2. Classical phase transitions and universality

2.1 Definitions

Order parameter (OP): The OP is an observable φ, for which

$$\langle\varphi\rangle \begin{cases} = 0 & \text{in disordered phase} \\ \neq 0 & \text{in ordered phase} \end{cases}$$

thermodynamic average ($T \neq 0$)
& quantum expectation value (quantum system)

Remarks:

- φ usually local observable: $\varphi = \varphi(\vec{r}, t)$

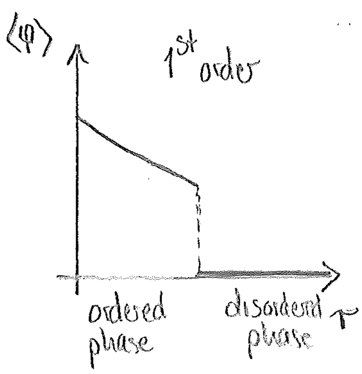
  [counter-example: volume enclosed by Fermi surface of a metal]

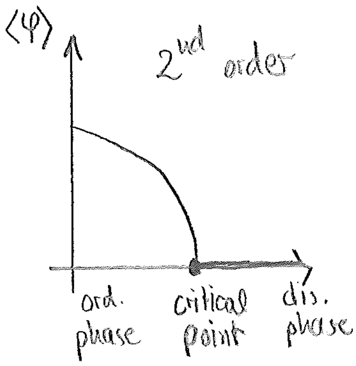
- φ not unique
- φ sometimes not known [e.g., interaction-driven metal-insulator transition]

Example [Ferromagnet (FM)]: $\vec{\varphi}(\vec{r}_i) = \vec{S}_i$ local magnetization at site i

First-order transition: OP changes discontinuously at the transition.

Continuous transition: OP varies continuously across the transition.





Critical point: Transition point of a continuous transition.

Correlations: For an order parameter $\varphi = \varphi(\vec{r},t)$, correlation functions can be defined by $\langle \varphi(\vec{r},t)\, \varphi(\vec{r}',t')\rangle$ ("two-point function")

Correlation length ξ: In stable phase the OP correlation function typically follows an exponential law

$$\langle \varphi(\vec{r})\, \varphi(\vec{r}')\rangle - \langle \varphi(\vec{r})\rangle \langle \varphi(\vec{r}')\rangle \propto e^{-\frac{|\vec{r}-\vec{r}'|}{\xi}}$$

with ~~the~~ correlation length ξ.

Remarks:

- ξ diverges at a critical point, then

$$\langle \varphi(\vec{r})\varphi(\vec{r}')\rangle - \langle \varphi(\vec{r})\rangle\langle \varphi(\vec{r}')\rangle \propto \frac{1}{|\vec{r}-\vec{r}'|^{d-2+\eta}}$$

where η is the anomalous dimension.

$\Rightarrow$ correlation function becomes a power law [scale invariance!]

- Near criticality, ξ is large and becomes the only length scale characterizing the low-energy physics $[a/\xi \to 0]$

Spontaneous symmetry breaking: Consider a Hamiltonian $\hat{H}$ that is invariant under a symmetry generated by $\hat{S}$; $[\hat{H},\hat{S}]=0$.
If the system's density operator $\hat{\varrho}$ is not symmetric under $\hat{S}$, $[\hat{\varrho},\hat{S}] \neq 0$, then the symmetry $\hat{S}$ is spontaneously broken.

Remarks:

- Spontaneous symmetry breaking requires nonanalyticity of thermodynamic potential (otherwise: $[\hat{H},\hat{S}]=0$ would imply $[e^{-\beta\hat{H}},\hat{S}]=0$)

  $\Rightarrow$ phase transition

- Singularity can be seen by including a small <u>conjugate field</u> h:

  $$\hat{H} \mapsto \hat{H} - h\varphi$$

  Spontaneous symmetry breaking: $\lim_{h\to 0^+} \hat{S}(h) \neq \hat{S}(h=0)$

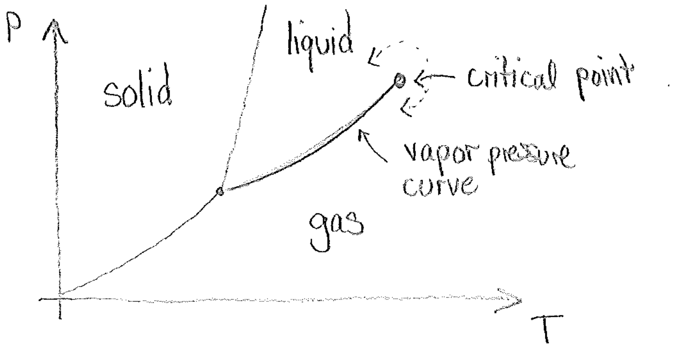
- Spontaneous symmetry breaking impossible in a finite-size system ($e^{-\beta\hat{H}}$ not singular for $N<\infty$)

  $\Rightarrow$ spontaneous symmetry breaking means $\lim_{h\to 0}\lim_{N\to\infty}(\dots) \neq \lim_{N\to\infty}\lim_{h\to 0}(\dots)$

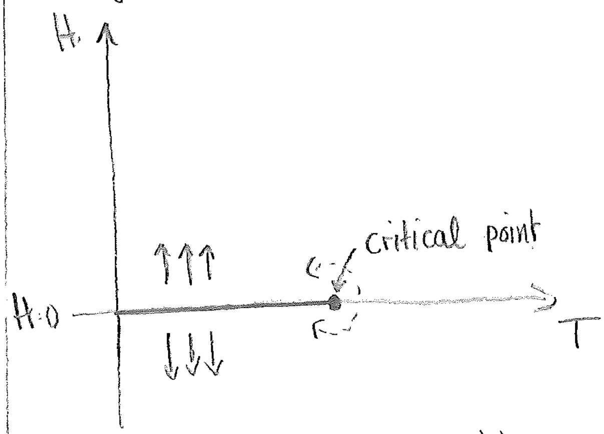
2.2 Generic phase diagrams of fluids and magnets

Fluid	Magnet

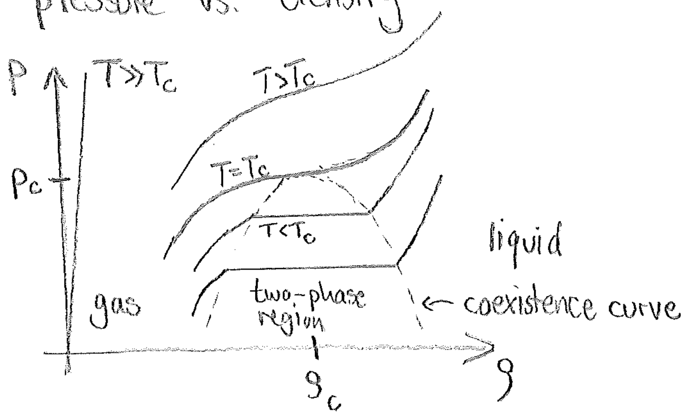
pressure vs. temperature



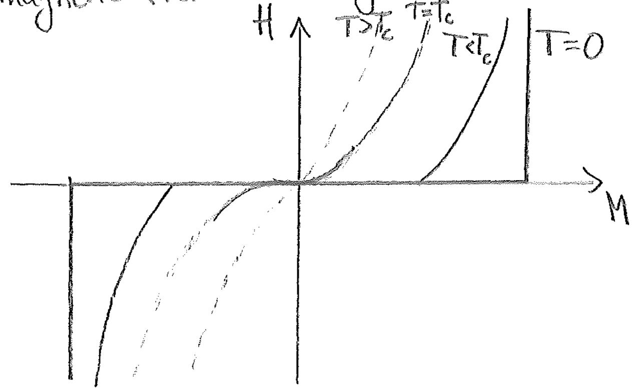
magnetic field vs. temperature



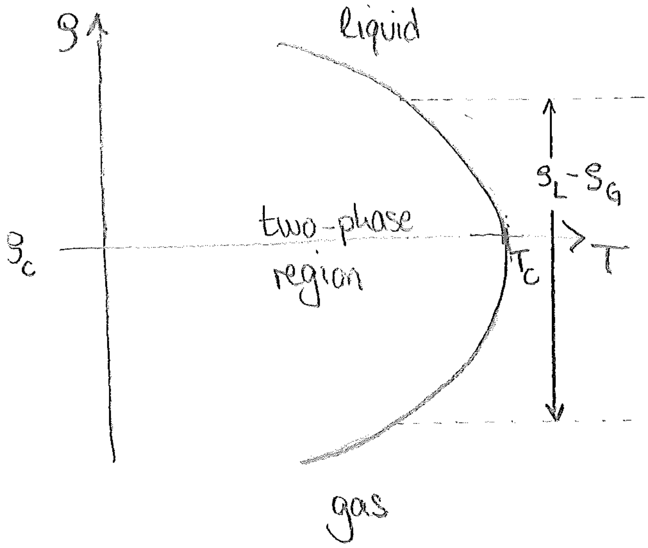
pressure vs. density

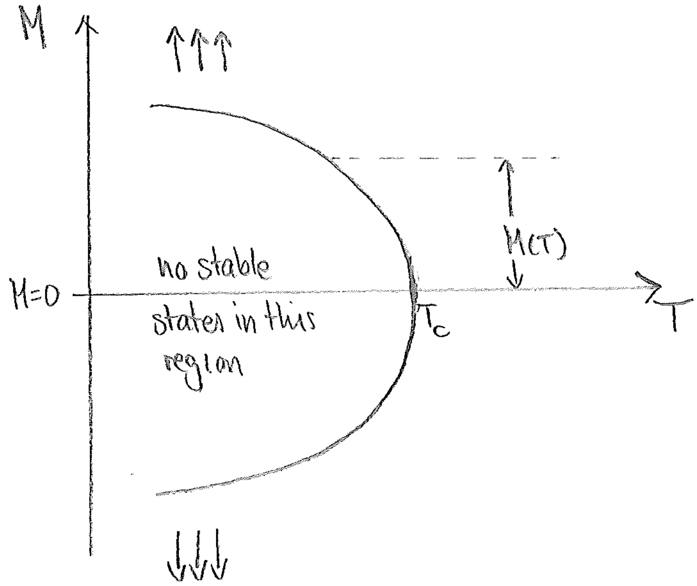


magnetic field vs. magnetization



density vs. temperature





2.3 Landau theory of phase transitions

Assumption: phase transition uniquely described in terms of a local order parameter φ

Idea: Expand a generalized thermodynamic potential f ("Landau functional") in terms of φ (conventional potential is singular at transition!)

Landau functional

Example (ferromagnet):

Specifying magnetic field H and temperature T fixes magnetization $\varphi \equiv M$.

Generalized potential:

$$\underbrace{f(T,H)}_{\text{thermod. pot.}} \longmapsto \underbrace{f(T,H,\varphi)}_{\text{Landau potential}}$$

and assume that $f(T,H,\varphi)$ is non-singular.

Equilibrium state:

$$\left.\frac{\partial f(T,H,\varphi)}{\partial \varphi}\right|_{\varphi=\varphi_{eq}} = 0 \quad \text{and} \quad f(T,H) = f(T,H,\varphi_{eq}(T,H))$$

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Expansion of Landau potential (valid near criticality):

$$f(T,H) = f_n + f_0 \left(\frac{a(T)}{2}\varphi^2 + \frac{b(T)}{4}\varphi^4 + \frac{c(T)}{6}\varphi^6 + \ldots - \varphi \cdot h \right)$$

where $h \equiv \frac{H}{f_0}$ is the magnetic field ("conjugate to OP") and f_n only weakly T dependent.

Remarks:

- f includes all symmetry-allowed terms, e.g. for $H=0$: [liquid-gas trans. Ising trans.]

  $\mathbb{Z}_2: \quad \varphi \mapsto -\varphi$ ("Ising symmetry")

  $\Rightarrow$ only even powers in φ allowed

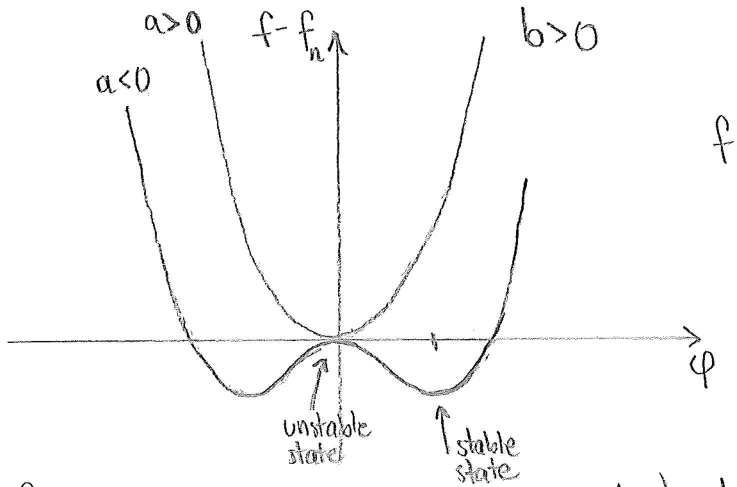
- Vector order parameter $\vec{\varphi}$: [H'berg FM]

  $O(N): \quad \vec{\varphi} \to \underset{\substack{\uparrow \\ \text{rotation matrix}}}{R}\,\vec{\varphi}$

  $\Rightarrow$ only $\vec{\varphi}^2 = \vec{\varphi}\cdot\vec{\varphi}$, $(\vec{\varphi}^2)^2$, $(\vec{\varphi}^2)^3$, ... allowed.

- coefficients $a(T)$, $b(T)$, ... are smooth functions of external parameters that preserve the symmetry (in particular, of the temperature)

Discussion for $h=0$ and $b>0$



$$f - f_n = \frac{a}{2}\varphi^2 + \frac{b}{4}\varphi^4$$

If $b(T)>0$ for $T \approx T_c$, then we can neglect higher-order terms $\propto O(\varphi^6)$ for φ near φ_{eq}:

$$\left.\frac{\partial f}{\partial \varphi}\right|_{\varphi_{eq}} = 0, \quad \left.\frac{\partial^2 f}{\partial \varphi^2}\right|_{\varphi_{eq}} > 0 \Rightarrow \varphi_{eq} = \begin{cases} 0, & a>0 \quad \text{disordered state} \\ \pm\sqrt{\frac{(-a)}{b}}, & a<0 \quad \text{ordered state} \end{cases}$$

Phase transition:

$$T = T_c \iff a(T) = 0$$

Expansion in <u>reduced temperature</u> $t = \frac{T - T_c}{T_c}$ (deviation from critical point):

$$a(T) = \alpha t + \mathcal{O}(t^2)$$

where we have assumed that $a(T)$ is smooth across the transition.

Order parameter:

$$\langle \varphi \rangle (T) = \begin{cases} 0 & , \; T > T_c \\ \pm\sqrt{\frac{\alpha}{b}(-t)} & , \; T < T_c \end{cases}$$

Remarks:

- In general $\langle \varphi \rangle (t<0) \propto (-t)^{\beta}$ with a critical exponent β ($\beta = \frac{1}{2}$ in Landau theory)
- Spontaneously broken $\mathbb{Z}_2$: $\langle \varphi \rangle (t<0) = \pm\sqrt{\frac{-a}{b}}$
  Spontaneously broken $O(N)$: $\langle \vec{\varphi} \rangle (t<0) = \sqrt{\frac{-a}{b}} \; \vec{e}_0$
  arbitrary direction

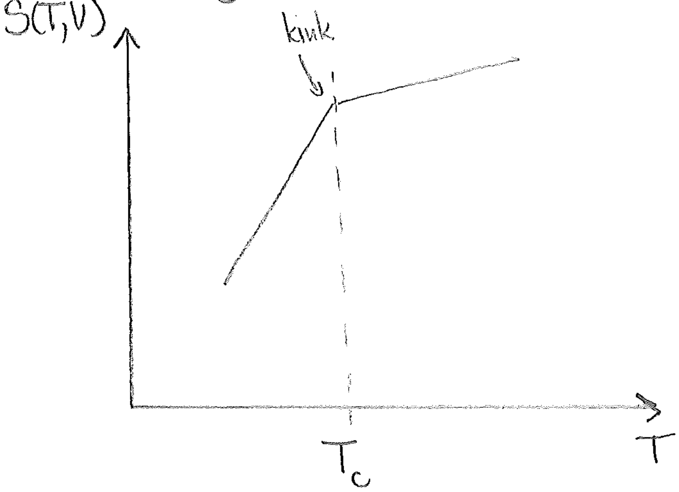
Thermodynamic observables:

$$f(T) = f(T, \varphi_{eq}) = \begin{cases} f_n(T) & , \; T > T_c \\ f_n(T) - f_0 \frac{\alpha^2}{4b} \left(\frac{T_c - T}{T_c}\right)^2 & , \; T < T_c \end{cases}$$

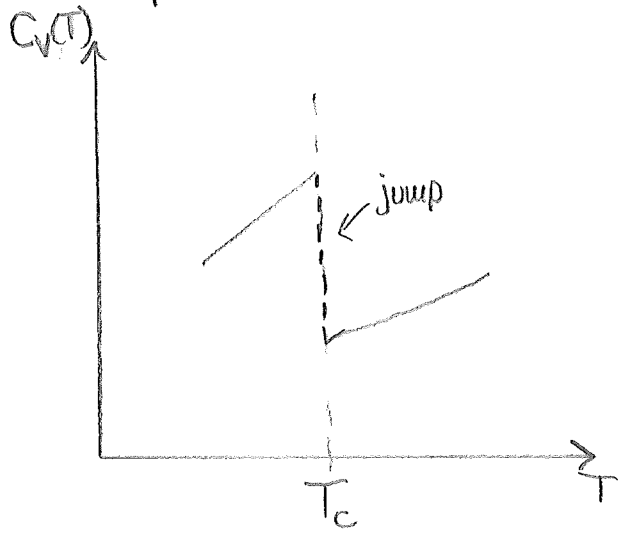
$$\frac{S}{V} = -\left(\frac{\partial f}{\partial T}\right)_V = \begin{cases} S_0(T) & , \; T > T_c \\ S_0(T) - f_0 \frac{\alpha^2}{2b} \frac{T_c - T}{T_c^2} & , \; T < T_c \end{cases}$$

$$C_V = \frac{T}{V}\left(\frac{\partial S}{\partial T}\right)_V = \begin{cases} C_0 & , \; T > T_c \\ C_0 + f_0 \frac{\alpha^2}{2b} \frac{T}{T_c^2} & , \; T < T_c \end{cases}$$

Entropy:



Specific heat:



In general: $C_V(T) = C_\pm \, |t|^{\alpha} + \mathcal{O}(t^2)$

with critical exponent α ($\alpha = 0$ in Landau theory)

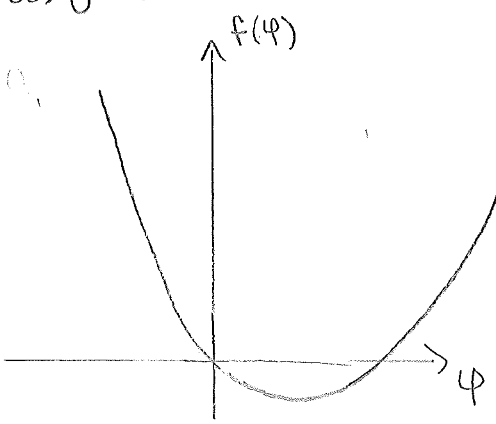
<u>Discussion for $h=0$ and $b<0$</u> : see exercises

<u>Discussion for $h \neq 0$ and $b>0$</u>

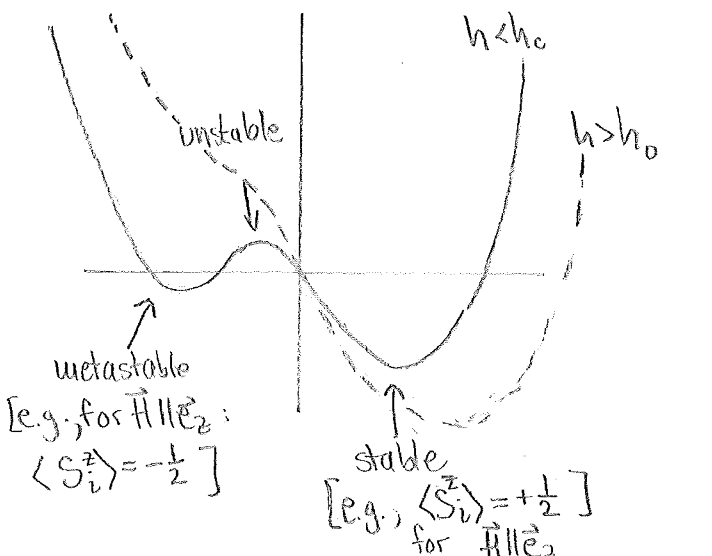
Equilibrium state:

$$\frac{\partial f}{\partial \varphi} = 0 \quad \Rightarrow \quad \underset{(*)}{a\varphi + b\varphi^3} = h \quad \text{with } a = a(T) = \alpha_0 t + \mathcal{O}(t^2)$$

$a>0$: one solution



$a<0$: $\begin{cases} \text{three solutions}, & h<h_0 \\ \text{one solution}, & h>h_0 \end{cases}$



Susceptibility χ:

$$\varphi(h) = \varphi_{spont} + \chi(T) \cdot h + \mathcal{O}(h^2)$$

with $\chi := \left.\frac{\partial \varphi}{\partial h}\right|_{h \to 0}$ the <u>order-parameter susceptibility</u>

and φ_{spont} the zero-field OP ("spontaneous order")

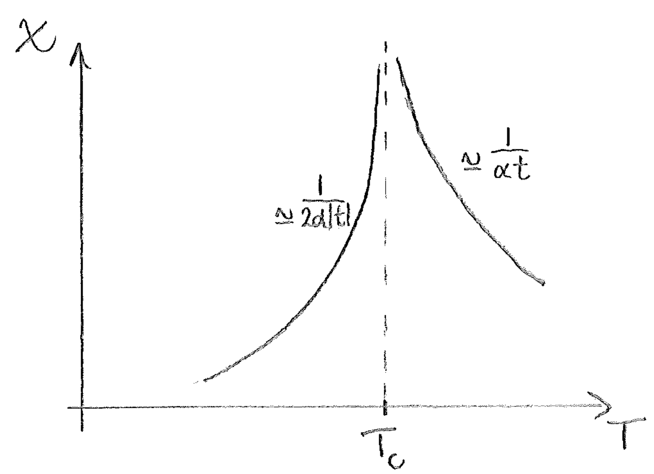
From (*) for small h:

$$a(T)\left[\varphi_{spont} + \chi(T) h\right] + b\left[\varphi_{spont} + \chi(T) h\right]^3 = h$$

with $\varphi_{spont} = \begin{cases} 0 & , T > T_c \\ \sqrt{\frac{-a}{b}} & , T < T_c \end{cases}$

we get by expanding in h to the leading order:

$$\chi(T) = \begin{cases} \frac{1}{\alpha t} & , \quad T > T_c \\ \frac{1}{2\alpha |t|} & , \quad T < T_c \end{cases} \qquad \Rightarrow \lim_{T \to T_c} \chi(T) = \infty$$



In general:

$$\chi(T) \propto |t|^{-\gamma} + \mathcal{O}(t^2) \quad \text{with critical exponent } \gamma$$

($\gamma = 1$ in Landau theory)

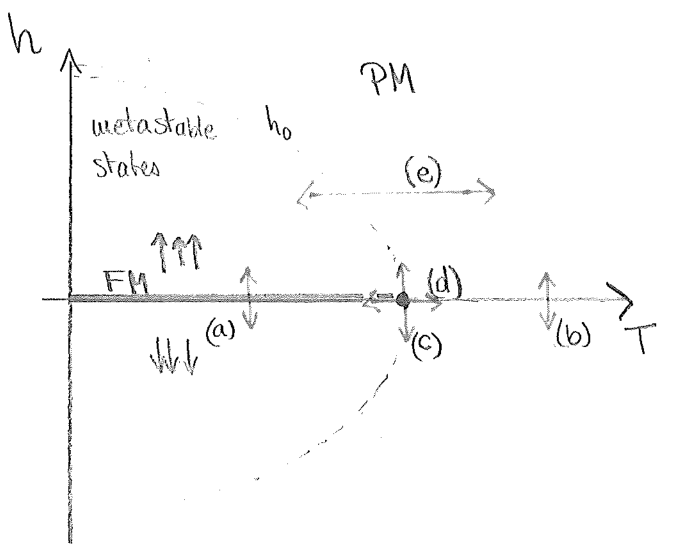
From (*) for finite h at $T=T_c \Leftrightarrow a(T)=0$:

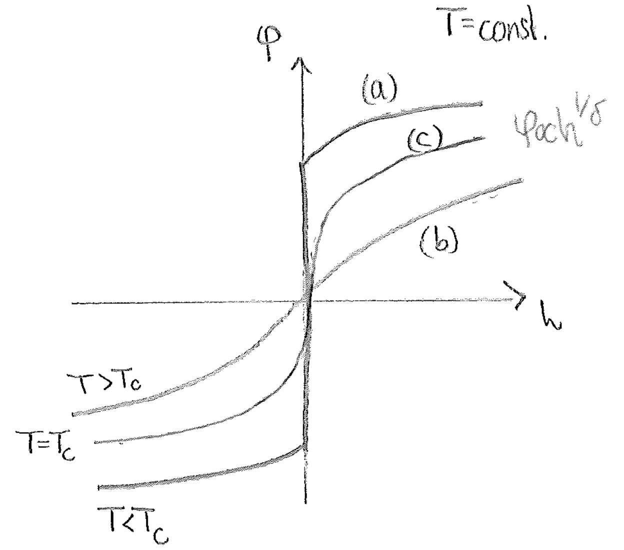
$$\varphi = \left(\frac{h}{b}\right)^{1/3} \qquad \text{"critical isotherm"}$$

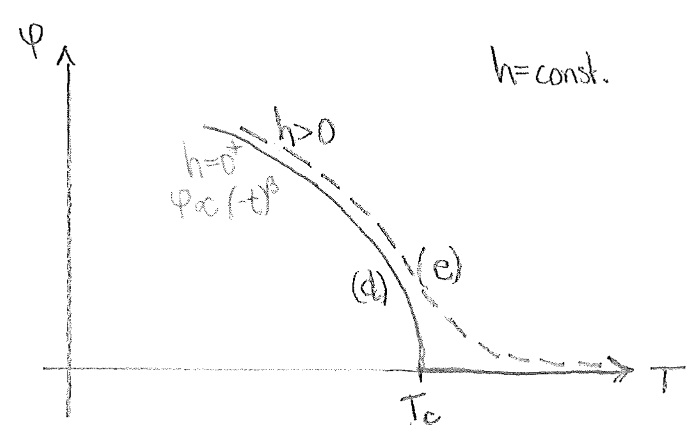
In general : $\varphi \propto |h|^{1/\delta}$ with critical exponent δ

($\delta = 3$ in Landau theory)

Phase diagram :







Remarks:

- Line of first-order transition at $h=0$ for $T<T_c$ (a)
- Here: the two states at $h=0^+$ and $h=0^-$ are related by $\mathbb{Z}_2$ symmetry
  $\Rightarrow$ latent heat $Q = \Delta S = 0$ (typically: $Q \neq 0$)
- Metastable states for $h<h_0$ and $T<T_c$
  $\Rightarrow$ hysteresis in $\varphi(h)$ near $h \approx 0$
- Continuous transition at $T=T_c$ and $h=0$ (c,d)
- "Crossover" for $T>T_c$ (b) or $h \neq 0$ (e) (no phase transition)

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Ginzburg-Landau theory and spatial correlations

Allow spatial variations for OP or fluctuations:

$$\varphi \longmapsto \varphi(\vec{r})$$

where $\vec{r}$ is a continuous space coordinate and $\varphi(\vec{r})$ is a smooth function, capturing variations on lengths scales much larger than microscopic lengths ("continuum-limit description")

[important to compute correlations, but also for inhomogeneous condensates $\rightarrow$ superconductors in field!]

Ginzburg-Landau functional:

$$f(T, H, \varphi(\vec{r})) = f_n + f_0 \left[\frac{a}{2} \varphi(\vec{r})^2 + \frac{b}{4} \varphi(\vec{r})^4 + \xi_0^2 \left(\vec{\nabla}_{\vec{r}} \varphi(\vec{r})\right)^2 - \varphi(\vec{r}) h \right]$$
$$+ \mathcal{O}(\varphi^6, \nabla^4, \nabla^2 \varphi^4)$$

energy cost of spatial variation

Ginzburg-Landau (free) energy:

$$F = \int d^d \vec{r} \, f(\vec{r})$$

Correlations:

$$G(\vec{r},\vec{r}\,') = \langle \varphi(\vec{r})\varphi(\vec{r}\,')\rangle - \langle \varphi(\vec{r})\rangle\langle \varphi(\vec{r}\,')\rangle = \langle \varphi(\vec{r})\varphi(\vec{r}\,')\rangle - \varphi_0^2$$

"propagator"

with $\varphi_0 \equiv \langle \varphi(\vec{r})\rangle$ homogenous OP.

In the large-distance limit for $T < T_c$:

$$\lim_{|\vec{r}-\vec{r}\,'|\to\infty} \langle \varphi(\vec{r})\varphi(\vec{r}\,')\rangle = \varphi_0^2 \neq 0 \qquad \text{"long-range order"}$$

and thus $G(\vec{r},\vec{r}\,')$ measures <u>correlations of fluctuations around φ_0</u>.

Expansion of φ around φ_0:

$$\varphi(\vec{r}) = \varphi_0 + \delta\varphi(\vec{r})$$

Free energy:

$$F(\varphi(\vec{r})) = F(\varphi_0) + \delta F \quad \text{with} \quad \delta F = \frac{f_0}{2}\int d^d\vec{r}\; \delta\varphi(\vec{r})\left(\alpha t + 3b\varphi_0^2 - \xi_0^2 \vec{\nabla}_{\vec{r}}^{\,2}\right)\delta\varphi(\vec{r})$$

with $a(T) = \alpha t + O(t^2)$ and the terms linear in $\delta\varphi$ vanish due to the equilibrium condition $\left.\frac{\delta F}{\delta\varphi}\right|_{\varphi_0} = 0$.

Fourier decomposition $\delta\varphi(\vec{r}) = \int \frac{d^d k}{(2\pi)^d}\, \delta\varphi(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}$:

$$\delta F = \frac{k_B T}{2}\int \frac{d^d\vec{k}}{(2\pi)^d}\, \delta\varphi(-\vec{k})\, G^{-1}(\vec{k})\, \delta\varphi(\vec{k})$$

with

$$G(\vec{k}) = \langle \delta\varphi(\vec{k})\delta\varphi(-\vec{k})\rangle = \frac{k_B T}{f_0\left[A(T) + \xi_0^2 \vec{k}^2\right]}$$

and $A(T) \equiv \alpha t + 3b\varphi_0^2 = \begin{cases} \alpha t & , T > T_c \\ -2\alpha t & , T < T_c \end{cases}$

Fourier back transform:

$$G(\vec{r},\vec{r}') = \int \frac{d^d\vec{k}}{(2\pi)} G(\vec{k})\, e^{i\vec{k}(\vec{r}-\vec{r}')} \propto \frac{e^{-\frac{r}{\xi(T)}}}{r^{\frac{d-1}{2}}}\, \xi(T)^{\frac{3-d}{2}} \quad , \quad r = |\vec{r}-\vec{r}'|$$

with <u>correlation-length ξ</u>:

$$\xi(T) = \begin{cases} \dfrac{\xi_0}{\sqrt{\alpha t}} & , \quad T > T_c \\[2ex] \dfrac{\xi_0}{\sqrt{2\alpha|t|}} & , \quad T < T_c \end{cases}$$

which diverges for $T \to T_c$.

In general: $\xi(T) \propto |t|^{-\nu}$ with critical exponent ν

($\nu = \frac{1}{2}$ in Ginzburg-Landau theory)

Remarks:

- Divergent length scale ξ: locally ordered "islands" of increasing size
- $\varphi(\vec{r})$ varies slowly near criticality $\Rightarrow$ justifies gradient expansion a posteriori
- Also: divergent correlation time $\tau_c \to \infty$ ("critical slowing down")

At criticality ($A(T)=0$):

$$G(\vec{k}) \propto \frac{1}{k^2} \quad \Rightarrow \quad G(r) \propto r^{2-d} \qquad (d>2)$$

In general: $G(r) \propto r^{2-d-\eta}$ with <u>"anomalous dimension" η</u>.

($\eta = 0$ in Landau-Ginzburg theory)

Fluctuations and Ginzburg criterion

Landau theory can be "derived" as a saddle-point solution of a field theory formulated as a functional integral (see chapter 3)
$\Rightarrow$ neglects fluctuations ("mean-field approximation")

Ginzburg criterion for the validity of Landau theory:

$$\underbrace{\frac{\langle \delta\varphi(\vec{r}=\xi(T)\vec{e})\,\delta\varphi(0)\rangle}{\varphi_0^2}}_{\text{"effective relative size of fluctuations"}} \propto \frac{\xi(T)^{2-d}}{|t|} \propto |t|^{\frac{d-4}{2}} \xrightarrow{|t|\to 0} \begin{cases} 0 & d>4 \\ \infty & d<4 \end{cases}$$

$\langle\delta\varphi\,\delta\varphi\rangle \propto \xi^{2-d}$, $\quad \xi \propto |t|^{-1/2}$, $\quad \varphi_0 \propto (-t)^{1/2}\ (T<T_c)$

$\Rightarrow$ Landau theory asymptotically exact for $d>4$

Remarks:

- $d_c^+ = 4$ is called "upper critical dimension"
- d_c^+ depends on (some general) system properties
- Critical exponents of Landau theory ("mean-field exponents") exact for $d>d_c^+$
- Logarithmic corrections directly at $d=d_c^+$
- Landau theory fails <u>at criticality</u> for $d<d_c^+$
- Mean-field exponents still observable in systems in which the numerical prefactor in the Ginzburg criterion is small (e.g., conventional superconductors: $t_{cr} \approx 10^{-10} \ll 1$)
- Consistent account for fluctuations beyond mean field: renormalization group (see chapter 4)

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2.4 Critical exponents and universality

At criticality:

$\xi \to \infty \quad \Rightarrow$ fluctuations on all length scales "scale invariance"

Observables follow <u>power laws</u>:

$$\underset{(\varphi,\, C_v,\, \chi,\, \xi,\, \dots)}{A} \sim \underset{(t,\, h,\, \dots)}{x}{}^{y}$$

with some critical exponent $y = \alpha, \beta, \gamma, \delta, \eta, \nu, \dots$

Common critical exponents:

Observable	Exponent	Definition	Conditions	MF value (GL) $d > d_c$	Example: Ising ($d=3$)
Specific heat	α	$C \propto \lvert t\rvert^{-\alpha}$	$t \to 0,\ h=0$	$\alpha = 0$	$\alpha \approx 0.110$
Order parameter	β	$\varphi \propto (-t)^{\beta}$	$t \to 0^-,\ h=0$	$\beta = \frac{1}{2}$	$\beta \approx 0.326$
Susceptibility	γ	$\chi \propto \lvert t\rvert^{-\gamma}$	$t \to 0,\ h=0$	$\gamma = 1$	$\gamma \approx 1.237$
Critical isotherm	δ	$h \propto \lvert\varphi\rvert^{\delta}\, \mathrm{sgn}(\varphi)$	$t=0,\ h \to 0$	$\delta = 3$	$\delta \approx 4.789$
Correlation length	ν	$\xi \propto \lvert t\rvert^{-\nu}$	$t \to 0,\ h=0$	$\nu = \frac{1}{2}$	$\nu \approx 0.630$
Correlation function	η "anomalous dimension"	$G(r) \propto \lvert r\rvert^{-d+2-\eta}$	$t=0,\ h=0$	$\eta = 0$	$\eta \approx 0.0363$
Correlation time	z "dynamical exponent"	$\tau_c \propto \xi^{z} \propto \lvert t\rvert^{-\nu z}$	$t \to 0,\ h=0$	n/a	n/a

Remark:

- z will play a special role in quantum phase transitions, c.f. chapter 6
- Scale invariance of power laws: E.g.,

$$C \propto |t|^{-\alpha} \propto \xi^{\alpha/\nu} \xrightarrow{\xi \mapsto b\xi} b^{\alpha/\nu}\, C$$

Universality:

- Critical exponents identical for microscopically completely different systems
- Systems fall into universality classes: E.g., $\mathbb{Z}_2$ universality = {Ising model, liquid-gas critical point, ...}
- Universality classes characterized by only very few general properties:

  dimension d, symmetry of order parameter, presence or absence of long-range interactions
- Phenomenological reason: $\xi \to \infty$ $\Rightarrow$ microscopic details become irrelevant
- Deeper understanding: renormalization group (RG), see Chapter 4

2.5 Scaling hypothesis

Assumption: ξ is only length scale near criticality

Scaling transformation:

$$x \to b\,x \qquad \text{lengths}$$
$$t \to b^{y_t}\,t \qquad \text{reduced temperature}$$
$$h \to b^{y_h}\,h \qquad \text{external field}$$

Scale invariance: change in length can be compensated by change in t and h (for appropriate y_t, y_h)

Scaling hypothesis for free energy density:

$$f_s(t,h) = b^{-d}\, f_s(b^{y_t}\,t,\; b^{y_h}\,h)$$

singular part of free energy

"f_s is homogenous in both t and h."

Consequence:

All critical exponents can be related to y_t and y_h and there exist thus only two independent exponents in static critical phenomena

Example (correlation length):

Scaling transf.: $\xi \propto |t|^{-\nu} \xmapsto{t \to b^{y_t} t} b^{-y_t \nu} |t|^{-\nu} \propto b^{-y_t \nu} \xi \xmapsto{x \to bx} b^{1-y_t\nu} \xi$

Scale invariance: $\xi \mapsto \xi \Rightarrow \underline{\underline{\nu = \frac{1}{y_t}}}$

Example (free energy density at $h=0$):

$$f_s(t, h=0) = b^{-d} f_s(b^{y_t} t, 0)$$

Choose b such that $b^{y_t}|t| = 1$: $b^{-d} = |t|^{\frac{d}{y_t}} = |t|^{d\nu}$,

$$f_s(t, h=0) = |t|^{d\nu} f_s(\pm 1, 0) \Rightarrow \underline{\underline{f_s(t, h=0) \propto |t|^{d\nu}}}$$

Example (specific heat):

$$C_V \propto T \frac{\partial^2 f}{\partial T^2} \propto |t|^{d\nu - 2} \Rightarrow \underline{\underline{\alpha = 2 - d\nu}} \qquad \text{"Josephson's law"}$$

Scaling hypothesis for correlation function ($h=0$):

$$G(r; t, h=0) = \frac{f_G\left(\frac{r}{\xi(t)}\right)}{r^{d-2+\eta}}$$

Critical point ($t=0$):

$$G(r; t=0, h=0) = \frac{f_G(0)}{r^{d-2+\eta}}$$

Susceptibility:

$$\chi = \left.\frac{\partial \langle \varphi \rangle}{\partial h}\right|_{h\to 0} \propto \int d^d r\, G(r; t) \propto \int dr\, f_G(r|t|^{\nu})\, r^{1-\eta} \qquad \begin{bmatrix} x = r|t|^{\nu} \\ dx = |t|^{\nu} dr \end{bmatrix}$$

$$= \underbrace{\int dx\, f_G(x)\, x^{1-\eta}}_{\text{const.}} |t|^{-(2-\eta)\nu}$$

$$\Rightarrow \underline{\underline{\gamma = (2-\eta)\nu}} \qquad \text{"Fisher's law"}$$

Other scaling relations ($h>0$):

$$\alpha + 2\beta + \gamma = 2 \qquad \text{"Rushbrooke's law"}$$

$$\alpha + \beta(\delta+1) = 2 \qquad \text{"Griffiths' law"}$$

Remarks:

- Scaling hypothesis is an assumption that can be justified with RG (chapter 4)
- It holds for $d<d_c^+$, but not for $d>d_c^+$ ("hyperscaling violation")
- Mean-field exponents violate Josephson's law (unless $d=d_c^+$)

26.4.24