin{pmatrix} \sin\theta \cos\phi \\ \sin\theta \sin\phi \\ \cos\theta \end{pmatrix}$

$\Rightarrow \langle n_i n_j \rangle_{T=\infty} = \frac{1}{3} \delta_{ij} \neq 0$

Take $Q_{ij} = \langle n_i n_j \rangle - \frac{1}{3} \delta_{ij} \quad (\text{Tr} Q = 0)$

$\langle n_x^2 \rangle = \langle n_y^2 \rangle = \langle n_z^2 \rangle = 1/3$ by symmetry

- $\langle Q_{ij} \rangle = 0$ if random orientations
- if $\vec{n} = \vec{e}_z$ (fixed orientation): $Q = \begin{pmatrix} -1/3 & 0 & 0 \\ 0 & -1/3 & 0 \\ 0 & 0 & 2/3 \end{pmatrix} \neq 0$

Free energy: should be invariant under rotations $\vec{n} \rightarrow R\vec{n}$
 $Q(\vec{n}) \rightarrow R Q(\vec{n}) R^T$
 $RESO(3)$

$\Rightarrow F[Q] = a \text{Tr} Q^2 + b \text{Tr} Q^3 + c (\text{Tr} Q^2)^2 + \dots$ (look $Q(\vec{n}) = Q$ uniform)

Represent $Q = \begin{pmatrix} -x/3 & 0 & 0 \\ 0 & -x/3 & 0 \\ 0 & 0 & 2x/3 \end{pmatrix} \rightarrow F \sim \alpha x^2 + \beta x^3 + \gamma x^4 \dots$
 First order transition \rightarrow agrees with experiments!!!