Critical Phenomena and Simple Models

(A) Phase transitions and universality

· **Phase transition:** Abrupt change in macroscopic properties of many-body system as external parameter is changed (Temperature, pressure, magnetic field, ...)
Happens only in the thermodynamic limit ⊕ interactions (or quantum effects: BEC)

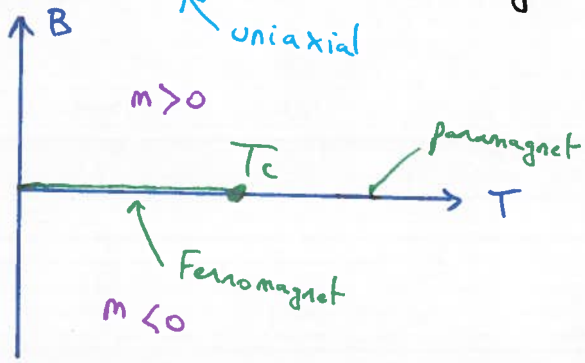
· **Continuous vs discontinuous:** Basically come in two flavors:

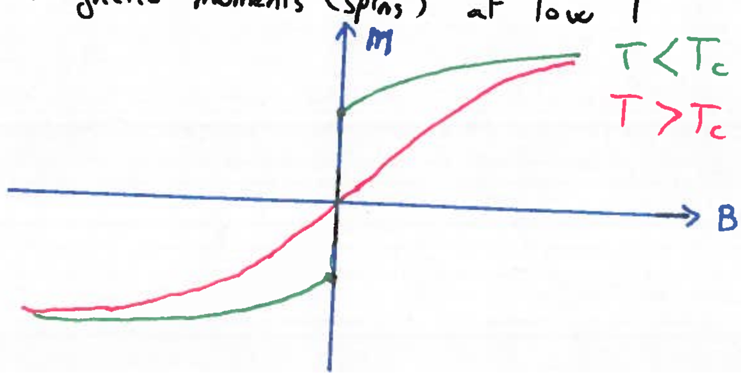
* **Discontinuous ("1st order"):** At the phase transition between phases A and B, the two phases coexist. Expect discontinuous behavior in various thermodynamic quantities. In particular: latent heat $h = T(S_A - S_B)$ Ex: melting of 3D solid, condensation gas → liquid

* **Continuous ("2nd order"):** Phase transition = critical point is its own state, thermodynamic quantities like energy density or magnetization vary smoothly across the transition. Ex: Critical point of water, Curie temperature in a ferromagnet.

* **Ehrenfest classification** (⚠ Outdated!) n^{th} order derivative of thermodynamic potential (F or G) discontinuous at "n^{th} order" phase transition. Actually: quantities like specific heat (C_v) or susceptibility (χ) diverge at 2nd order transition.

Ferromagnets: spontaneous alignement of magnetic moments ("spins") at low T
uniaxial





- Magnetization m = order parameter $\left(\begin{array}{l} m \neq 0: \text{ Ferromagnet} \\ m = 0: \text{ Paramagnet} \end{array} \right)$

- For $T < T_c$ and $B = 0$: $m = \pm m_0$ → example of spontaneous symmetry breaking

(System spontaneously breaks symmetry of the Hamiltonian)

Critical exponents: Near the critical point, singular behavior:

$t = \dfrac{T - T_c}{T_c}$ (reduced temperature).

- Specific heat: $\boxed{C_V \sim |t|^{-\alpha}}$

- Susceptibility: $\boxed{\chi = \dfrac{\partial m}{\partial B}\Big|_{B \to 0} \sim |t|^{-\gamma}}$

- Magnetization: $\boxed{m \sim (-t)^{\beta}}$ $(B \to 0^+, t < 0)$

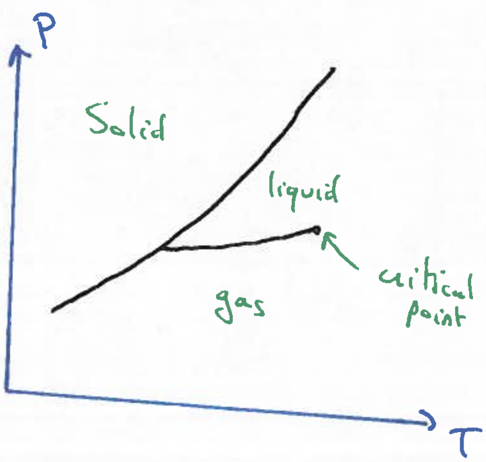
- Field: at $T = T_c$, $\boxed{m \sim B^{1/\delta}}$

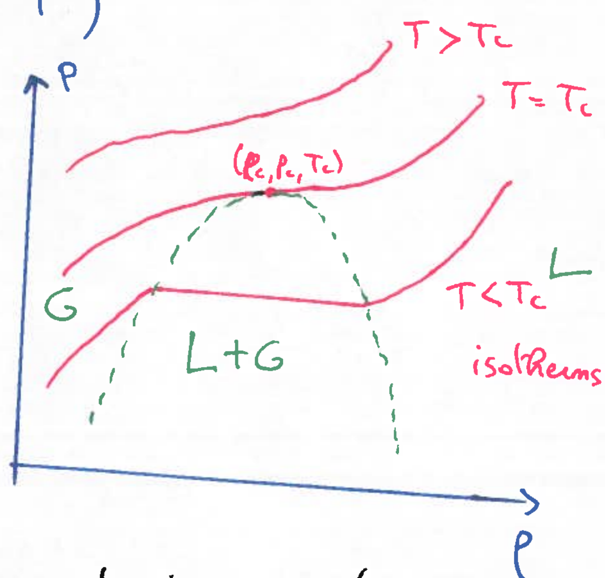
- The exponents $\alpha, \beta, \gamma, \delta$ are known as the thermodynamic critical exponents.
(we will introduce two more exponents ν and η below).

- Same exponents for many different materials ⟶ universality

Experiments $DyAlO_3$: $m \sim (T_c - T)^{0.311 \pm 0.005}$

Fluids:





$P - P_c \longleftrightarrow B$

$\rho - \rho_c \longleftrightarrow m$

But in fluids, overall average density fixed ($\neq$ from magnets magnetization not fixed)

at $\rho = \rho_c$: $C_V \sim |t|^{-\alpha}$ $\qquad \chi_T = -\dfrac{1}{V}\dfrac{\partial V}{\partial p}\Big|_T \sim |t|^{-\gamma}$

$\rho_L - \rho_G \sim (-t)^{\beta}$ $\qquad P - P_c \sim |\rho_L - \rho_G|^{\delta}$

Remarkably: . same exponents for many fluids $\beta \simeq 0.320 \pm 0.005$

. also coincide with ferromagnet/paramagnet exponents within error bars!!

Universality: at a continuous critical point, many properties of a system turn out to be largely independent of microscopic details (chemical make up etc...). Instead, they fall into a relatively small number of universality classes which depend only on global features: symmetry properties, # of dimensions, ...

. Very different systems can enjoy the same critical exponents (= same universality class) $\Rightarrow$ Physicist's dream! Crude toy models can capture the correct physics!

. Scaling: $m = f(B,t) \Rightarrow \boxed{m \sim B^{1/\delta}\, \Phi\left(t/B^{1/\delta\beta}\right)}$ (near critical point) t, B small

Same function $\Phi(x)$ for different materials: universal!

Goal of this course: Explain universality and describe framework to compute critical exponents. Near critical point: ignore lattice spacing and continuum approach based on symmetry (Landau theory). Critical exponents and scaling behavior
Ginzburg

then follow from dimensional analysis ($\sim$ Mean-field). Not correct: lattice spacing cannot be set to $a=0$ entirely $\Rightarrow$ Renormalization Group.

B Simple Models:

B.1 Ising Model: "Drosophila" of phase transition model

. Spins $s_i = \pm 1$ on a lattice $\boxed{\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - B \sum_i S_i}$

⚠ Not a classical or quantum "Hamiltonian": No Dynamics!

. Microstates: configurations $\{S_i\}$. $J > 0$ favors aligned spins.

· Partition function: $\boxed{Z = \sum_{\{S_i\}} e^{-\beta \mathcal{H}(\{S_i\})}}$

Probability of given microstate: $P(\{S_i\}) = \dfrac{e^{-\beta \mathcal{H}(\{S_i\})}}{Z}$

Free Energy per spin

magnetization: $m = \frac{1}{N}\sum_{i=1}^{N} \langle S_i \rangle = \frac{1}{N\beta}\frac{\partial \log Z}{\partial B} = -\left.\frac{\partial f}{\partial B}\right|_T$ with $\boxed{f = -\frac{k_B T}{N}\log Z}$

$d=1$: easy (transfer matrix or other): no transition

$d=2$: exact solution due to Onsager 1944 phase transition

$d=3$: no exact solution

Ising model is clearly a very simplified model for a ferromagnet. Yet, thanks to universality, its critical exponents are the same as in more realistic models and as in experiments!

· Symmetry: $\mathcal{H}(\{S_i\}) = \mathcal{H}(\{-S_i\})$ if $B=0$. $S_i \to -S_i$ (flip all spins) symmetry

Group: $\mathbb{Z}_2 = \mathbb{Z}/2\mathbb{Z}$ (two elements: $1, g$ with $g^2=1$)

B.2 $O(n)$ model:

n-component spins: $\vec{S}_i = (S_i^1, \dots S_i^n)$, $\vec{S}_i^2 = 1$ and $\boxed{\mathcal{H} = -J\sum_{\langle i,j\rangle}\vec{S}_i\cdot\vec{S}_j - \sum_i \vec{B}\cdot\vec{S}_i}$

. For $\vec{B}=\vec{0}$, $\mathcal{H}$ has an $O(n)$ symmetry: $\vec{S}_i \longrightarrow R\vec{S}_i$ with $R \in O(n)$ (rotation of all spins)

. $n=1$: Ising ($O(1) = \mathbb{Z}_2$), $n=2$: XY model, $n=3$: Heisenberg model.

even $n \to 0$ has a meaning (Polymers, Self avoiding walks)

B.3 Correlation functions and correlation length

. Cut a magnet in half: still a magnet. Repeat the process: at some point, chunk stop being ferromagnetic: characteristic lengthscale $\equiv$ Correlation length $= \xi$

. Characterize correlations of the fluctuations in a material (see below)

System of linear size $L \gg \xi$: effectively in the thermodynamic limit even if L finite

Correlation functions:

at large distances: rotation and translation invariance

$$\boxed{\begin{aligned} G(|\vec{r}_i - \vec{r}_j| = r) &= \langle S_{\vec{r}_i} S_{\vec{r}_j} \rangle - \langle S_{\vec{r}_i} \rangle \langle S_{\vec{r}_j} \rangle \\ &= \langle (S_{\vec{r}_i} - \langle S_{\vec{r}_i} \rangle)(S_{\vec{r}_j} - \langle S_{\vec{r}_j} \rangle) \rangle \end{aligned}}$$

(say, for Ising model)

. In the phases (paramagnetic or ferromagnetic), we have $\boxed{G(r) \sim e^{-r/\xi}}$ ← decay of correlations
(we will show this later in the course)

. At a second order transition, ξ diverges : $\xi \sim |K - K_c|^{-\nu}$ ($K = \beta J$ for Ising)

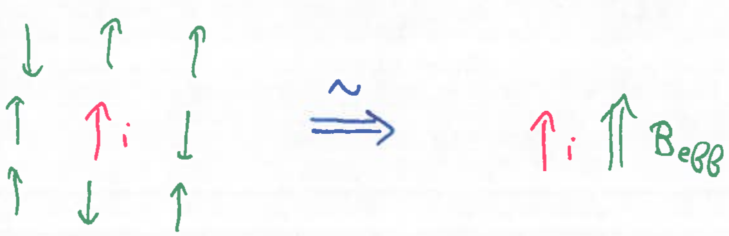
or $\boxed{\xi \sim |T - T_c|^{-\nu}}$

for $T = T_c$: scale invariance ($\xi = \infty$) : $\boxed{G(r) \sim \dfrac{1}{r^{d-2+\eta}}}$ → exponent η : "anomalous dimension"

Ⓒ Mean Field Theory

C.1 MF approximation for the Ising Model

. Computing Z is very hard in general: try some approximation



Replace neighboring spins by effective magnetic field

. More precisely: neglect fluctuations $S_i = m + \overbrace{(S_i - m)}^{\delta S_i}$ with $m = \langle S_i \rangle$

$$-J \sum_{\langle i,j \rangle} \left(m^2 + m(\delta S_i + \delta S_j) + \delta S_i \delta S_j \right)$$ and $\displaystyle\sum_{\langle i,j \rangle} = \frac{1}{2} \sum_i \sum_{j\ \mathrm{n.n.}\ i}$: $\dfrac{Nz}{2}$ terms

$z = \#$ neighbors $= 2d$ for square cubic lattice

$$\Rightarrow -J\sum_{\langle i,j\rangle} S_i S_j = \frac{JNz}{2} m^2 - Jzm \sum_i S_i - J \underbrace{\cancel{\sum_{\langle i,j\rangle} \delta S_i \delta S_j}}_{\text{neglect: "small"}}$$

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

this yields: $\boxed{\mathcal{H} \simeq \frac{JNz}{2} m^2 - B_{eff}(m) \sum_i S_i}$ $\Rightarrow Z = e^{-\beta\frac{JNzm^2}{2}} \times \left(e^{-\beta B_{eff}} + e^{\beta B_{eff}}\right)^N$

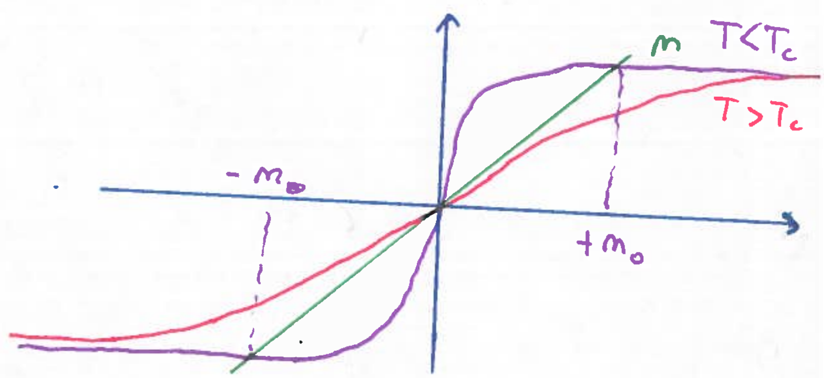
$= B + Jzm$: effective field

. Non interacting spins: $F = \frac{JNzm^2}{2} - Nk_BT \log\left[2\cosh(\beta B_{eff}m)\right]$

and $m = \langle S_i \rangle = \frac{e^{\beta B_{eff}} - e^{-\beta B_{eff}}}{e^{\beta B_{eff}} + e^{\beta B_{eff}}} \Rightarrow \boxed{m = \tanh\left(\beta\left(B + Jmz\right)\right)}$ self-consistency equation

. Focus on $B=0$: $\tanh x \simeq x - x^3/3 + \dots$

critical temperature $\boxed{T_c = \frac{Jz}{k_B}}$



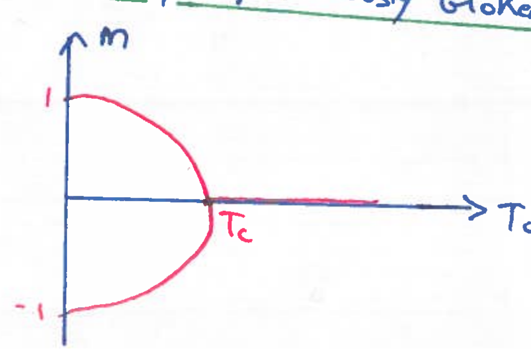
. if $\beta J z < 1$ $(T > T_c)$: only solution $m=0$
paramagnet

. if $\beta J z > 1$ $(T < T_c)$: 3 solutions: $m=0$, $m = \pm m_0$. $m=0$ unstable (see next chapter)

Ferromagnet: $m \neq 0$ ordered phase, $S_i \to -S_i$ symmetry spontaneously broken

Spins tend to align themselves: $\uparrow\uparrow\uparrow$ $\uparrow\uparrow\uparrow$ or $\downarrow\downarrow\downarrow$ $\downarrow\downarrow\downarrow$

$\Rightarrow$ simple picture of spontaneous symmetry breaking
(will become even clearer within Landau-Ginzburg theory)



Critical exponents: $B = 0$, $\tanh x \simeq x - x^3/3 + \dots \Rightarrow m \simeq \frac{T_c}{T} m - \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m^3 + \dots$ (m small near transition)

$$\Rightarrow m^2 = 3\left(\frac{T}{T_c}\right)^3 \left[\frac{T_c - T}{T}\right] \xrightarrow[\text{in } \frac{T_c - T}{T_c}]{\text{expand}} \boxed{\begin{array}{c} m \sim \pm\sqrt{T_c - T} \\ \beta = 1/2 \end{array}}$$

- $T = T_c$ and $B \neq 0$: $m \simeq B/Jz + m - \frac{1}{3} m^3 + \dots \Rightarrow \boxed{\begin{array}{c} m \sim B^{1/3} \\ \delta = 3 \end{array}}$

- Susceptibility: $\chi = \left.\frac{\partial m}{\partial B}\right|_{B=0} = \frac{\beta\,(1 + Jz \overbrace{\frac{\partial m}{\partial B}}^{\chi})}{\cosh^2(\beta J z m)} \underset{\substack{T \to T_c^+ \\ m = 0}}{\Rightarrow} \chi = \frac{\beta}{1 - Jz\beta}$

$$\boxed{\chi \sim \frac{1}{T - T_c}, \quad \gamma = 1}$$

In the next chapter, we will show that $\alpha = 0$, $\nu = 1/2$ and $\eta = 0$ within MF theory

C.2 Validity of Mean-Field Theory

How good is MF theory? Depends on dimensionality d.

- Turns out to be exact for $d = \infty$ (!)
- In the next chapter, we will show that mean-field predicts the correct exponents for $\boxed{d > 4}$ (= upper critical dimension)
- Completely wrong in $\boxed{d = 1}$: exact solution, no phase transition

  lower critical dimension
- Qualitatively OK for $d = 2$ and $d = 3$, but exponents wrong

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

  $d = 3$: $\beta \simeq 0.32$, $\gamma \simeq 1.2$,

Same exponents as in experiments

Universality! Need to take into account fluctuations

$\Rightarrow$ rest of the course!

C.3 General remarks about spontaneous symmetry breaking

. $\mathcal{H}(\{s_i\}) = \mathcal{H}(\{-s_i\})$

$$\begin{matrix}\uparrow&\uparrow&\downarrow\\ \downarrow&\downarrow&\uparrow\\ \uparrow&\downarrow&\uparrow\end{matrix} \quad \xleftrightarrow[\text{flip}]{\text{spin}} \quad \begin{matrix}\downarrow&\downarrow&\uparrow\\ \uparrow&\uparrow&\downarrow\\ \downarrow&\uparrow&\downarrow\end{matrix}$$

Proba $P(\{s_i\}) = \dfrac{e^{-\beta \mathcal{H}(\{s_i\})}}{Z}$

$P(\{s_i\}) = P(\{-s_i\})$

$\Rightarrow \langle s_i \rangle = \sum_{\{s_i\}} s_i P(\{s_i\})$

$= 0$ (!)

by symmetry

How did we get $m = \langle s_i \rangle \neq 0$? Focus on groundstates (all spins $\uparrow$ or $\downarrow$)

add a small field: $E_\pm = -\underbrace{\dfrac{NzJ}{2}}_{\text{all spins aligned}} \mp BN$ $\Rightarrow \dfrac{e^{-\beta E_-}}{e^{-\beta E_+}} = e^{-2\beta BN} \underset{\substack{N\to\infty \\ (B>0)}}{\longrightarrow} 0$

$\Rightarrow$ B splits the 2 states, and in the thermodynamic limit, $\{s_i = -1\}$ has negligible proba!

Key point: $\boxed{\lim_{B\to 0} \lim_{N\to\infty} \langle s_i \rangle \neq \underbrace{\lim_{N\to\infty} \lim_{B\to 0} \langle s_i \rangle}_{= 0 \text{ by symmetry}}}$

. Phase transitions occur only in the thermodynamic limit: $N \to \infty$

This is also why there can be non analyticities in $f = -k_B T \lim_{N\to\infty} \frac{1}{N} \log Z$

($e^{-\beta E_n}$ analytic function $\Rightarrow$ so are Z and F in N finite!)