

2 Classical phase transitions and universality

(6)

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)

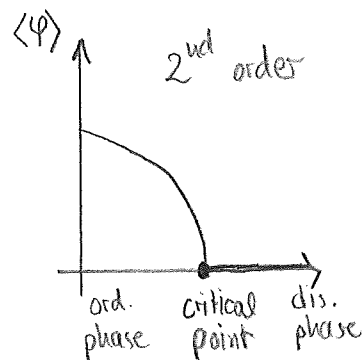
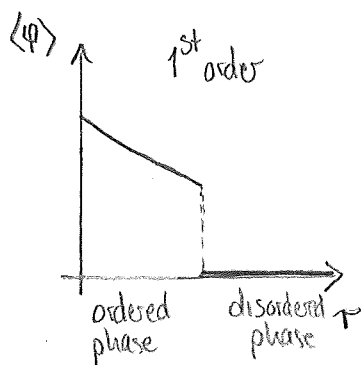
Remarks:

- 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") (7)

Correlation length ξ : In stable phases 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 [$a/\xi \rightarrow 0$]

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 $\hat{\rho}$ is not symmetric under \hat{S} , $[\hat{\rho}, \hat{S}] \neq 0$, then the symmetry \hat{S} is spontaneously broken.

Remarks:

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- Spontaneous symmetry breaking requires nonanalyticity of thermodynamic potential (otherwise: $[\hat{H}, \hat{S}] = 0$ would imply $[\hat{S}, \hat{S}] = \frac{1}{2} [e^{-\beta \hat{H}}, \hat{S}] = 0$)
 \Rightarrow phase transition

- Singularity can be seen by including a small conjugate field h :

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

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

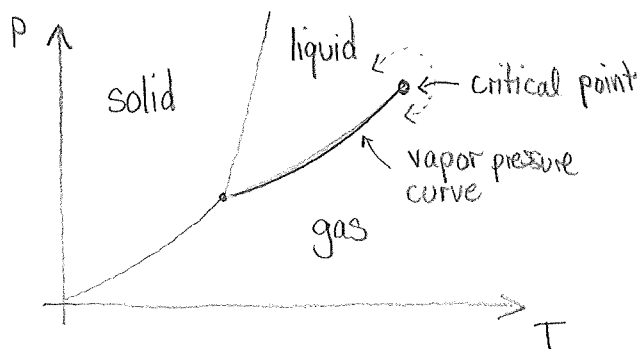
- Spontaneous symmetry breaking impossible in a finite-size system
($e^{-\beta \hat{H}}$ not singular for $N < \infty$)

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

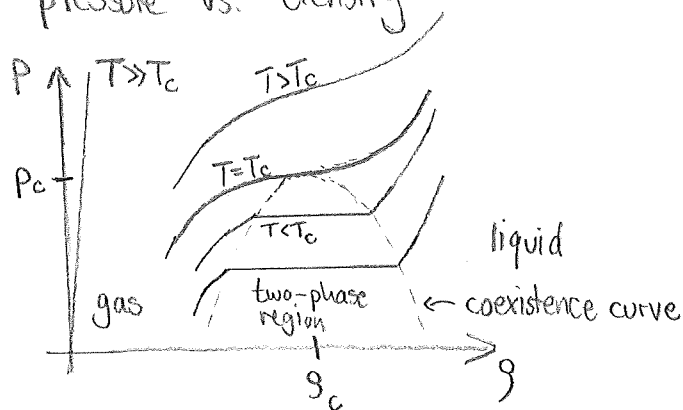
2.2 Generic phase diagrams of fluids and magnets

Fluid

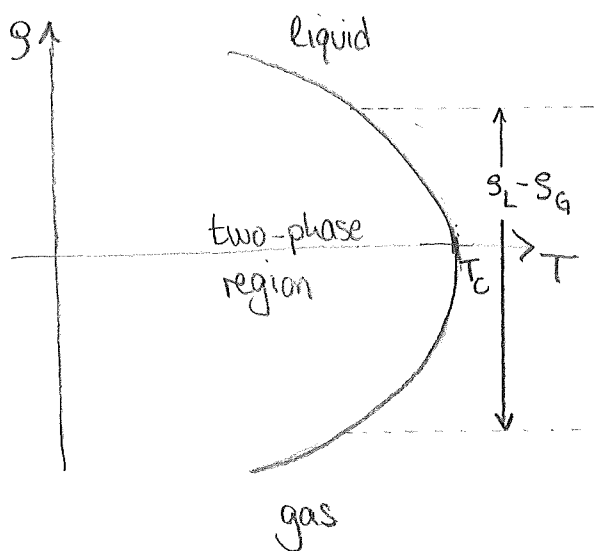
Pressure vs. temperature



pressure vs. density

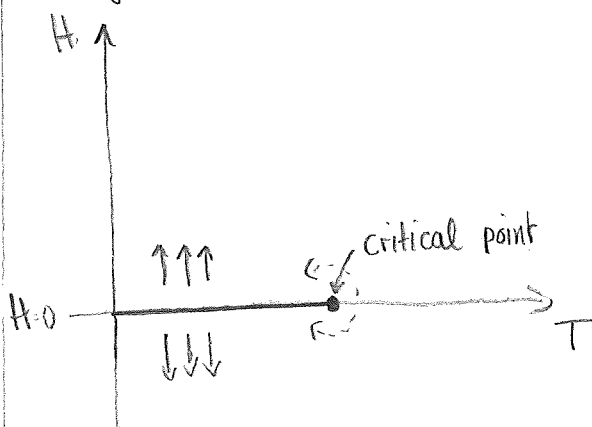


density vs. temperature

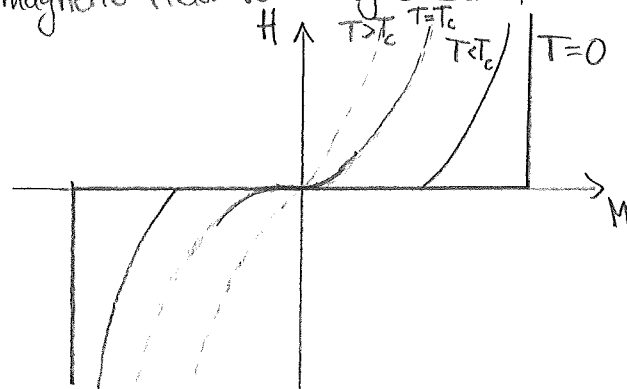


Magnet

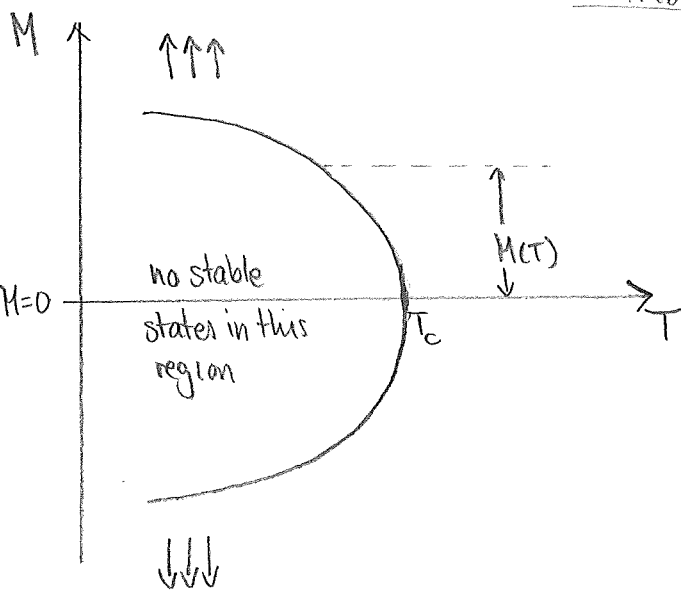
magnetic field vs. temperature



magnetic field vs. magnetization



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2.3 Landau theory of phase transitions

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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:

$$\begin{array}{ccc} f(T, H) & \longmapsto & f(T, H, \varphi) \\ \uparrow & & \uparrow \\ \text{thermod. pot.} & & \text{Landau potential} \end{array}$$

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

Equilibrium state:

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

Expansion of Landau potential:

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

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

Remarks:

- f includes all symmetry-allowed terms, e.g. for $H=0$:

[liquid-gas trans.]
[Ising trans.]

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

\Rightarrow only even powers in φ allowed

- Vector order parameter $\vec{\varphi}$:

[H'beg FM]

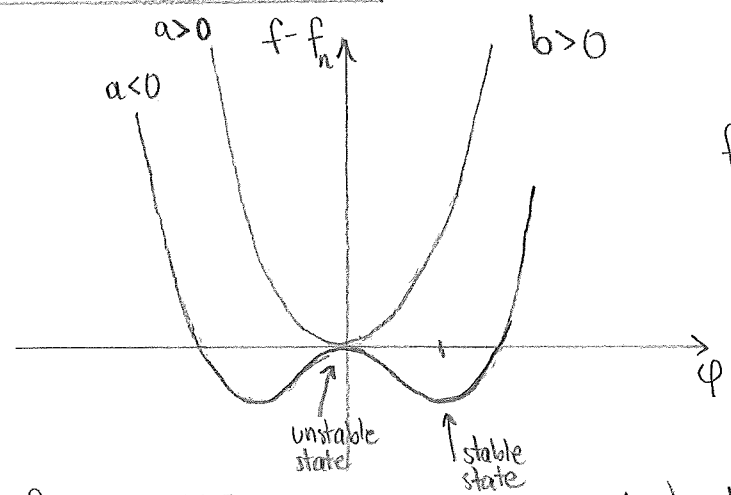
$$O(N): \quad \vec{\varphi} \rightarrow R \vec{\varphi}$$

↑
rotation matrix

\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 (e.g., temperature) that preserve symmetry

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} :

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

Phase transition:

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

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

$$a(T) = a_1 t + \mathcal{O}(t^2)$$

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

Order parameter:

$$\langle \varphi \rangle(T) = \begin{cases} 0 & , T > T_c \\ \pm \sqrt{\frac{a_1}{b}(-t)} & , T < T_c \end{cases}$$

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 : $\langle \varphi \rangle(t < 0) = \pm \sqrt{\frac{-a}{b}}$

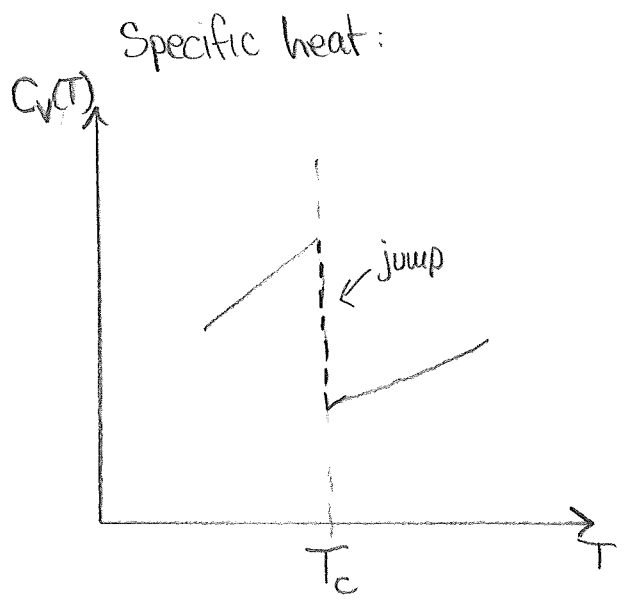
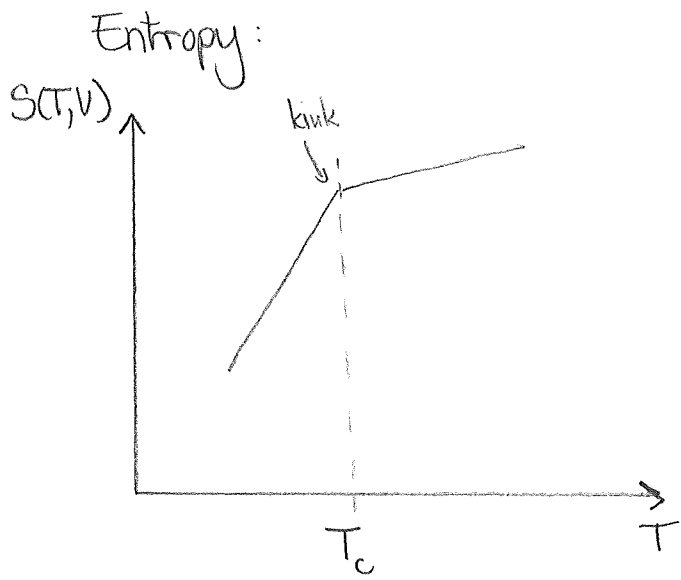
Spontaneously broken $O(N)$: $\langle \vec{\varphi} \rangle(t < 0) = \sqrt{\frac{-a}{b}} \vec{e}_0$
↑ arbitrary direction

Thermodynamic observables:

$$f(T) = f(T, \varphi_{eq}) = \begin{cases} f_n(T) & , T > T_c \\ f_n(T) - f_0 \frac{a_1^2}{4b} \left(\frac{T_c - T}{T_c}\right)^2 & , T < T_c \end{cases}$$

$$\frac{S}{V} = - \left(\frac{\partial f}{\partial T} \right)_V = \begin{cases} s_0(T) & , T > T_c \\ s_0(T) - f_0 \frac{a_1^2}{2b} \frac{T_c - T}{T_c^2} & , T < T_c \end{cases}$$

$$C_v = \frac{T}{V} \left(\frac{\partial S}{\partial T} \right)_V = \begin{cases} c_0 & , T > T_c \\ c_0 + f_0 \frac{a_1^2}{2b} \frac{T}{T_c^2} & , T < T_c \end{cases}$$



In general: $C_V(T) = C_{\pm} |t|^{\alpha} + O(t^2)$
 with critical exponent α ($\alpha=0$ in Landau theory)

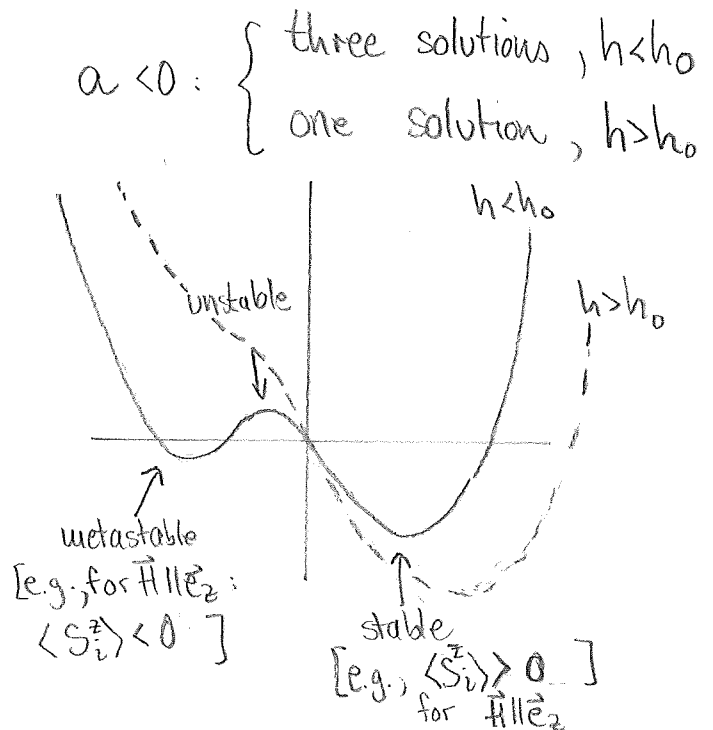
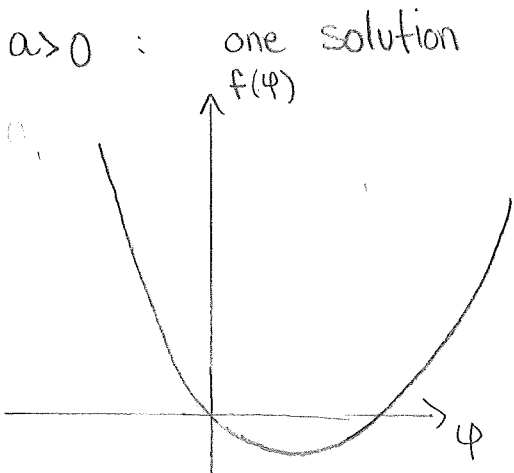
Discussion for $h=0$ and $b < 0$: see exercises

Discussion for $h \neq 0$ and $b > 0$

Equilibrium state:

$$\frac{\partial f}{\partial \varphi} = 0 \Rightarrow a\varphi + b\varphi^3 = h \quad \text{with } a = a(T) = a_1 t + O(t^2)$$

(*)



Susceptibility χ :

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$$\Psi(h) = \Psi_{\text{spont}} + \chi(T) \cdot h + \mathcal{O}(h^2)$$

with $\chi := \left. \frac{\partial \Psi}{\partial h} \right|_{h \rightarrow 0}$ the order-parameter susceptibility

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

From (*) for small h :

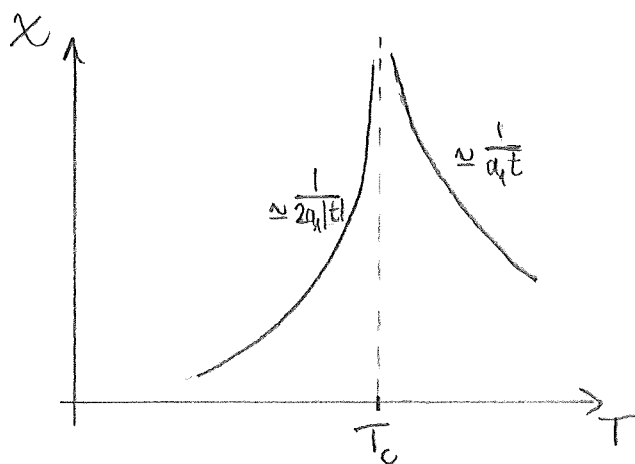
$$a(T) [\Psi_{\text{spont}} + \chi(T)h] + b [\Psi_{\text{spont}} + \chi(T)h]^3 = h$$

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

We get by expanding in h to the leading order:

$$\chi(T) = \begin{cases} \frac{1}{aT} & , T > T_c \\ \frac{1}{2a|t|} & , T < T_c \end{cases}$$

$$\Rightarrow \lim_{T \rightarrow T_c} \chi(T) = \infty$$



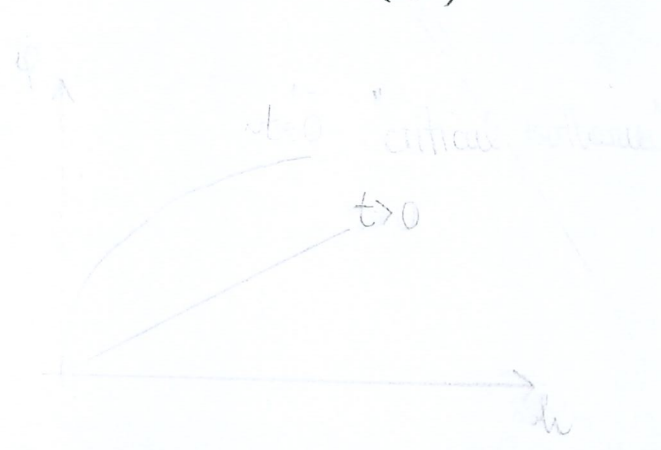
In general:

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

($\gamma = 1$ in Landau theory)

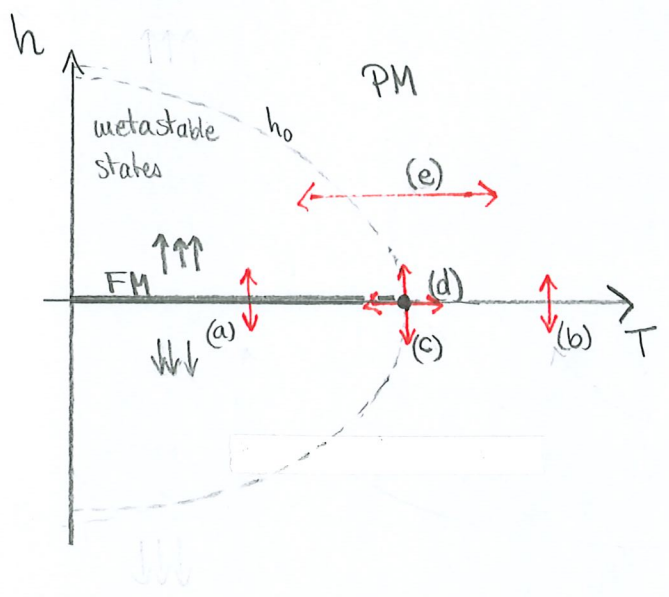
From (*) for finite h at $T=T_c \Leftrightarrow a(T)=0$:

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

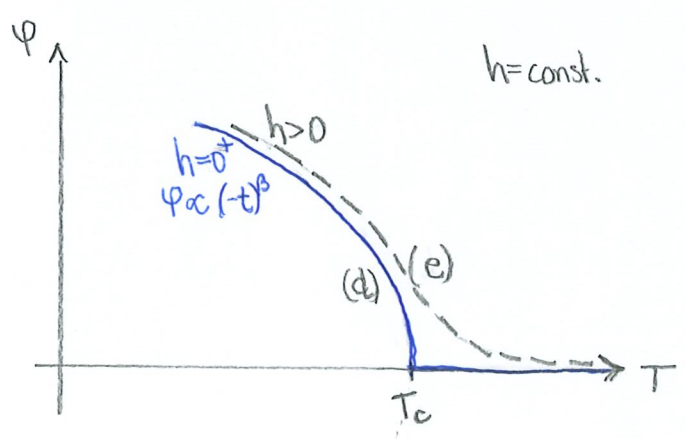
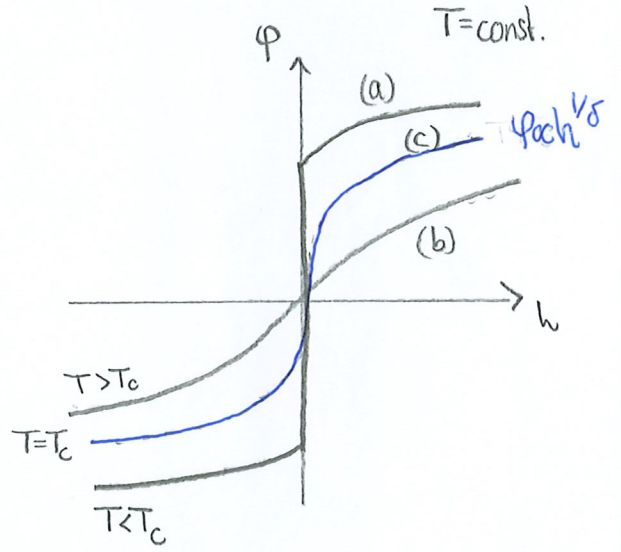


In general : $\varphi \propto |h|^{1/\delta}$ with critical exponent δ
 ($\delta=3$ in Landau theory)

Phase diagram :



Order parameter :



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 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 $\Psi(h)$ 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)

Ginzburg-Landau theory and spatial correlations

Allow spatial variations for OP or fluctuations:

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

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:

$$f(T, H, \varphi(\vec{r})) = f_n + f_0 \left[\frac{a}{2} \varphi(\vec{r})^2 + \frac{b}{4} \varphi(\vec{r})^4 + \sum_0^2 (\vec{\nabla}_{\vec{r}} \varphi(\vec{r}))^2 - \varphi(\vec{r}) h \right] + O(\varphi^6, \nabla^4, \nabla^2 \varphi^4)$$

\uparrow
energy cost of spatial variation

Ginzburg-Landau (free) energy:

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

Correlations :

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

"propagator"

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

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

$$\lim_{|\vec{r}-\vec{r}'| \rightarrow \infty} \langle \Psi(\vec{r}) \Psi(\vec{r}') \rangle = \varphi_0^2 \neq 0 \quad \text{"long-range order"}$$

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

Expansion of Ψ around φ_0 :

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

Free energy ($h=0$):

$$F(\Psi(\vec{r})) = F(\varphi_0) + \delta F \quad \text{with} \quad \delta F = \frac{f_0}{2} \int d^d \vec{r} \delta\Psi(\vec{r}) \left(a_1 t + 3b\varphi_0^2 - \sum_0^2 \vec{\nabla}_{\vec{r}}^2 \right) \delta\Psi(\vec{r})$$

with $a(T) = a_1 t + \mathcal{O}(t^2)$ and the terms linear in $\delta\Psi$ vanish due to the equilibrium condition $\left. \frac{\delta F}{\delta \Psi} \right|_{\varphi_0} = 0$.

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

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

with

$$G(\vec{k}) = \langle \delta\Psi(\vec{k}) \delta\Psi(-\vec{k}) \rangle = \frac{k_B T}{f_0 \left[A(\pi) + \sum_0^2 \vec{k}^2 \right]}$$

$$\text{and} \quad A(\pi) \equiv a_1 t + 3b\varphi_0^2 = \begin{cases} a_1 t & , T > T_c \\ -2a_1 t & , T < T_c \end{cases}$$

Fourier back transform:

$$G(\vec{r}, \vec{r}') \propto \int \frac{d^d k}{(2\pi)^d} G(\vec{k}) e^{i\vec{k}(\vec{r}-\vec{r}')} \propto \frac{e^{-\frac{r}{\xi(T)}}}{r^{\frac{d-1}{2}}} \xi(T)^{\frac{3-d}{2}}, \quad r = |\vec{r}-\vec{r}'| \quad (18)$$

with correlation-length ξ :

$$\xi(T) = \begin{cases} \frac{\xi_0}{\sqrt{a_1 t}} & , T > T_c \\ \xi_0 & , T < T_c \\ \sqrt{2a_1 |t|} & \end{cases}$$

which diverges for $T \rightarrow T_c$.

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 $\tau_c \rightarrow \infty$ ("critical slowing down")

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

$$G(\vec{k}) \propto \frac{1}{k^2} \Rightarrow G(r) \propto r^{2-d} \quad (d > 3)$$

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

($\eta = 0$ 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)
 ⇒ neglects fluctuations ("mean-field approximation")

Ginzburg criterion for the validity of Landau theory:

$$\frac{\langle \delta\psi(\vec{r}=\xi(T)\vec{e}) \delta\psi(0) \rangle}{\varphi_0^2} \propto \frac{\xi(T)^{2-d}}{|t|} \propto |t|^{\frac{d-4}{2}} \xrightarrow{|t| \rightarrow 0} \begin{cases} 0 & d > 4 \\ \infty & d < 4 \end{cases}$$

$\leftarrow \propto \xi^{2-d}$
 $\leftarrow \propto |t|^{-1/2}$
 $\leftarrow \propto (-t)^{1/2} \quad (T < T_c)$

↑ effective relative size of fluctuations"

⇒ 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 at criticality 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)

2.4 Critical exponents and universality

At criticality:

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

Observables follow power laws:

$A \sim x^y$ with some critical exponent $y = \alpha, \beta, \gamma, \delta, \nu, \dots$
↑ (φ, C_v, χ, ξ, ...) ↑ (t, h, ...)

Common critical exponents:

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

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

Universality :

- Critical exponents identical for microscopically completely different systems
- Systems fall into universality classes : E.g., 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: $\xi \rightarrow \infty \Rightarrow$ microscopic details become irrelevant
- Deeper understanding: renormalization group (RG), see Chapter 4

2.5 Scaling hypothesis

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Assumption: ξ is only length scale near criticality

Scaling transformation:

$$x \rightarrow x' = \frac{x}{b} \quad \text{lengths} \quad (\text{"zoom out"})$$

$$t \rightarrow t' = b^{y_t} t \quad \text{reduced temperature}$$

$$h \rightarrow h' = b^{y_h} h \quad \text{external field}$$

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):

$$\text{Scaling transf.: } \xi \propto |t|^{-\nu} \xrightarrow{\substack{x=bx' \\ t=b^{y_t}t'}} b \xi' \propto b^{y_t \nu} |t|^{-\nu} \Rightarrow \xi \propto b^{y_t \nu - 1} |t|^{-\nu}$$

$$\text{Scale invariance: } y_t \nu - 1 = 0 \Rightarrow \underline{\underline{\nu = \frac{1}{y_t}}}$$

Example (free energy density at h=0):

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

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

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

Example (specific heat):

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

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:

$$\chi = \left. \frac{\partial \langle \varphi \rangle}{\partial h} \right|_{h \rightarrow 0} \propto \int d^d r G(r; t) \propto \int dr f_G(r|t|^\nu) r^{1-\eta} \quad \left[\begin{array}{l} x = r|t|^\nu \\ dx = |t|^\nu dr \end{array} \right]$$

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

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

Other scaling relations ($h > 0$):

$\alpha + 2\beta + \gamma = 2$ "Rushbrooke's law"

$\alpha + \beta(\delta + 1) = 2$ "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 $d = d_c^+$)

4.5.26