Thermodynamic laws

p.7-9 Huang

I: $dU = \delta Q - \delta W$ is an exact differential, therefore

$U_B = \cancel{A}U_A + \int_{\gamma_{AB}} dU$, where γ_{AB} arbitrary. It follows, that

$C_p - C_v = nR > 0$. p. 53 Landau

II: Kelvin: It is impossible to devise a cyclically operating device, the sole effect of which is to absorb energy in the form of heat from a single thermal reservoir and to deliver an equivalent amount of work.

Landau (Clausius): If a closed system is at some ~~point~~ instant in a non-equilibrium macroscopic state, the most probable consequence at later instants is a steady increase in the entropy of the system.

Using Carnot define $\oint \frac{\delta Q}{T} = 0 \Rightarrow S_B = S_A + \int_{\gamma_{AB}} \underbrace{\frac{\delta Q_{rev}}{T}}_{=:dS}$.

Alternatively, $S_B > S_A$. (defines an arrow of time)

→ No contradiction!

p. 192 Landau ↙

III: Planck-Nernst: the entropy tends to a constant value S_0, independent of pressure, Volume, state of aggregation, when the temperature is lowerd toward its absolute zero.

$\Rightarrow \alpha, \beta, C_V, C_p$ vanish for $T \to 0$. Remember $C_V \begin{array}{l} \propto T^3 \text{ phonons} \\ \propto T \text{ metals} \end{array}$

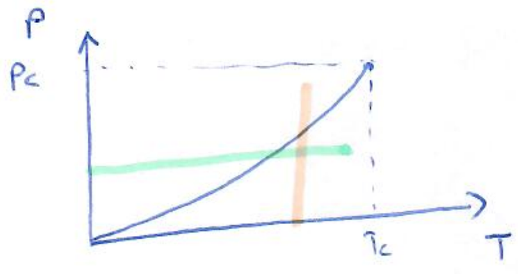
Beware: absolute zero cannot be reached

Phase diagrams

p. 251 - 259 Landau
p. 32 Huang

P-T

tells everything about the existinge phases and transitions

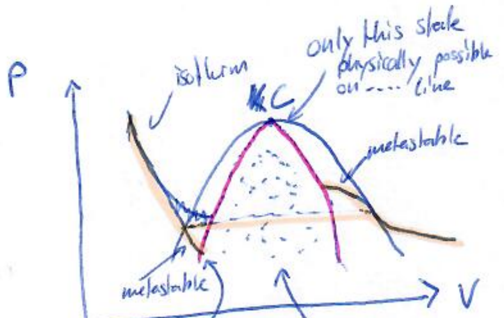


critical points only for phases differing purely quantitive (Liquid/Gas). Not possible for qualitatively different (solid/liquid), have different internal symmetry. Equilibrium curve to infinity or terminating by intersection of equilibrium-curve of other phases.

p. 136 Chaikin
eg. for ϕ for $P_{LG}(T)$

p-V

P(V) must be decreasing due to $\frac{\partial p}{\partial V}|_T < 0$, Stability



supercooling

line defined by $\frac{\partial p}{\partial V}|_T = 0$

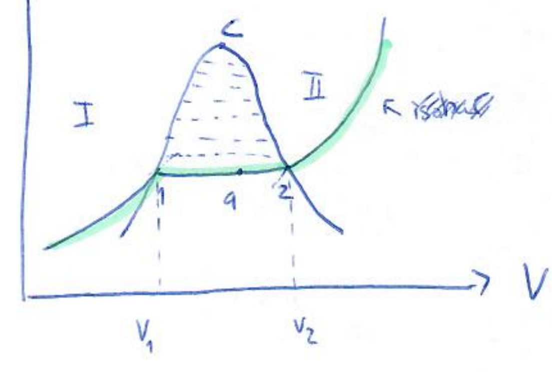
body cannot exist in homogeneous state, violates $\frac{\partial p}{\partial V}|_T \leq 0$

isotherms terminate there where $\frac{\partial p}{\partial V}|_T = 0$

spinodal line

supersaturation

T-V



lever-rule
quantities of phase I and II are inversely propotional to a1 and a2.

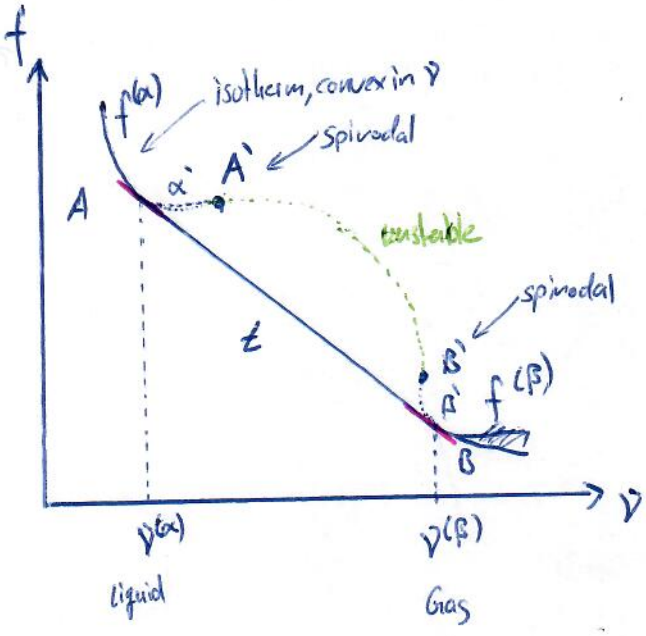
at C the $V_1 = V_2$.

The location of phase coexistance in a p-V,-T diagram are ruled surfaces which projecte on the p-T plane define $P_{\alpha\beta}(T)$. Phases cannot be distinguished beyond the critical points.

Maxwell Construction

p.261 Landau

p41. Huang



no curvature $\Rightarrow \left.\frac{\partial^2 f}{\partial v^2}\right|_T = 0 \Rightarrow \kappa_T = \infty$

⇝ infinitely compressible

unstable $\Leftrightarrow \left.\frac{\partial^2 f}{\partial v^2}\right|_T = \frac{1}{\kappa_T v}$ changes sign

The point between metastable and unstable is called spinodal.

From $p^{(\alpha)}(T, v^{\alpha}) = p^{(\beta)}(T, v^{\beta}) = p_{\alpha\beta}(T)$ it follows that

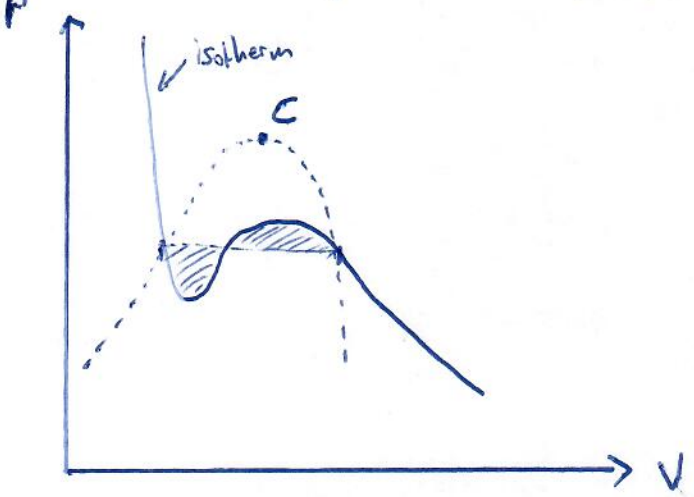
$$p = -\left.\frac{\partial f}{\partial v}\right|_T \Rightarrow \text{tangent } t$$

Definition of t comes from $\mu^{(\alpha)} = \mu^{(\beta)}$

$$\Rightarrow (f + pv)^{(\alpha)} = (f + pv)^{(\beta)}$$

$$\xRightarrow{\boxed{!\ p^{(\alpha)} = p^{(\beta)}}} \frac{f^{(\alpha)} - f^{(\beta)}}{v^{(\alpha)} - v^{(\beta)}} = -p_{\alpha\beta}$$

alternatively, $\mu^{(\alpha)} = \mu^{(\beta)} \Leftrightarrow \int_\alpha^\beta d\mu = 0 \xRightarrow[d\mu = vdp]{dG=0} \int_\alpha^\beta v\,dp = 0$



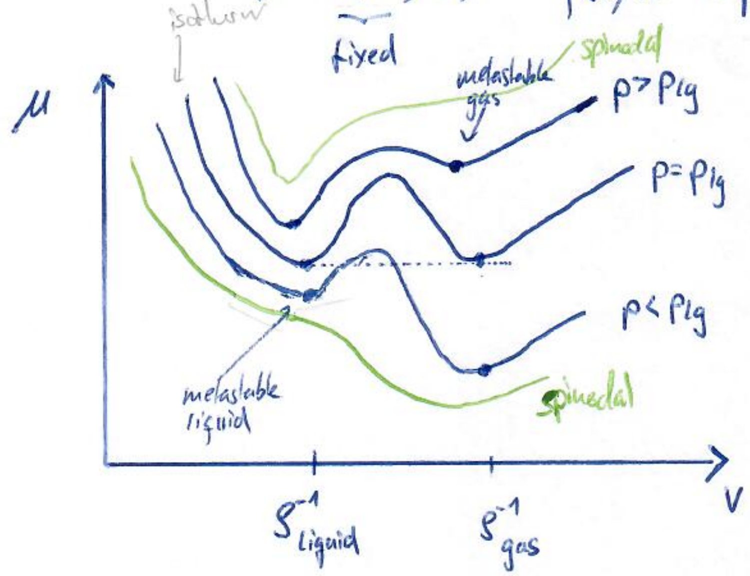
Constraining parameters in phase transitions

$$\underbrace{f = -pv + \mu}_{(T,V)} \Rightarrow \underbrace{g = f + pv}_{(T,p)} = \mu$$

Keeping the volume as a constraint parameter and plot

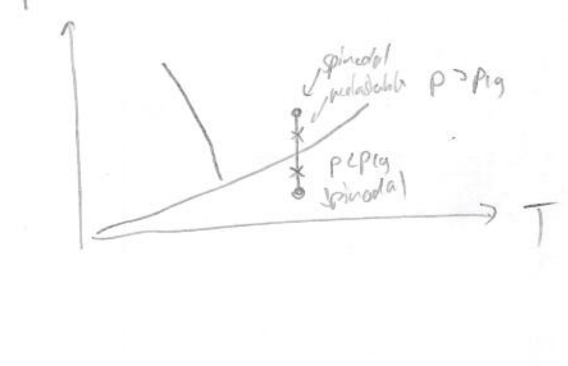
$$\mu(\underbrace{T,p}_{\text{fixed}}; v) = f(v,T) + pv$$ (partial legendre transformation)

First order transition



$$\frac{\partial \mu}{\partial v} = \frac{\partial f}{\partial v} + p = -p + p = 0 \Rightarrow \quad p = -\frac{\partial f}{\partial v} \text{ equivalent to } \frac{\partial \mu}{\partial v} = 0$$

Examples for metastable states: undercooled gas / overheated liquid phases



Nucleation in first order transitions

p.481 Chaikin

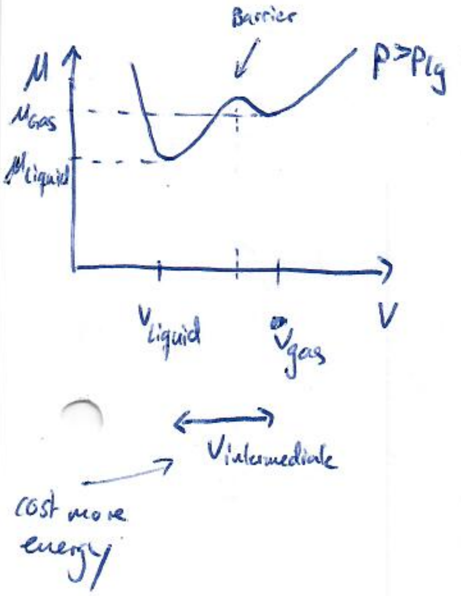
p36 Huang

Amount δn_{gas} condenses into an isotropic liquid droplet of radius r

$$\delta n_{gas} = -\delta n_{Li} = \underbrace{\frac{4}{3}\pi r^3 \cdot \rho_{Li}}_{\#\text{particles}} \frac{1}{N_A}$$

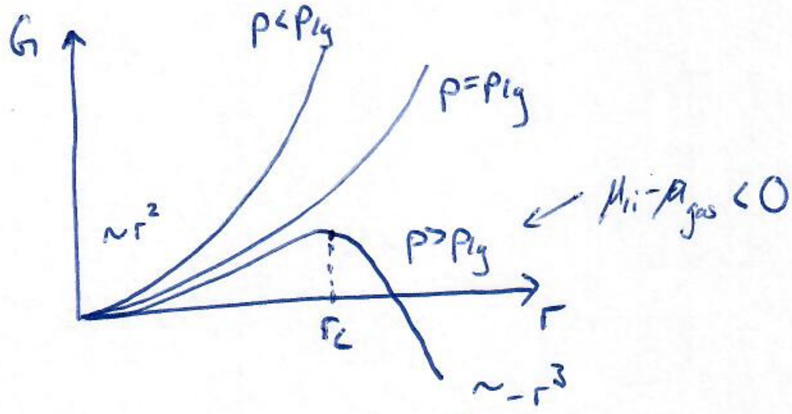
Avogadro n in mole

particle density



surface tension

$$G(r) = \frac{4}{3}\pi r^3 \rho_{Li} \frac{1}{N_A}(\mu_{Li} - \mu_{Gas}) + 4\pi r^2 \sigma_{lg}$$



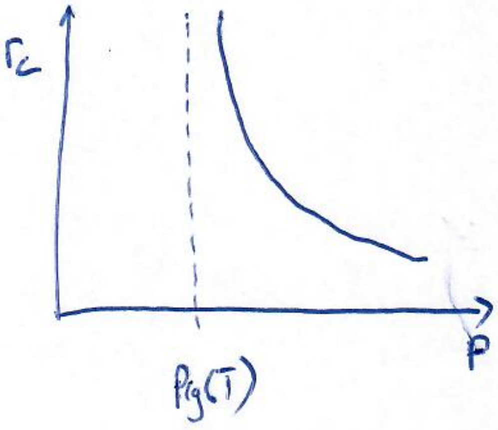
System runs away
droplet grows, Gas → liquid

To find r_c for $(\mu_{Li} < \mu_{Gas})$ $\frac{\partial G}{\partial r} = 0$

$$\Rightarrow r_c = \frac{2\sigma_{lg} N_A}{\rho_{Li}} \frac{1}{\mu_{Gas} - \mu_{Li}}$$

Calculations →

$$r_c(p,T) = \frac{2\sigma v_{Li}}{RT \log(P/P_{Liquid})}$$



Canonical Distrib.

Fluctuation: $\Gamma \approx \underbrace{\omega_{mikro}}_{} e^{-G(r_c)/k_B T}$

~ collision time between gas particles

Gibbs - Duhem

A function $f(x_1,\dots,x_N)$ is homogeneous of order k, if

$$f(\lambda x_1,\dots,\lambda x_N) = \lambda^k f(x_1,\dots,x_N).$$

If $k=1$ then Eulers Theorem applies

$$f(x_1,\dots,x_n) = \sum_{i=1}^{n} x_i \frac{\partial f}{\partial x_i}\Big|_{x_j \neq x_i}$$

Starting from $U = TS - pV + \mu N$ and taking the derivative

$$dU = TdS + SdT - pdV - Vdp + \mu dN + Nd\mu$$

and using $dU = Td - pdV + \mu dN$ we get the equation of Gibbs-Duhem

$$SdT - Vdp + Nd\mu = 0.$$

alternatively use

$$G - \mu N = 0$$

$$\Big\downarrow d/dx$$

$$SdT - Vdp + Nd\mu = 0$$

Gibbs' phase rule

p. 264 Landau

pressure p, temperature T and amount of substances (in moles) n_i, $i \in \{1, --, r\}$ is prescribed. ⤳ appropriate thermodynamic potential is G. The associated equilibrium parameters are the chemical potentials $\mu_i^{(\alpha)}$ of the i-th substance in the α-th phase, $\alpha \in \{I, --, \nu\}$

$$\mu_i^{(\alpha)}(p, T, x_1^{(\alpha)}, \dots, x_{r-1}^{(\alpha)}) \quad \Rightarrow \quad r+1 \text{ intensive variables}$$

Gibbs-Duhem

$$\underbrace{\overset{p,T}{2} + r - 1}_{\text{Gibbs duhem}}$$

$$\underset{p,T}{2} + \underset{\text{phase}}{\nu}\underbrace{(r-1)}_{\text{Gibbs-duhem}} \text{ intensive variables}$$

Equilibrium imposes $r(\nu-1)$ conditions:

r ↓ ~~phase~~ component

$$\begin{rcases} \mu_1^{I} \overset{1}{=} \mu_1^{II} \overset{2}{=} \dots \overset{\nu-1}{=} \mu_1^{\nu} \\ \mu_2^{I} = \mu_2^{II} = \dots = \mu_2^{\nu} \\ \vdots \qquad\qquad\qquad \vdots \\ \mu_r^{I} = \mu_r^{II} = \dots = \mu_r^{\nu} \end{rcases}$$

determines a system of equation with $r\underbrace{(\nu-1)}_{\#\text{of "=" signs}}$ equations

for a substance all chemical potentials in different phases must be equal →

$\xrightarrow{\qquad}$ phases ν

The degrees of freedom is therefore given by

$$f = 2 + \nu\overbrace{(r-1)}^{\text{Gibbs duhem}} - r(\nu-1)$$

leading to

$$f = 2 + \underset{\text{components}}{r} - \underset{\text{phase}}{\nu}. \qquad \text{(Gibbs phase rule)}$$

E.g. one component system $r=1$

only Gas $\Rightarrow$ $\nu = 1$ $\Rightarrow$ $f = 2$ $\Rightarrow$ possible in an area in a p-T diagram

e.g. Gas and liquid $\Rightarrow$ $\nu = 2$ $\Rightarrow$ $f = 1$ $\Rightarrow$ along a line ⤳ $p_{\text{Gas, liquid}}(T)$

Gas, liquid, solid $\Rightarrow$ $\nu = 3$ $\Rightarrow$ $f = 0$ $\Rightarrow$ triple point $P_{\alpha\beta\gamma}\, T_{\alpha\beta\gamma}$, system of equation determined fully

Clausius - Clapeyron

p.255 Landau

We start by the equilibrium condition $\mu_1(p_{\alpha\beta}(T), T) = \mu_2(p_{\alpha\beta}(T), T)$. Differentiating,

$g = \mu$

$\frac{\partial g}{\partial T} = -s \overset{?}{=} \frac{\partial \mu}{\partial T}$

$$\underbrace{\frac{\partial \mu_1}{\partial T}}_{-s_1} + \underbrace{\frac{\partial \mu_1}{\partial p_{\alpha\beta}}}_{v_1} \frac{d p_{\alpha\beta}}{dT} = \underbrace{\frac{\partial \mu_2}{\partial T}}_{-s_2} + \underbrace{\frac{\partial \mu_2}{\partial p_{\alpha\beta}}}_{v_2} \frac{d p_{\alpha\beta}}{dT}$$

$$\Rightarrow \qquad \frac{dp(T)}{dT} = \frac{s_1 - s_2}{v_1 - v_2}$$

and use $T \Delta s = L$, (latent heat)

$$T \frac{d p_{\alpha\beta}(T)}{dT} = \frac{L}{\Delta v}$$

Measuring L and Δv at fixed p and T for different values of T allows us to find the transition line $p_{\alpha\beta}$ through simple integration.

Ehrenfest Classification

phase transition $\longleftrightarrow$ non analyticity in thermodyn. potential

↳ can only appear in thermodyn. limit, i.e. infinitely many degrees of freedom.

phase transition of n-th order $\overset{\text{def.}}{\Longleftrightarrow}$ jump appears in n-the derivative

modern
- with latent heat, first order with jump in order parameter
- second order transition, smooth developement of order parameter with divergent susceptibility and correlation length ⇝ "continuous transition"

Beware: Kosterlitz - Thouless

- does not break symmetry and does not have order parameter

⇒ typical characteristics of second order transition (critical exponent) manifest themselves along continuation of the first order phase line.

Statistical Description (Introduction)

p.10 Landau

$$\begin{pmatrix}\dot{q}_i\\ \dot{p}_i\end{pmatrix}=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}\begin{pmatrix}\frac{\partial H}{\partial q_i}\\ \frac{\partial H}{\partial p_i}\end{pmatrix}\ , \quad \langle M\rangle = \frac{\int d^{3N}p\, d^{3N}q\ M(p,q)\,\rho(p,q)}{\underbrace{\int d^{3N}p\, d^{3N}q\ \rho(p,q)}}$$

(Ensemble average)

density function ← probability that the system is around (p,q) in Γ

Liouville

$$\partial\rho/\partial t \ \underbrace{+\,\mathrm{div}(\rho \overset{=\dot{x}_i}{v})}_{\substack{=0\\ \text{steady flow}}} = 0 \quad \Rightarrow \sum_{i=1}^{N}\left[\frac{\partial}{\partial q_i}(\rho\dot{q}_i)+\frac{\partial}{\partial p_i}(\rho\dot{p}_i)\right]=0$$

$$\Rightarrow \underbrace{\sum_{i=1}^{N}\left[\dot{q}_i\frac{\partial\rho}{\partial q_i}+\dot{p}_i\frac{\partial\rho}{\partial p_i}\right]}_{\frac{d\rho}{dt}}+\rho\underbrace{\sum_{i=1}^{N}\left[\frac{\partial\dot{q}_i}{\partial q_i}+\frac{\partial\dot{p}_i}{\partial p_i}\right]}_{\substack{=0\\ \text{Hamilton equations}}}=0 \quad\Rightarrow\quad \frac{d\rho}{dt}=0\ ,\ \text{where}$$

$\frac{\partial\rho}{\partial t}$ not necessarily zero.

⇝ ρ is an incompressible fluid in Γ-space.

isolated/closed system

Microcanonical Ensemble (Entropy definition)

$\mathcal{H} \to \Gamma$, $dw = \rho\, dp\, dq$, Liouvill $\Downarrow$ $\rho = \text{const}$ along path

A system with fixed E, V, N in equilibrium is described by

$\sim \frac{1}{h^{3N} N!}$ ← Gibbs paradox $[h]$ = action, vanishes from $\langle M \rangle$

$$\rho(p,q) = \text{const} \cdot \delta(E - E_0) \cancel{\delta(P-P_0)\delta(M-M_0)}$$

and is called the microcanonical distribution. As $\rho(p,q) = \rho(H(p,q))$ one gets $\partial_t \rho = 0$, i.e. ρ is time independant in thermodynamic equilibrium.

The fundamental idea of statistical mechanics is that $\overline{M}^T = \langle M \rangle$

time average Ensemble average.

The assumption made here is that the system covers $\Gamma_{N,E,V}$ homogeneously. This ergodic hypothesis is however not true in general. Ergodicity is broken in the physics of glasses.

$$\Gamma(E) := \int d^{3N}p\, d^{3N}q\, \rho(p,q) \overset{\text{microcan.}}{=} \int_{E < H(p,q) < E+\Delta} \frac{d^{3N}p\, d^{3N}q}{N!\, h^{3N}}$$

$$\Sigma(E) := \int_{H(p,q) < E} \frac{d^{3N}p\, d^{3N}q}{N!\, h^{3N}}$$ (dimensionless due to h)

$$\omega := \frac{d\Sigma(E)}{dE}$$ (density of states)

$$\Rightarrow \quad \Gamma(E) = \Sigma(E+\Delta) - \Sigma(E) \simeq \omega(E)\Delta$$

additivity on p. 26 Landau

$$S(E,V,N) := k_B \log \Gamma(E)$$

- extensive in E, V, N
- in isolated system maximal

} Entropy counts the number of available states in Γ-space and its maximization directs the isolated system towards a homogeneous distribution of states compatible with E, V, N.

Entropy following Landau

p. 23. Landau

Landau

$dw = \varrho(p_1,\dots,p_N,q_1,\dots,q_N)\,dp\,dq$,

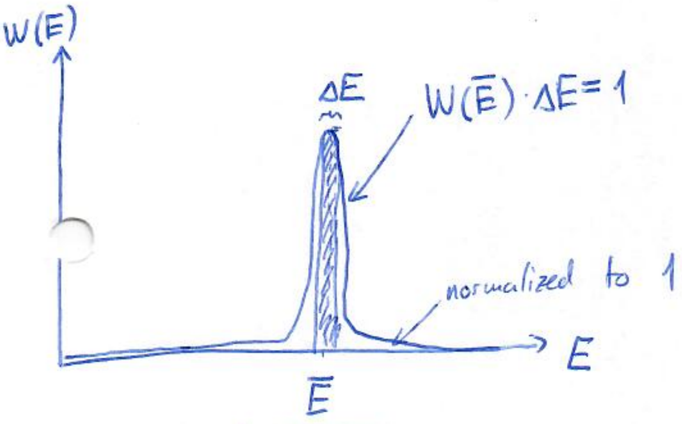
$W(E)dE$ = probability that system Energy E and E+dE

$\Gamma(E)$ = # states with Energy $\leq$ E

$\boxed{\frac{d\Gamma(E)}{dE}}dE$ = # states with energy between E and E+dE

$$\underbrace{W(E)}_{\text{max. at } \bar{E}} = \underbrace{\frac{d\Gamma(E)}{dE}}_{\#\text{ states for } E}\ \underbrace{w(E)}_{\text{probability to be in } E}$$

not necessarily maximum at $\bar{E}$



$$\Rightarrow W(\bar{E})\Delta E = \boxed{\underbrace{\boxed{\frac{d\Gamma(\bar{E})}{dE}}\Delta E}_{=\Delta\Gamma}}\cdot w(\bar{E}) = \Delta\Gamma\, w(\bar{E}) = 1$$

$\boxed{\Delta\Gamma}$ = # states corresponding to ΔE

$\Delta E \sim$ mean fluctuation

$$S = \log \boxed{\Delta\Gamma}$$

Blatter

$$\Gamma(E) = \int d^{3N}p\, d^{3N}q\ \varrho(p,q)$$

$$\Sigma(E) = \int_{H<E} \frac{d^{3N}p\, d^{3N}q}{N!\, h^{3N}}$$

$$\boxed{\omega(E) = \frac{d\Sigma(E)}{dE}}$$ (Density of states)

$$\Gamma(E) \approx \boxed{\boxed{\omega(E)}\,\Delta}$$

Δ

$$S = k_B \log \boxed{\Gamma(E)}$$

(microcanonical derivation)

Entropy of an ideal gas

following p. 138 Huang

$\int_0^{p^*}$ $p^* \leftarrow$ where $\sum \frac{p_i^*}{2m} = E$

$$H = \frac{1}{2m} \sum_{i=1}^{N} p_i^2 \quad , \; N, \; U \quad \text{are fixed}$$

$$\Sigma(E) = \frac{1}{N!\,h^{3N}} \int_{H<E} d^3p_1 \cdots d^3p_N \underbrace{\int d^3q_1 \cdots d^3q_N}_{V^N}$$

Define $R := \sqrt{2mE} = \sqrt{\sum_i p_i^2}$

$$\Rightarrow \quad \Sigma(E) = \frac{1}{N!}\left(\frac{V}{h^3}\right)^N \Omega_{3N}(R) \overset{\text{n-sphere}}{=} \left(\frac{V}{h^3}\right)^N C_{3N} R^{3N}$$

$$= \frac{1}{N!} C_{3N} \left[\frac{V}{h^3} (2mE)^{3/2} \right]^N$$

$$\overset{\text{Stirling}}{\Rightarrow} \quad S(E,V,N) = k_B \log \Sigma = N k_B \left[\log \frac{V}{N} + \log \left(\frac{4\pi m E}{3 N h^2} \right)^{3/2} + \frac{5}{2} \right]$$

$$\overset{\text{inversion}}{\Rightarrow} \quad U(S,V,N) = \frac{3h^2}{4\pi m} \left(\frac{N}{V} \right)^{2/3} N \exp\left(\frac{2}{3} \frac{S}{N k_B} - \frac{5}{3} \right)$$

$$T = \frac{\partial U}{\partial S}\Big|_V = \frac{2}{3} \frac{U}{N k_B} \, , \quad U = \frac{3}{2} N k_B T = E$$

also via equipartition Theorem

$$C_V = \frac{\partial U}{\partial T}\Big|_V = \frac{3}{2} N k_B$$

$$\Rightarrow \quad S = N k_B \log \frac{V}{N} + C_V \log T + \text{const}$$

$$p = -\frac{\partial U}{\partial V}\Big|_S = \frac{2}{3} \frac{U}{V} = \frac{N k_B T}{V}$$

(microcanonical Ensemble)

Equipartition Theorem

p. 136 Huang / 129. landau

$$\boxed{\left\langle x_i \frac{\partial H}{\partial x_j} \right\rangle = \delta_{ij} k_B T}$$

Example: $H = \sum_{i=1}^{N} \frac{p_i^2}{2m} \Rightarrow \left\langle \frac{p_i^2}{2m} \right\rangle = \frac{1}{2} k_B T$, i.e. in equilibrium every motional degree of freedom carries the energy $\frac{k_B T}{2}$. Therefore,

$$\langle H \rangle = U = \underset{\text{N-particles}}{\overset{\text{3-dimensions}}{\frac{3}{2} N k_B T}}$$

Example: Harmonic oscillator: $H = \sum_i a p_i^2 + b q_i^2$

$$\sum_i \left\langle p_i \frac{\partial H}{\partial p_i} + q_i \frac{\partial H}{\partial q_i} \right\rangle = \langle 2H \rangle = \sum 2 k_B T$$

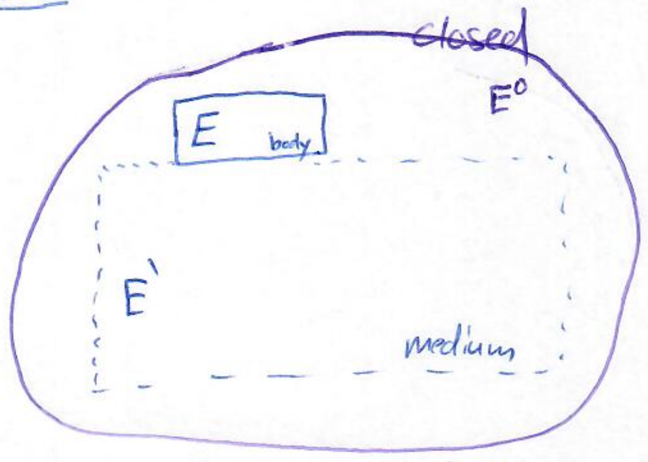
$\Rightarrow$ As a result, every kinetic and potential degree of freedom carries the energy $\frac{k_B T}{2}$.

Beware! $C_V = \frac{f}{2} k_B N$ is only true for classical ~~degree~~ System where every degree of freedom can be excited by arbitrarily small energy. In quantum mechanics a finite energy δE is requireled and equipartition is only valid for $k_B T > \delta E$.

The Gibbs Distribution

p. 79 landau

Apply the microcanonical distribution to



$$dw = \text{const.}\ \delta(E+E'-E^0)\,d\Gamma\,d\Gamma'$$

w_n = probability of state of the whole system, such that body concerned is in microscopically defined state (E_n).

$E^0 = E + E'$

$$\Gamma'(E') \Rightarrow \underset{\text{Substitution}}{d\Gamma'} = \underbrace{\frac{d\Gamma'(E')}{dE'}}_{\text{eq. 7.4}}dE'$$

$$\frac{e^{S'(E')}}{\Delta E'}$$

$d\Gamma = 1$

$E = E_n$

$$\Rightarrow w_n = \text{const.} \cdot \int \delta(E_n + E' - E^0)\,d\Gamma'$$

$$\Rightarrow w_n = \text{const.} \cdot \int \frac{e^{S'}}{\Delta E'}\,\delta(E' + E_n - E^0)\,dE'$$

$$\Rightarrow w_n = \text{const.}\ \frac{e^{S'}}{\Delta E'}\bigg|_{E' = E^0 - E_n}$$

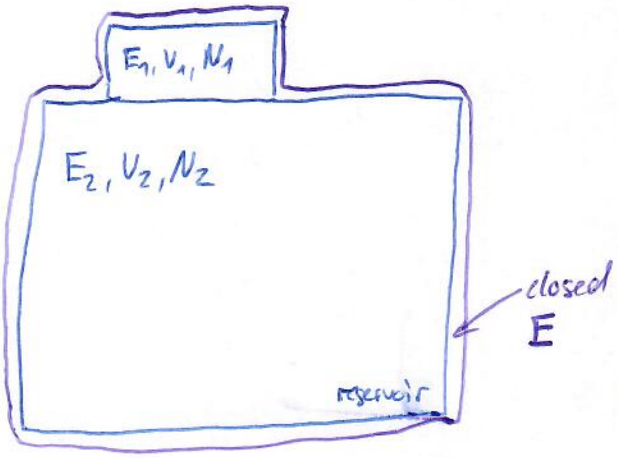
Assume the body is small $\Rightarrow E_n \ll E^0$. $\Delta E'$ doesn't vary much $\Rightarrow \Delta E' = \Delta E^0 = \text{const.}$

$$S'(E^0 - E_n) \underset{\text{Taylor}}{=} \underbrace{S'(E^0)}_{\text{const.}} - E_n \underbrace{\frac{dS'(E^0)}{dE^0}}_{\frac{1}{T}} \xrightarrow{T \to k_B T} \boxed{w_n = A e^{-E_n/k_B T}}$$

The Gibbs distribution gives the statistical distribution of any macroscopic body which is comparatively small part of a large closed system.

Canonical Ensemble

p. 143 Huang



$$\rho(p_1,q_1) \propto \underbrace{\Gamma_1(E_1)}_{\substack{=1 \\ \text{for fixed} \\ \text{State } (p,q)}} \Gamma_2(E_2) = \Gamma_2(E-E_1)$$

?

Using that $E_1 \ll E$

$$\Rightarrow k_B \log \Gamma_2(E-E_1) \overset{\text{def}}{=} S_2(E-E_1) = S_2(E) - E_1 \frac{\partial S(E_2)}{\partial E_2}$$

$$= S_2(E) - \frac{E_1}{T}$$

$$\Rightarrow \quad \Gamma(E-E_1) = \text{const}\; e^{-\frac{E_1}{k_B T}}$$

We define: $\rho(p,q) := \frac{1}{h^{3N} N!} e^{-H(p,q)/k_B T}$

$$Z_N := \int d^{3N}p\, d^{3N}q\; \rho(p,q) = \int \frac{d^{3N}p\, d^{3N}q}{N!\, h^{3N}} \exp\left[-\frac{H(p,q)}{k_B T}\right]$$

(partition function)

$$F(T,V,N) := -k_B T \log Z_N(V,T)$$

$$1 = \frac{1}{Z_N}\int d^{3N}p\, d^{3N}q\; \rho(p,q) \Rightarrow Z_N = e^{-\beta F} = \int d^{3N}p\, d^{3N}q \frac{1}{h^{3N}N!} e^{-\beta H}$$

$$\overset{\partial_\beta}{\Rightarrow} \frac{1}{Z_N}\int \frac{d^{3N}p\, d^{3N}q}{h^{3N}N!} e^{\beta[F-H]} \Big[\underbrace{F - H + \beta\frac{\partial F}{\partial \beta}}_{e^{-\beta F}}\Big] = 0$$

(products rule)

$$\Rightarrow \langle H \rangle = F + \beta\frac{\partial F}{\partial \beta} \Rightarrow U = F - T\frac{\partial F}{\partial T}$$

$$\beta\frac{\partial}{\partial\beta} = \beta\frac{\partial}{\partial T}\frac{\partial T}{\partial \beta} = -T\frac{\partial}{\partial T}$$

Grand canonical Ensemble p. 149 Huang

We start from the (Canonical Ensemble) the partition function

$$Z_N(T,V) = \int d^{3N}p\, d^{3N}q \; \frac{e^{-\beta H(p,q)}}{N!\, h^{3N}}$$

written as a product over the subsystems where $N_1 = N - N_2$

$$Z_N = \frac{1}{N!\, h^{3N}} \sum_{N_1=0}^{N} \frac{N!}{N_1!\, N_2!} \int d^{3N_1}p_1\, d^{3N_1}q_1\, e^{-\beta H(p,q,N_1)} \int d^{3N_2}p_2\, d^{3N_2}q_2\, e^{-\beta H(p,q,N_2)}$$

$$=: \sum_{N_1=0}^{N} \int d^{3N_1}p_1\, d^{3N_1}q_1\, \rho(p_1,q_1,N_1)\, Z_N ,$$

where

$$\rho^{(p_1,q_1,N_1)} = \frac{Z_{N_2}(T,V_2)}{Z_N(T,V)} \, \frac{e^{-\beta H(p_1,q_1,N_1)}}{N_1!\, h^{3N_1}}$$

$$\mathcal{Z}(T,V,z) = \sum_{N=0}^{\infty} z^N Z_N(T,V) \quad , \qquad z = e^{\beta\mu}$$

$$= \sum_{N=0}^{\infty} \int \frac{d^{3N}p\, d^{3N}q}{N!\, h^{3N}} e^{-\beta[H(p,q) - \mu N]}$$

$$\Omega = -k_B T \log \mathcal{Z}(T,V,z)$$

$$U = -\frac{\partial}{\partial\beta} \log \mathcal{Z}(\beta,V,z)\Big|_{V,z} \quad \text{(3.54) derivation}$$

$$N = z \frac{\partial}{\partial z} \log \mathcal{Z}(\beta,V,z)\Big|_{\beta,V}$$

$$p = k_B T \frac{\partial}{\partial V} \log \mathcal{Z}(\beta,V,z)$$

Quantum Statistical Mechanics

Expectation value: $\langle M\rangle = \dfrac{\langle\psi|M|\psi\rangle}{\langle\psi|\psi\rangle} \overset{\text{def.}}{=} \dfrac{\sum_{n,m} c_n^* c_m \langle\phi_n|M|\phi_m\rangle}{\sum_n |c_n|^2}$

$\psi = \sum_n c_n \phi_n$ ← states of the subsystem (ϕ_n)

↳ amplitudes of the reservoir (c_n)

random phases

inelastic collisions

, $\overline{\langle c_n|c_m\rangle_{res}}^T = 0$ for $n\neq m$

$\overline{\langle c_n|c_n\rangle_{res}}^T = \begin{cases} 1 & E<E_n<E+\Delta \\ 0 & \text{otherwise}\end{cases}$

$$\Rightarrow \overline{\langle M\rangle}^T = \frac{\sum_n w_n \langle\phi_n|M|\phi_n\rangle}{\sum_n w_n} \quad , \quad w_n = \begin{cases} 1 & E<E_n<E+\Delta \\ 0 & \text{otherwise}\end{cases}$$

$\rho = \sum_n w_n \underbrace{|\phi_n\rangle}_{\text{normalized}}\langle\phi_n|$, if $w_n = \delta_{n0} \Rightarrow$ state is pure

else mixed

$$\Rightarrow \overline{\langle M\rangle}^T = \frac{tr(\rho M)}{tr(\rho)} \quad \text{and} \quad i\hbar\partial_t \rho = \underbrace{[H,\rho]^{\rho(H)}}_{=0} = 0$$

$\Rightarrow \rho$ is time independant.

Free particle

~~p. 179 Huang~~

Classical:

$$H = \frac{p^2}{2m} \Rightarrow Z_1 = \int \frac{d\vec{p}\,d\vec{q}}{h^3} e^{-p^2/2mk_BT}$$

Gauss

$$= V\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}$$

Beware: h is just an action

Quantum

$$Z_1 \overset{def}{=} \mathrm{tr}\left(e^{-\beta H}\right) = \sum_{\vec{p}} \langle \vec{p} | e^{-\beta H} | \vec{p} \rangle = V \int \frac{d\vec{p}}{(2\pi\hbar)^3} e^{-p^2/2mk_BT}$$

$$= V\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{3/2} = \frac{V}{\lambda^3} \quad , \quad \lambda = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$$

(thermal de Broglie wavelength)

→ fixes $h = 2\pi\hbar$, because of Heisenberg $d\vec{p}\,d\vec{q} = (2\pi\hbar)^3$

$Z_N = \frac{1}{N!} Z_1^N$ for independent particles

Classical, ~~interacting~~, in a potential / interacting

$$H = \frac{p^2}{2m} + V(q) \Rightarrow Z_1 = \frac{V}{\lambda^3} \int \frac{d^3q}{V} e^{-\beta V(\vec{q})}$$

↖ cancel the V above
no ∫ over $d\vec{q}$

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i,j} V(|q_i - q_j|) \Rightarrow Z_N = \frac{1}{N!}\left(\frac{V}{\lambda^3}\right)^N \int \frac{d^{3N}q}{V^N} \exp\left[-\frac{\beta}{2}\sum_{i \neq j} V(|q_i - q_j|)\right]$$

Quantum particle in a potential

lecture 7.10

$$Z_1 = \sum_{\vec{p}} \langle \vec{p} | e^{-\beta\left(\frac{p^2}{2m} + V(q)\right)} | \vec{p} \rangle$$

Using $\mathbb{1} = \int d^3\vec{q}\, |\vec{q}\rangle\langle\vec{q}|$ and the Baker-Hausdorf formula we get

$$e^{-\beta(H_0+V)} \approx e^{-\beta H_0} e^{-\beta V} e^{-\frac{\beta^2}{2}[H_0, V]}$$

and therefore to lowest order in β, $(T \to \infty)$

$$Z_1 = \sum_{\vec{p}} \int d^3\vec{q}\, \langle \vec{p} | e^{-\beta\frac{p^2}{2m}} | \vec{q} \rangle \langle \vec{q} | e^{-\beta V(\vec{q})} | \vec{p} \rangle = \frac{V}{\lambda^3} \int \frac{d^3\vec{q}}{V} e^{-\beta V(\vec{q})}$$

$Z_1 = \sum_{\vec{p}} \int d\vec{q}\, \langle \vec{p} | e^{-\beta H} | q \rangle \langle q | \vec{p} \rangle$ ← cancel by S_0

In a next step we study $\langle \vec{p} | e^{-\beta \mathcal{H}} | q \rangle$ in an expansion in $\hbar$. Note that

(imaginary time S.E.) $\Rightarrow$ $-\frac{\partial}{\partial\beta} \langle \vec{p} | e^{-\beta H} | \vec{q} \rangle = \left[-\frac{\hbar^2}{2m}\Delta + V \right] \langle \vec{p} | e^{-\beta H} | \vec{q} \rangle$ Bender Orszag

$\frac{it}{\hbar} \hat{=} \beta$

WKB- Ansatz: $\langle \vec{p} | e^{-\beta H} | \vec{q} \rangle = \dfrac{e^{-\frac{i}{\hbar}\sum_{n=0}^{\infty}\left(\frac{\hbar}{i}\right)^n S_n(\beta, \vec{q})}}{\sqrt{V}}$

$$\Rightarrow \frac{\partial S}{\partial \beta} = \frac{\hbar}{i}\left[\frac{1}{2m}(\vec{\nabla}S)^2 + V(\vec{q})\right] - \left(\frac{\hbar}{i}\right)^2 \frac{1}{2m}\Delta S$$

coefficient comparison $\Rightarrow$ in $\frac{\hbar}{i}$

$$\begin{cases} \partial_\beta S_0 = 0 \Rightarrow S_0 = \vec{p}\cdot\vec{q} \qquad \left(e^{-\frac{i}{\hbar}\vec{p}\vec{q}}\right) \langle \vec{q} | \vec{p} \rangle = 1 \\ \partial_\beta S_1 = \frac{1}{2m}(\vec{\nabla}S_0)^2 + V \Rightarrow S_1 = \beta H \\ \partial_\beta S_2 = \frac{1}{2m} 2(\nabla S_0)(\nabla S_1) - \frac{1}{2m}\Delta S_0 \\ \quad \Rightarrow S_2 = \frac{\beta^2}{2m}\vec{p}\cdot\vec{\nabla}V \\ \partial_\beta S_3 = \ldots,\ S_3 = \frac{\beta^3}{6m}(\vec{\nabla}V)^2 + \frac{\beta^3}{6m^2}(\vec{p}\cdot\vec{\nabla})^2 V - \frac{\beta^2}{4m}\Delta V \end{cases}$$

$$Z_1 = \sum_{\vec{p}} \int \frac{d^3\vec{q}}{V} \exp\left[-\beta H - \frac{\hbar}{i}S_2 - \left(\frac{\hbar}{i}\right)^2 S_3 + \ldots\right] \underset{\exp[-\frac{\hbar}{i}S_2]}{\overset{\text{Taylor in}}{\approx}} Z_1^{cl}\left(1 - \frac{\hbar}{i}\langle S_2 \rangle_{cl} + \hbar^2 \langle S_3 - \frac{1}{2}S_2^2 \rangle_{cl} + \ldots\right)$$

not done in lecture

calc. $\langle \cdots \rangle$ and (ΔV) p.I.

$$\Longrightarrow \quad Z_1 = Z_1^{cl}\left(1 - \frac{\beta^2\hbar^2}{24m}\langle \Delta V \rangle\right) \underset{\text{Taylor } \hbar^2 \text{ small}}{\overset{\text{reverse exponentiating}}{\Longrightarrow}} Z_1 \approx \frac{V}{\lambda^3}\int \frac{d^3\vec{q}}{V} \exp\left(-\beta\left(V(q) + \frac{\beta\hbar^2}{24m}\Delta V(q)\right)\right)$$

$\hookrightarrow \sim \lambda^2$

Canonical ensemble

The classical ideal gas

$$Z_N = \mathrm{tr}(e^{-\beta H}) = \sum_{\{n_{p_i}\}_N} e^{-\beta \sum_{p_i} n_{p_i} \varepsilon_{p_i}} \cdot g \quad \leftarrow \text{counting factor}$$

$$\boxed{H = \frac{p^2}{2m}}$$

$\{n_{p_i}\}_N$: # particles with momentum p_i

$$, \quad \sum_{p_i} n_{\vec{p}_i} = N$$

$$Z_N = \sum_{\{n_{p_i}\}_N} \prod \frac{e^{-\beta n_{\vec{p}_i} \varepsilon_{\vec{p}_i}}}{n_{p_i}!} \underset{\uparrow \text{multinomial}}{=} \frac{1}{N!} \Big(\underbrace{\sum_i e^{-\beta \varepsilon_{p_i}}}_{V/\lambda^3} \Big)^N = \frac{1}{N!} \left(\frac{V}{\lambda^3} \right)^N$$

$$\left(\sum_{p_i} e^{-\beta \varepsilon_{p_i}} = V \int \frac{d\vec{p}}{(2\pi\hbar)^3} \exp\left(-\frac{p^2}{2mk_BT}\right) = \frac{V}{\lambda^3} \right)$$

Stirling $\log N! = N \log N - N$

$$\Rightarrow \quad F = Nk_BT\left[\log(n\lambda^3) - 1\right]$$

$F = U - TS$

$$S = -\frac{F}{T} + \frac{U}{T} \underset{U = \frac{3}{2}Nk_BT}{=} Nk_B\left[-\log n\lambda^3 + \frac{5}{2}\right] \qquad (\text{Sackur - Tedrode})$$

$$p = \frac{Nk_BT}{V}$$

Classical limit of ideal quantum gases p. 199 Huang

Calculate the canonical partition of ideal quantum gases in the limit of $\beta \to 0$.

$$\overset{\sum_i \frac{p_i^2}{2m}}{\downarrow}$$

$$Z_N = \mathrm{tr}(e^{-\beta H_0}) = \sum_n \langle \phi_n | e^{-\beta E_n} | \phi_n \rangle$$

$$H_0 |\phi_n\rangle = E_n |\phi_n\rangle \ , \quad \langle \vec{q}_1, \vec{q}_2, \dots, \vec{q}_N | \phi_n \rangle \overset{\text{Slater}}{=} \frac{1}{\sqrt{N!}} \sum_{\pi \in S_n} (\overset{\text{Bosons}}{\pm} 1)^{\pi} \phi_{\vec{p}_1}(\vec{q}_{\pi_1}) \cdots \phi_{\vec{p}_N}(\vec{q}_{\pi_N})$$

Fermions

with $\phi_{\vec{p}}(\vec{q}) = \dfrac{e^{i\vec{p}\vec{q}/\hbar}}{\sqrt{V}}$

9.48 Huang

$\sum_n \Rightarrow \int d\vec{p}$ and identity $\mathbb{1}$

$$Z_N = \frac{V^N}{N!\,(2\pi\hbar)^{3N}} \boxed{\int d^{3N}p}\, d^{3N}q \underbrace{|\phi_n(\vec{q}_1, \dots, \vec{q}_N)|^2}_{\frac{1}{V^N} \sum_{\pi} (\pm 1)^{\pi} \boxed{e^{i\vec{p}_1(q_1 - q_{\pi_1})/\hbar}} \cdots} e^{\boxed{-\beta E_n}}$$

$$\int \frac{d^3p}{(2\pi\hbar)^3} e^{-\beta p^2/2m + i\vec{p}\vec{q}/\hbar} = \frac{1}{\lambda^3} e^{-\frac{\pi q^2}{\lambda^2}} \sim e^{-\beta V}$$

exact

$$\Rightarrow Z_N = \underbrace{\frac{1}{N!}\left(\frac{V}{\lambda^3}\right)^N}_{\text{classical result}} \int \frac{d^{3N}q}{V^N} \overbrace{\sum_{\pi \in S^N} (\pm 1)^{\pi} \Big[\underbrace{e^{-\frac{\pi}{\lambda^2}(q_1 - q_{\pi_1})^2}}_{\text{gets smaller if } \pi \neq \mathbb{1}} \cdots e^{-\frac{\pi}{\lambda^2}(q_N - q_{\pi_N})^2} \Big]}$$

For $T \to \infty \Leftrightarrow \lambda^2 \to 0$ only $\pi = \mathbb{1}$ survives giving the classical result.

For $T < \infty$ the terms in $\sum_{\pi}$ become smaller the more particles are permuted.

Under the assumption that $\langle (\vec{q}_i - \vec{q}_j)^2 \rangle > \lambda^2$ (i.e. low ~~den~~ densities), expansion

gives $\Rightarrow \sum_{\pi} (\pm 1)^{\pi} [--] = \underset{\pi = \mathbb{1}}{1} \pm \sum_{i \neq j} \exp\left[-\frac{2\pi}{\lambda^2}(q_i - q_j)^2\right]$ + 3 particle-terms + O(4part

Comparing ~~the~~ ~~co~~ coefficients by $e^{-\beta V}$ leads $\overset{x = e^{\log x}}{\text{to}}$ $\Rightarrow V^S(q) = -k_B T \log\left(1 \pm e^{-2\pi\left(\frac{q}{\lambda}\right)^2}\right)$

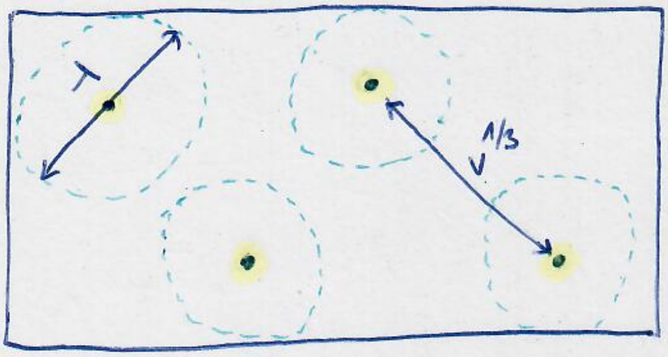
the statistical interaction, which is short ranged and only coming from symmetry properties of the N-particle wave function:

Quantum corrections to the interacting classical Gas

→ expansion in $\hbar$

$$Z_N(V,T) \simeq \underbrace{\frac{1}{N!}\left(\frac{V}{\lambda^3}\right)^N}_{\substack{\text{Classical}\\ \text{ideal gas}}} \int \frac{d^{3N}q}{V^N} \exp\Big[-\beta \underbrace{\sum_{i<j}\big[V(\vec{q}_i-\vec{q}_j)}_{\substack{\text{Interaction}\\ \text{between particles}}} + \underbrace{V^s(\vec{q}_i-\vec{q}_j)}_{\substack{\text{Statistical}\\ \text{interaction}}} + \underbrace{\frac{\beta\hbar^2}{24m}\Delta_i V(\vec{q}_i-\vec{q}_j)\big]}_{\substack{\text{quantum}\\ \text{correction}\\ \text{to potential}\\ \text{due to smearing}}}\Big]$$

Interacting particles at $T \to 0$ p.230 Huang



$v^{1/3} \equiv$ average interparticle separation

$\lambda \equiv$ thermal wavelength

● $\cong$ range of interparticle potential

⇒ the details of the interparticle potential are unimportant as it only sees an averaged effect of the potential due to smearing.

$\{ a>0$ repulsive, $a<0$ attractive

at low energies potential only depends on a (the scattering length). The total cross-section is $4\pi a^2$, similar to a hard sphere. This is well described by s-wave scattering.

effective range

$$k\cot\delta_0 \approx -\frac{1}{a} + \frac{r_0}{2}k^2 + \dots$$

s-wave phase shift

and to lowest order in k ⇒ $\cot\delta_0 \approx -\frac{1}{ak}$. Hard spheres are conveniently described by

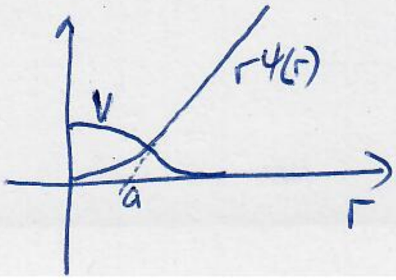
$$V^a_{L=0}(\vec{r}) = \frac{4\pi a\hbar^2}{m}\delta(\vec{r})\left(\frac{\partial}{\partial r} r\right)$$

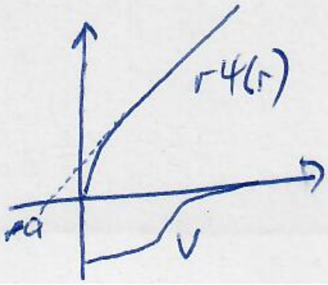
$$H = \frac{p^2}{2m} + V^a_{L=0}(\vec{r})$$

Calculation

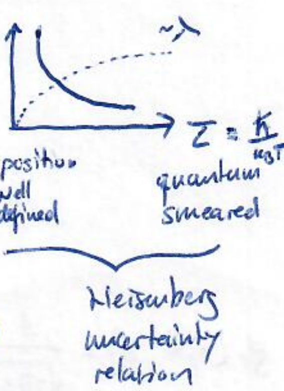
I: Calculate spectrum of $H = \sum \frac{p_i^2}{2m} + \frac{4\pi a\hbar^2}{m}\sum_{i<j}\delta(\vec{q}_i - \vec{q}_j)$ in perturbation the

II: Calculate canonical partition function.





Path Integrals



$$\langle \phi_i | \rho(\beta) | \phi_j \rangle = \langle \phi_i | e^{-\beta H} | \phi_j \rangle \Rightarrow \rho_{ij}(\beta) = e^{-\beta E_i}\delta_{ij}$$

$$\Rightarrow \frac{\partial}{\partial\beta}\rho_{ij}(\beta) = -E_i\, e^{-\beta E_i}\delta_{ij} = -E_i \rho_{ij} \underset{\tau=\hbar\beta}{\Rightarrow} -\hbar\frac{\partial\rho}{\partial\tau} = H\rho(\tau)$$

evolves as a diffusive particle

In position representation, this is ~~solved~~ given by

$$-\hbar\frac{\partial\rho(x,x';\tau)}{\partial\tau} = \overset{\text{acts on } x}{H_x\rho(x,x';\tau)}$$

with the initial condition $\rho(x,x';0) = \delta(x-x')$

Example: **Free particle**

$$H_0 = -\frac{\hbar^2}{2m}\partial_x^2$$

$$\Rightarrow \quad -\hbar\frac{\partial\rho_0}{\partial\tau} = -\frac{\hbar^2}{2m}\partial_x^2\rho_0 \quad , \quad \rho_0(x,x';0) = \delta(x-x')$$

$$\Rightarrow \quad \rho_0(x,x';\tau) = \left(\frac{m}{2\pi\hbar\tau}\right)^{1/2} \exp\left[-\frac{m}{2\hbar\tau}(x-x')^2\right]$$

For a system at length L and temperature k_BT

$$Z_1 = \mathrm{tr}(\rho_0) = \int dx \langle x|\rho_0|x\rangle = \int dx\, \rho_0(x,x;\beta\hbar) = \int dx \left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2} = L\left(\frac{mk_BT}{2\pi\hbar^2}\right)^{1/2} = \frac{L}{\lambda}$$

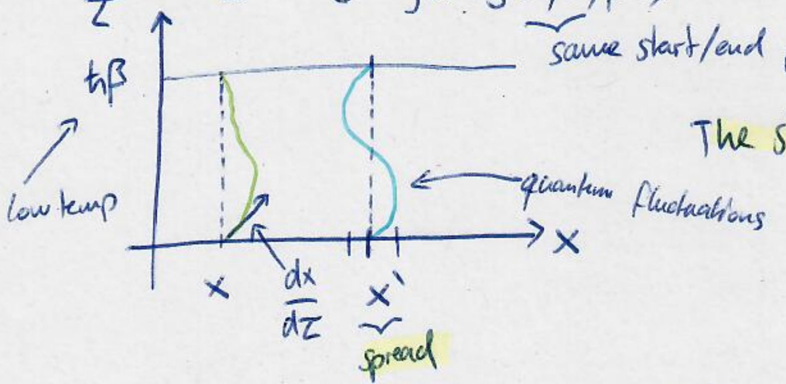
Path Integral representation

$$e^{-\tau H/\hbar} = \left[e^{(-\tau/n)H}\right]^n \quad \Rightarrow \quad \rho(\tau) = \rho(\varepsilon)\rho(\varepsilon)\cdots\rho(\varepsilon) \quad , \quad \varepsilon = \frac{\tau}{n}$$

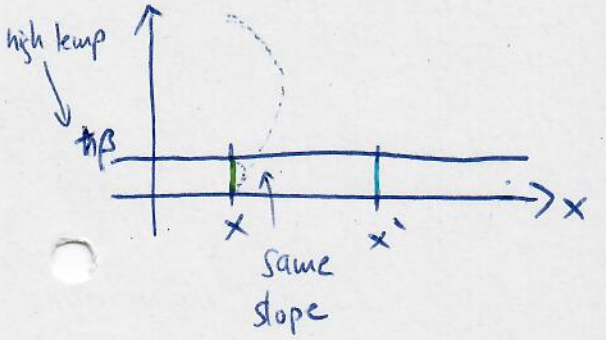
$$\rho(x,x';\tau) = \int\cdots\int dx_1\cdots dx_{n-1}\, \rho(x,x_{n-1};\varepsilon)\,\rho(x_{n-1},x_{n-2};\varepsilon)\cdots\rho(x_2,x_1;\varepsilon)\,\rho(x_1,x';\varepsilon)$$

Interpretation of Path Integrals

$$Z = \mathrm{tr}(\varrho) = \int \overset{\text{sum along } x}{dx}\, \varrho(\underbrace{x,x}_{\text{same start/end point}},\beta\hbar)$$



The straight line gives the biggest contribution.

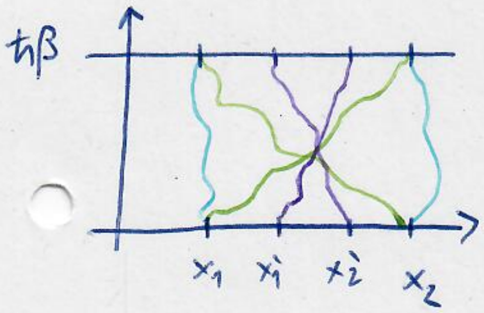


mostly straight. For a given slope $\left(\frac{dx}{d\tau}\right)$ a much further away point can be reached in ~~high~~ low temperature

In quantum, you get $+1$ dimension.

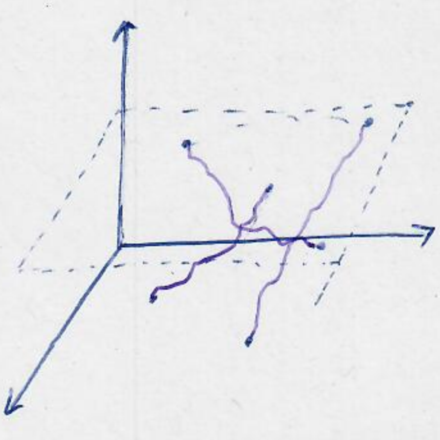
additional imaginary time τ.

Bosonic Attraction



reduced action ⇒ attraction, "try to straighten up"

Condensation



3 lines not distinguishable, are shared (properties/identity) could also be only one boson.

cooperative ring exchanges

Fermions

p. 243 Huang

$$n = \frac{1}{V} z\partial_z \log \mathcal{Z} = \frac{1}{\lambda^3} f_{3/2}(z) \Rightarrow \delta := n\lambda^3 = f_{3/2}(z) \Rightarrow z = z(n) = e^{\beta\mu(n)}$$

$$\Rightarrow \mu(n) = k_B T \log z(n)$$

$$f_{3/2}(z) = \frac{4}{\sqrt{\pi}} \int_0^\infty dx \frac{x^2}{1+e^{x^2}/z} = \sum_{l=1}^\infty \frac{(-1)^{l+1} z^l}{l^{3/2}}$$

monotonically increasing function of z

classical gas

$$f_{3/2}(z) = \delta = n\lambda^3 \ll 1$$

We want to find $z(n)$.

$\delta \ll 1 \Rightarrow z$ small

monoton increasing

$$f_{3/2}(z) = z - \underset{\approx\delta^2}{\frac{z^2}{2^{3/2}}} + \frac{z^3}{3^{3/2}} \mp O(z^4)$$

$$\Rightarrow \delta = z - \frac{z^2}{2\sqrt{2}} \Rightarrow z \approx \delta + \frac{1}{2\sqrt{2}}\delta^2$$

$$\Rightarrow \begin{matrix} z \longrightarrow 0 \\ \delta \longrightarrow 0 \end{matrix}$$

$$\Rightarrow \langle n_p \rangle \overset{\text{def.}}{=} \frac{1}{\frac{e^{\beta\varepsilon_p}}{z} + 1} \xrightarrow[z\to 0]{} z e^{-\beta\varepsilon_p}$$

$$\longrightarrow n \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{3/2} \exp\left[-\frac{p^2}{2mk_BT}\right] = h^3 f_{MB}(\vec{p})$$

Maxwell Boltzmann

Analogously,

$$pV \approx \frac{V}{\lambda^3} k_B T \left(z - \frac{z^2}{2^{5/2}} + \dots\right)$$

$$\approx Nk_BT\left(1 + \frac{n\lambda^3}{4\sqrt{2}} + \dots\right)$$

classical ideal Gas with quantum corrections $\propto \delta$

quantum gas

$$f_{3/2}(z) = \delta = n\lambda^3 \gg 1$$

$$f_{3/2}(z) = \frac{4}{\sqrt{\pi}} \int_0^\infty dx \frac{x^2}{1+e^{x^2-\beta\mu}} = \frac{4}{3\sqrt{\pi}} \int_0^\infty dy\, y^{3/2} \underbrace{\frac{e^{y-\beta\mu}}{(1+e^{y-\beta\mu})^2}}_{= -\frac{d}{dy}\frac{1}{1+e^{y-\beta\mu}}}$$

$$y^{3/2} \approx (\mu\beta)^{3/2} + \frac{3}{2}(\mu\beta)^{1/2}(y-\mu\beta) + \dots$$

sharply peaked around $\beta\mu$

$$\Rightarrow f_{3/2}(z) \approx \frac{4}{3\sqrt{\pi}}\left[(\log z)^{3/2} + \frac{\pi^2}{8}(\log z)^{-1/2} + \dots\right] + \dots$$

Sommerfeld expansion

Degenerate Fermi Gas

p. 244 Huang

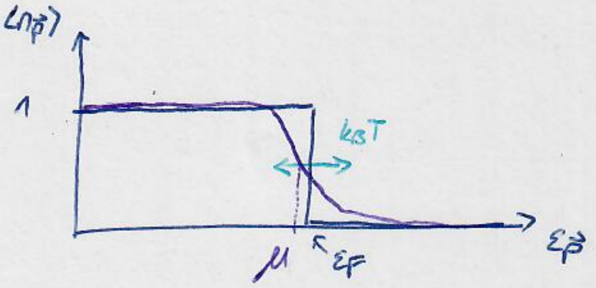
$$1 \ll \delta = n\lambda^3 \simeq \frac{4}{3\sqrt{\pi}}\left[(\beta\mu)^{3/2} + \frac{\pi^2}{8}\frac{1}{(\beta\mu)^{1/2}}\right]$$

Sommerfeld

lowest order $\Rightarrow$ $\mu(T=0) = \frac{\hbar^2}{2m}(6\pi^2 n)^{2/3} = \varepsilon_F$

second term $\Rightarrow$ $\mu(T) \simeq \varepsilon_F\left[1 - \frac{\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2\right]$, decreasing with increasing temperature

$$f_{FD}(\vec{p}) = \langle n_{\vec{p}}\rangle \simeq \frac{1}{e^{\beta(\varepsilon_p-\mu)}+1}$$



$$U \overset{\text{def}}{=} \sum_p \varepsilon_p \langle n_{\vec{p}}\rangle = \frac{V}{(2\pi\hbar)^3}\int_0^\infty dp\, 4\pi p^2 \frac{p^2}{2m}\langle n_p\rangle = \frac{3}{5}N\varepsilon_F\left[1 + \frac{5\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2 + \dots\right]$$

$$c_V = \frac{\partial U}{\partial T}\Big|_V = Nk_B\frac{\pi^2}{2}\frac{k_B}{\varepsilon_F}T \xrightarrow[T\to 0]{} 0$$ in agreement with third law

$$p = \frac{2}{3}\frac{U}{V} = \frac{2}{5}n\varepsilon_F\left[1 + \frac{5\pi^2}{12}\left(\frac{k_BT}{\varepsilon_F}\right)^2 + \dots\right] \xrightarrow{T\to 0} \frac{2}{5}n\varepsilon_F$$

{ arises from pauli as only a single particle can occupy the zero momentum state

This pressure corresponds to a system with degeneracy temperature

$$k_BT_F = \varepsilon_F \xRightarrow{n\sim 10^{22}/\text{cm}^3} T_F \simeq 2\cdot 10^4\,\text{K}$$

Dilute Fermi gas

p. 243 Huang

$$\sigma \overset{\text{def}}{=} n\lambda^3 = f_{3/2}(z) = z - \frac{z^2}{2\sqrt{2}} + O(z^3) \quad \Rightarrow \quad z \approx n\lambda^3$$

$$\langle n_{\vec{p}} \rangle \overset{\text{def.}}{=} \frac{1}{e^{\beta(\varepsilon_p - \mu)} + 1} \underset{8.66}{\overset{\text{Huang}}{=}} \frac{z e^{-\beta \varepsilon_p}}{1 + \underbrace{z e^{-\beta\varepsilon_p}}_{\text{irrelevant}}} \overset{\overset{z}{n\lambda^3 \to 0}}{\approx} z e^{-\beta\varepsilon_p} = n \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{3/2} e^{-\frac{p^2}{2mk_BT}}$$

$$\simeq h^3 f_{MB}(\vec{p})$$

Electrons in a magnetic field (overview)

intrinsic magnetic moment of nucleus is 10^{-3} times smaller than electrons.

$$\mathcal{H} = \underbrace{\sum_i \frac{[\vec{p}_i + \frac{e}{c}\vec{A}(\vec{q}_i)]^2}{2m}}_{\mathcal{H}_{orb}} - \sum_i \vec{\mu}_i \cdot \vec{H} \quad , \quad \vec{\mu}_i = -\underset{\frac{e\hbar}{2mc}}{\mu_B}\,\underset{\simeq 2}{g}\,\overset{s_i/2}{\vec{S}_i}$$

legendre transform

$-H\sum\mu_i \Leftrightarrow Hm$

$$m = \frac{k_B T}{V}\frac{\partial}{\partial H}\log\begin{cases} Z_N \\ \tilde{Z}_N \end{cases}$$ (magnetization density)

$$m = -\frac{1}{V}\left\langle\frac{\partial \mathcal{H}}{\partial H}\right\rangle = \underbrace{\frac{1}{V}\left\langle\sum_i \mu_{z,i}\right\rangle}_{\text{spin}} - \underbrace{\frac{1}{V}\left\langle\frac{\partial \mathcal{H}_{orb}}{\partial H}\right\rangle}_{\text{orbital}}$$

$B = H + 4\pi m_{spin} > H$

increase, paramagnetic

use $>H$

$\chi_{para} > 0$

Pauli

$B = H - 4\pi|m_{orb}| < H$

cost Energy, diamagnetic

simply use $<H$

$\chi_{dia} < 0$

Landau

$$\chi = \frac{\partial M}{\partial H}$$

Landau Diamagnetism

p.254 Huang
→p.253 Huang

$$\boxed{\begin{gathered}\mathcal{H} = \frac{[\vec{p} + \frac{e}{c}\vec{A}(\vec{q})]^2}{2m} \\ \mathcal{H}\psi_\lambda = \varepsilon_\lambda \psi_\lambda\end{gathered}} \xrightarrow[\vec{A} = (-Hy, 0, 0)]{\vec{H} = (0,0,H)} -\frac{\hbar^2}{2m}\left[\left(\partial_x - \frac{2\pi i}{\phi_0}Hy\right)^2 + \partial_y^2 + \partial_z^2\right]\psi_\lambda = \varepsilon_\lambda \psi_\lambda$$

$$\xrightarrow[\psi_\lambda = e^{ik_x x} e^{ik_z z}\phi(y)]{\text{Separation}} \left[-\frac{\hbar^2}{2m}\partial_y^2 + \frac{1}{2}m\omega_c^2(y-y_0)^2\right]\phi = \left(\varepsilon_\lambda - \frac{\hbar^2 k_z^2}{2m}\right)\phi$$

(Schrödinger equation for a displaced harmonic oscillator)

$\omega_c = \frac{h}{m\phi_0}H = \frac{eH}{mc}$ ← cyclotron frequency

$y_0 = \frac{\phi_0}{2\pi H}k_x = L^2 k_x$ ← magnetic length

Solution

$$\Rightarrow \begin{cases} \varepsilon_\lambda = \hbar\omega_c\left(n + \frac{1}{2}\right) + \frac{\hbar^2 k_z^2}{2m} \\ \psi_\lambda = e^{ik_x x} e^{ik_z z} N_n \underset{\text{Hermite}}{H_n}[(y - \overset{\text{shift}}{y_0})/L] \underbrace{e^{-(y-y_0)^2/2L^2}}_{\text{Gauss}} \end{cases}$$

$L^3 = V$

The degeneracy is given by $g = \frac{eH}{hc}L^2 = \frac{\phi}{\phi_0}$ of the landau levels.

B[illegible]uperposition $\sum_{i=1}^{\phi/\phi_0} a_{n_i}\psi_n(y - y_{0i})$ and the Gauge $\vec{A} = \frac{B}{2}(y, -x, 0)$ one obtains the circular solution

$$\tilde{Z} \overset{\text{def.}}{=} \prod_\lambda (1 + ze^{-\beta\varepsilon_\lambda}) \Rightarrow \log \tilde{Z} = \underbrace{\sum_1^{\phi/\phi_0}}_{\text{degeneracy in } k_x} \underbrace{\sum_n}_{\text{Landau level}} \underbrace{\sum_{k_z}}_{\text{degen. in } k_z \text{ free motion}} \log\left(1 + ze^{-\beta\varepsilon(n,k_z)}\right)$$

high temperature limit → Taylor in z

$$\overset{\text{Taylor in } z}{\approx} \frac{\phi}{\phi_0}\sum_n L_z \int \frac{dk_z}{2\pi} z \overbrace{\exp\left[-\frac{\beta\hbar^2 k_z^2}{2m}\right]\exp\left[-\beta\hbar\omega_c\left(n + \frac{1}{2}\right)\right]}^{\varepsilon(n,k_z)}$$

$$= N\left(1 - \frac{1}{96\pi^2}\frac{\lambda^4}{L^4}\right)$$

p.841 ashcroft

Pauli spin paramagnetism

$$\vec{H} = (0,0,H)$$

$$\mathcal{H} = \sum_i \left(\frac{p_i^2}{2m} + \mu_B \sigma_i H \right) \quad , \quad \sigma_i = \pm 1$$

$$\varepsilon_{\vec{p},\sigma} = \frac{p^2}{2m} + \sigma \mu_B H \quad \text{(single particle energy)}$$

$$\Rightarrow E[\{n_{\vec{p},\sigma}\}] = \sum_{\vec{p},\sigma} \underbrace{n_{\vec{p},\sigma}}_{\in\{0,1\}} \frac{p^2}{2m} - \mu_B H (N_+ - N_-)$$

$$Z_{0N} = e^{-\beta F_0(N)} = \sum_{\{n_{\vec{p}}\}_N} \exp\left[-\beta \sum_{\vec{p}} \frac{p^2}{2m} n_{\vec{p}}\right]$$

Canonical partition function

$$Z_N = \sum_{\{n_{\vec{p},\sigma}\}_N} e^{-\beta E[\{n_{\vec{p},\sigma}\}]} = e^{-\beta \mu_B H N} \sum_{N_+=0}^{M} e^{\boxed{2\beta\mu_B H N_+ - \beta F_0(N_+) - \beta F_0(N_-)}} \leftarrow \beta f(N_+)$$

$$N_- = N - N_+$$

dominant role comes from the largest term, find $N_+ =: \bar{N}_+$ maximizing f

$$\left.\frac{\partial f}{\partial N_+}\right|_{\bar{N}_+} = 0$$

Remember chemical potential ideal spinless Fermi Gas

$$\mu(n) = \begin{cases} k_B T \log n\lambda^3 & < 0 \quad \text{(dilute gas)} \\ \varepsilon_F(n)\left(1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\varepsilon_F}\right)^2\right) & \gg 0 \quad \text{(degenerate gas)} \end{cases}$$

$$\left.\frac{\partial f}{\partial N_+}\right|_{\bar{N}_+} \overset{!}{=} 0 \Rightarrow \mu(\bar{N}_+) - \mu(N - \bar{N}_+) = 2\mu_B H \quad , \quad \bar{N}_\pm = \left(\frac{1}{2} \pm \varepsilon\right) N \quad \Rightarrow \varepsilon = \frac{\mu_B H V}{\frac{\partial \mu}{\partial n} N}$$

$$\overset{\mu(n)}{\Rightarrow} \frac{\partial \mu}{\partial n} \overset{T \to 0}{=} \frac{2}{3} \frac{\varepsilon_F}{n} \Rightarrow M = \frac{\overbrace{(\bar{N}_+ - \bar{N}_-)}^{2\varepsilon N} \mu_B}{V} = \frac{3}{2} \frac{\mu_B^2 H}{\varepsilon_F} n$$

$$\Rightarrow \chi_P = \frac{3n}{2\varepsilon_F} \mu_B^2 = g(\varepsilon_F) \mu_B^2 \quad , \quad \chi_P = -3\chi_L$$

degenerate gas

Photons

p. 278 Huang

→ Grand canonical Ensemble , $\mu = 0 \Rightarrow \mathcal{Z} = Z$

$$\mathcal{Z} = \prod_{\vec{k},\lambda} \frac{1}{1-e^{-\beta\hbar\omega_k}} \quad , \log \mathcal{Z} = -2 \sum_{\vec{k}} \log(1- e^{-\beta\hbar\omega_k})$$

$$\langle n_{\vec{k},\lambda} \rangle = -\frac{1}{\beta} \frac{\partial \log \mathcal{Z}}{\partial \hbar\omega_k} = \frac{1}{e^{\beta\hbar\omega_k}-1}$$

(Planck distribution)

derivation also via

$\bar{n}_k = -\frac{\partial a_k}{\partial \mu}$ and then

setting $\mu = 0$

$\frac{\partial}{\partial \hbar\omega_k}$ [illegible] $\frac{\partial}{\partial \mu}$

think before calculating

$$U = -\frac{\partial}{\partial \beta} \log \mathcal{Z} = \sum_{\vec{k},\lambda} \hbar\omega_k \langle n_{\vec{k},\lambda} \rangle$$

$$p = \underbrace{\frac{\partial}{\partial V} k_B T \log \mathcal{Z}}_{Z = \mathcal{Z}} = \frac{U}{3V}$$

$\omega_k(V)$

$$\sum_{\vec{k},\lambda} \xrightarrow{V\to\infty} 2V \int \frac{d\vec{k}}{(2\pi)^3} = \frac{V}{\pi^2} \int_0^\infty dk\, k^2 = \frac{V}{\pi^2 c^3} \int_0^\infty d\omega\, \omega^2$$

$$U = \frac{V\hbar}{\pi^2 c^3} \int_0^\infty d\omega \frac{\omega^3}{e^{\beta\hbar\omega}-1} \overset{x=\beta\omega_k\hbar}{=} \frac{V\hbar}{\pi^2 c^3} \frac{1}{\hbar^4 \beta^4} \underbrace{\int_0^\infty dx \frac{x^3}{e^x - 1}}_{\pi^4/15} = \frac{\pi^2}{15} \frac{(k_B T)^4}{(\hbar c)^3} V = \frac{\pi^2 V}{15 \underbrace{\lambda^3}_{\hat{=} N}} k_B T$$

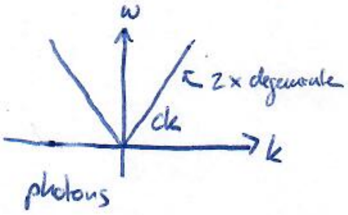
$2\pi k_B T = \frac{hc}{\lambda}$

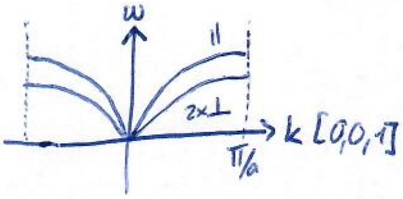
particles are created by T

Phonons

Condensed matter system has 3N modes. Spectrum is reduced to BZ, $\frac{\partial \omega}{\partial k}\Big|_{BZ} = 0$.

$\underbrace{\text{2 transversal}}_{\text{characteristic of condensed matter}}$, 1 longitudinal





Isotropic elastic medium (simplified)

result = $\frac{3}{2} \cdot \sum_{\vec{k}}$ from photons

$$\omega_\lambda = c_\lambda |\vec{k}| \qquad (I)$$

$$\rho(\omega)d\omega \overset{\text{def. } \rho, k}{\simeq} \sum_\lambda 4\pi k^2 \left(\frac{L}{2\pi}\right)^3 dk = \sum_\lambda \frac{V}{2\pi^2}\omega^2 d\omega \left(\frac{1}{c_\lambda^3}\right) \overset{\Sigma}{=} \frac{3V\omega^2}{2\pi^2 \bar{c}^3} d\omega \qquad (II)$$

$$\frac{3}{\bar{c}^3} = \frac{2}{c_\perp^3} + \frac{1}{c_\parallel^3}$$

$$\int_0^{\omega_{max}} \rho(\omega)d\omega \overset{(II)}{=} \frac{V}{2\pi^2}\frac{\omega_{max}^3}{\bar{c}^3} \overset{\text{def}}{=:} \frac{V}{2\pi^2} k_{BZ}^3 \overset{!}{=} 3N \Rightarrow k_{BZ} = (6\pi^2 n)^{1/3}$$

$$\Rightarrow \omega_{max} = \bar{c} k_{BZ}$$

$$\sum_{\vec{k},\lambda} \xrightarrow{V \to \infty} \frac{3V}{2\pi^2 \bar{c}^3} \int_0^\infty d\omega\, \omega^2$$

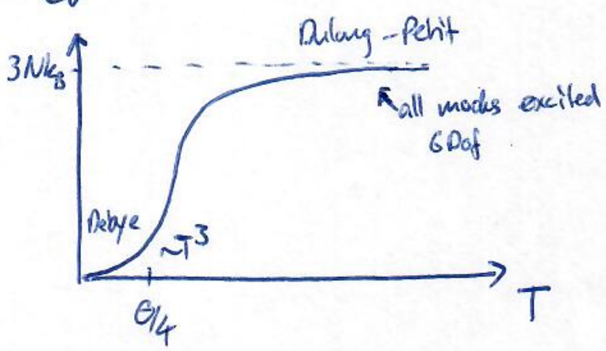
λ

polarization photon/phonon

$$U \overset{\text{def.}}{=} \sum_{\vec{k},\lambda} \hbar\omega_k \langle n_{k,\lambda} \rangle = \frac{3V}{2\pi^2 \bar{c}^3} \int_0^{\omega_{max}} d\omega\, \omega^2 \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1}$$

$$\Rightarrow \frac{U}{N} = \underbrace{\frac{3\hbar}{2\pi^2 n \bar{c}^3} \frac{1}{(\hbar\beta)^4}}_{\frac{9(k_B T)^4}{(\hbar\omega_{max})^3}} \underbrace{\int_0^{\beta\hbar\omega_{max}} dt \frac{t^3}{e^t - 1}}_{\text{Debye function}}$$

N ↑ $= nV$



$$\frac{U}{N} \approx 3k_B T \begin{cases} 1 - \frac{3}{8}\frac{\Theta}{T} + \ldots & T \gg \Theta \\ \frac{\pi^4}{5}\left(\frac{T}{\Theta}\right)^3 & T \ll \Theta \end{cases}$$

few 100 K

$k\Theta = \hbar\omega_{max}$

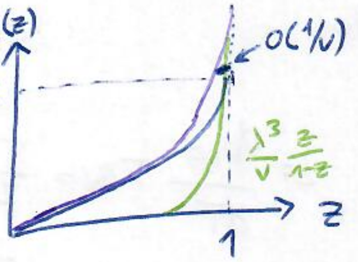
Bose - Einstein Condensation

p. 286 Huang

$$\tilde{Z} = \prod_{\vec{p}} (1 - z e^{-\beta \varepsilon_p})^{-1} \quad / \quad n = \frac{z}{V}\frac{\partial}{\partial z} \log \tilde{Z} = \frac{1}{\lambda^3} g_{3/2}(z) + \frac{1}{V}\frac{z}{1-z}$$

$$\langle n_p \rangle = \frac{1}{e^{\beta(\varepsilon - \mu)} - 1} \quad / \quad p = \frac{k_B T}{V} \log \tilde{Z} = \frac{k_B T}{\lambda^3} g_{5/2}(z) - \frac{k_B T}{V} \log(1-z)$$

$$\Rightarrow \quad n\lambda^3 = g_{3/2}(z) + \underbrace{\frac{\lambda^3}{V}\frac{z}{1-z}}_{\langle n_0 \rangle}$$



if $n\lambda^3 < 2{,}612$

$$\Rightarrow \quad n\lambda^3 = g_{3/2}(z) + O(\tfrac{1}{V}), \text{ for } V \to \infty$$

$$g_{3/2}(z) = \begin{cases} z + \frac{z^2}{2\sqrt{2}} + \dots & , z \ll 1 \\ 2{,}612 & , z = 1 \end{cases}$$

if $n\lambda^3 > 2{,}612$

$$\Rightarrow n\lambda^3 = 2{,}612 + \underbrace{\frac{\lambda^3}{V}\frac{z}{1-z}}_{\neq 0 \Rightarrow z = 1 \text{ for } V \to \infty}$$

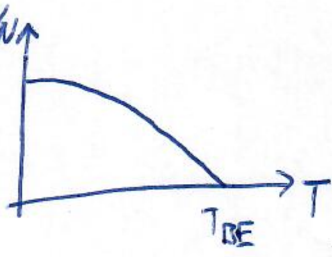
$$\Rightarrow \langle n_0 \rangle = \frac{V}{\lambda^3}(\underbrace{n\lambda^3}_{>2{,}612} - \underbrace{n_{BE}\lambda^3}_{2{,}612}) \propto V$$, finite fraction occupies $p=0$ state. ($\propto N$)

The condensation region is separated from the rest of the P-v-T space by

$$n\left(\frac{2\pi\hbar^2}{m k_B T}\right)^{3/2} = \frac{\lambda^3}{\underset{\frac{1}{n}}{V}} = g_{3/2}(1) = 2{,}612$$

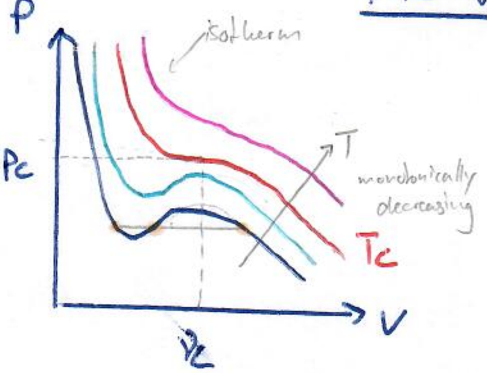
$$\Rightarrow \quad k_B T_{BE} = \frac{\hbar^2 n^{2/3}}{2m} \cdot 6{,}63 \quad / \quad n_{BE} = \frac{2{,}612}{\lambda^3}$$

$$\frac{\langle n_0 \rangle}{N} = \begin{cases} 1 - \left(\frac{T}{T_{BE}}\right)^{3/2} & T < T_{BE} \\ 0 & T > T_{BE} \end{cases}$$



The van der Waals Gas

p.38 Huang

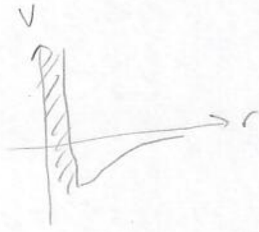


volume of atoms

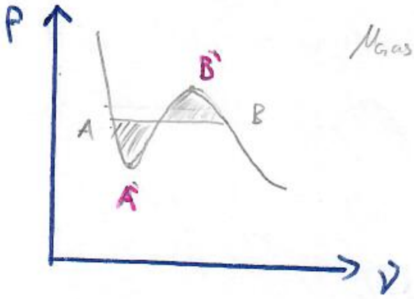
$$(v-b)\left(p+\frac{a}{v^2}\right) = RT$$

short range interaction

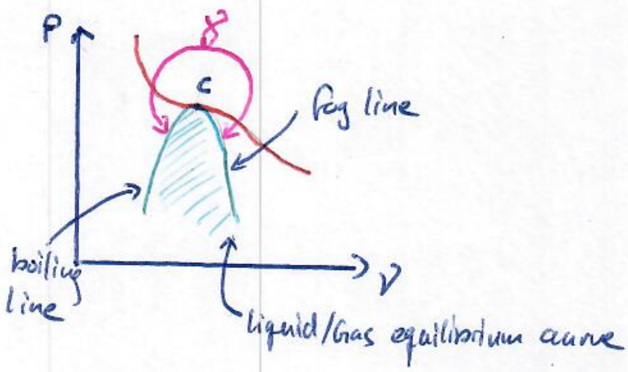
long range interaction



Using the maxwell construction we account for instability ⟹ phase transition



$\mu_{Gas} = \mu_{liquid}$



Spinodals

Continuous transition from gas to liquid

classical ⟹ canonical partition function

$$Z_N(V,T) = \frac{1}{N!}\left(\frac{V}{\lambda^3}\right)^N \int \frac{d\vec{q}^N}{V^N}\, e^{-\beta\sum_{i<j} V(\vec{q}_i-\vec{q}_j)}$$

$$V = V_{long\,range} + V_{short\,range} = -\frac{\pi}{8}\frac{V_0}{R_0^3}e^{-r/R_0} + V_{hard\,sphere}$$

$$Z_N(T,V) = \frac{1}{N!}\left(\frac{V}{\lambda^3}\right)^N e^{\beta \underbrace{V_0}_{a} N^2/2V}\left(\frac{V-Nb}{V}\right)^N$$

$$F(T,V,N) = -k_BT\log Z_N = F_{id\text{-}Gas} - \frac{aN^2}{V} - k_BTN\log\left(1-\frac{bN}{V}\right)$$

$p = -\frac{\partial F}{\partial V}$

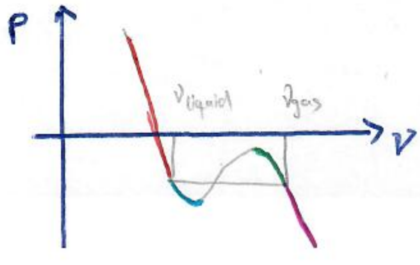
ausklammern gleichnamig

$$p = \frac{k_BT}{v} - \frac{a}{v^2} + \frac{k_BT}{v}\frac{b}{v-b} = \frac{k_BT}{v-b} - \frac{a}{v^2}$$

$F_{id\text{-}Gas} = Nk_BT[\log(n\lambda^3)-1]$

sackur tetrode mit $v \to v-b$

$$\Rightarrow f = k_BT\left[\log\left[\frac{\lambda^3}{v-B}\right]-1\right] - \frac{a}{v} \Rightarrow s = -\frac{\partial f}{\partial T} = k_B\left[\log\left[\frac{v-b}{\lambda^3}\right]+\frac{5}{2}\right]$$



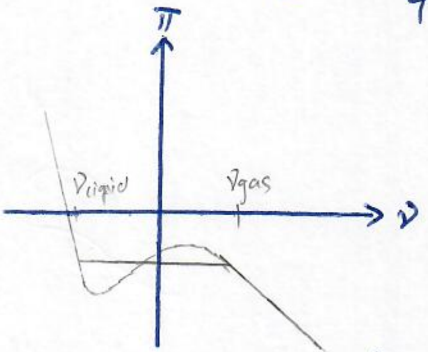
Critical region of the gas-liquid transition

$$\pi = \overset{\text{conjugate variable}}{\frac{p}{p_c}} - 1, \quad \nu = \overset{\text{order parameter}}{\frac{V}{V_c}} - 1, \quad \tau = \overset{\text{separates order}}{\frac{T}{T_c}} - 1$$

$$\pi(\nu) = 4\tau - 6\tau\nu + 9\tau\nu^2$$

$$\Rightarrow \quad (1+\pi) + \frac{3}{(1+\nu)^2} = \frac{8(1+\tau)}{2+3\nu} \quad \overset{\text{Taylor}}{\Rightarrow} \quad \pi(\nu) \overset{\tau=0}{=} -\frac{3}{2}\nu^3 + \frac{21}{4}\nu^4$$

$$\Rightarrow \quad \nu \propto \pi^{1/3} \Leftrightarrow \delta = 3$$



Asymmetric due to ν^4. Gas volume grows faster than liquid volume shrinks at $T < T_c$.

No conclusion about phase transition.
Constant path length: more gas than liquid in one unit length

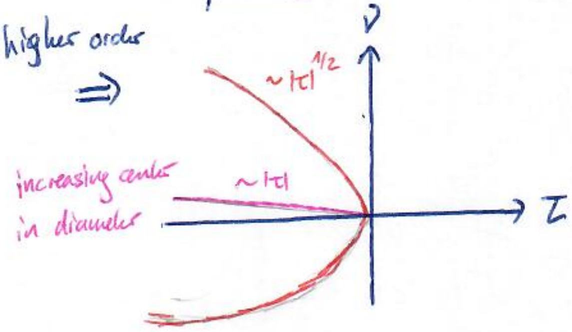
$$\overset{\text{Ansatz}}{\nu = \alpha\sqrt{|\tau|}}$$

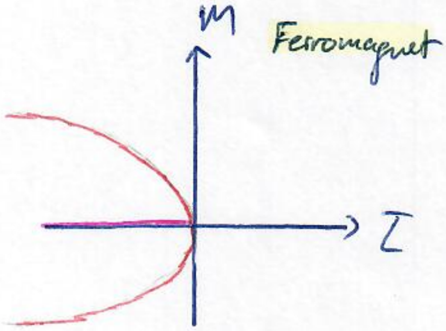
$$\overset{\text{Taylor}}{\Rightarrow} \pi - 4\tau = -\left(\frac{3}{2}\alpha^3 - 6\alpha\right)|\tau|^{3/2} + O(\tau^2)$$

$$\Rightarrow \nu_{gas} = 2\sqrt{|\tau|}, \quad \nu_{Li} = -2\sqrt{|\tau|}$$

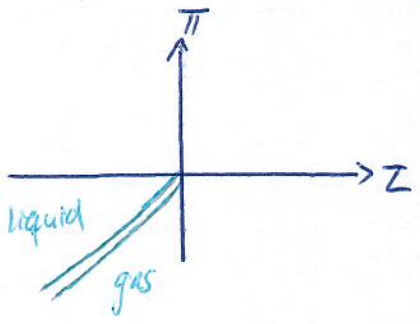
$$\Rightarrow \beta = 1/2$$

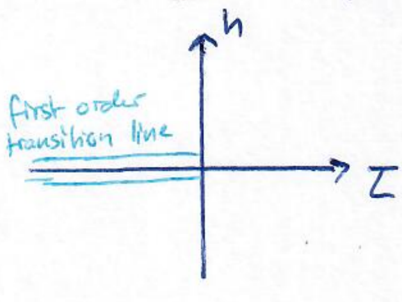
higher order ⇒





absence of m <-> -m symmetry

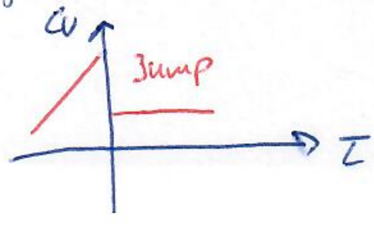




Compressibility ⇒ $\gamma = 1$

Speific heat ⇒ $\alpha = 0$

} treating the gas-liquid transition within MF, assuming long range interaction ⇒ MF-critical exponents by Landau



Magnetization and susceptibility

$$\langle n(\vec r)\rangle = \Big\langle \sum_i \delta(\vec r-\vec r_i)\Big\rangle \longleftrightarrow \langle \vec m(\vec r)\rangle = \Big\langle \sum_i \mu \vec S_i\, \delta(\vec r-\vec r_i)\Big\rangle$$

in homogeneous case: $\langle \vec m\rangle = \frac{\vec M}{V}$

$$\chi = \frac{\partial m}{\partial h} \qquad \text{(magnetic susceptibility)}$$

Partition function for a spin system

N spins fixed → Canonical Ensemble

$$Z_N(\underbrace{T,\vec h}_{\text{Intensive}}) = \sum_{\{S_i\}} \exp\left[-\frac{H[\{\vec S_i\}]}{k_B T}\right]$$

legendre transformation done in Hamiltonian.

$$G(T,\vec h,N) = -k_B T \log Z_N(T,\vec h)$$

$$\chi_{ij} = \frac{\partial m_i}{\partial h_j} = -\frac{1}{V}\frac{\partial^2 G}{\partial h_i \partial h_j}$$

via legendre: $F = G + \vec h\cdot\vec M = F(T,\vec M,N)$

$$\vec h = \frac{\partial F}{\partial \vec M}$$

$$\chi_{ij}^{-1} = V\frac{\partial^2 F}{\partial M_i \partial M_j}$$

Mean-field theory (Ising-model)

$$\mathcal{H} = -\frac{J}{2}\sum_{\langle i,j\rangle} S_i^z S_j^z - \mu h \sum_i S_i^z$$

effective, weiss field

external field

$$\frac{1}{z}\sum_j S_j^z = \langle S\rangle \cdot N \;\checkmark ?$$

(mean field approximation)

$$x = \mu h_i' \overset{\text{df.}}{=} \mu h + \sum_j J S_j^z = \mu h + z J \langle S\rangle$$

$$\Rightarrow \mathcal{H}_{MF} = \underbrace{\frac{J}{2} z N \langle S\rangle^2}_{\text{constant}} - \underbrace{\mu h' \sum_i S_i^z}_{\text{sum of single particle Hamiltonian}} ,$$

Graphical solution $\Rightarrow$ negative slopes lead to ~~finite~~ appearance of solution for $\langle S\rangle$ at $h=0$. Symmetry is spontaneously broken with finite $\langle S\rangle$.

For $T = T_c \Rightarrow \mu h = k_B T \frac{\langle S\rangle^3}{3}$

$$\Rightarrow \langle m\rangle = \frac{\mu}{V_{uc}}\left(\frac{3\mu h}{k_B T}\right)^{1/3}$$

$$\Rightarrow \langle m\rangle \propto h^{1/\delta} \quad , \delta = 3$$

close to T_c, $h = \frac{k_B}{\mu}(T\langle S\rangle - T_c\langle S\rangle)$

$$\Rightarrow \frac{\partial h}{\partial\langle S\rangle} = \frac{k_B T_c}{\mu}\left(\frac{T}{T_c} - 1\right)$$

$$\Rightarrow \chi = \frac{\partial m}{\partial h} = \frac{\mu}{V_{uc}}\frac{\partial\langle S\rangle}{\partial h} = \frac{\mu^2}{V_{uc} k_B T_c}\overset{\overset{?}{-\tau}}{\left(\frac{1}{\tau}\right.}$$

$$\chi \propto \frac{1}{\tau^\gamma} \Rightarrow \gamma = 1$$

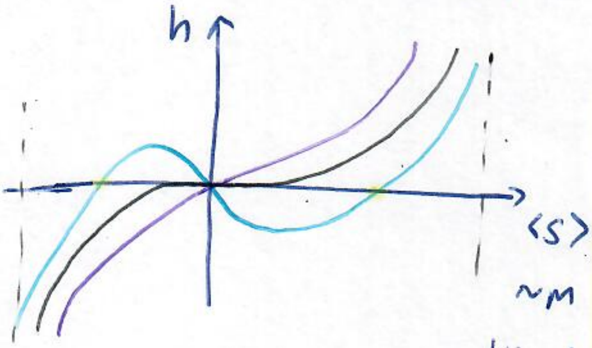
$$\langle S\rangle = \frac{\partial}{\partial\beta x}\log Z_1$$

$$\sim \langle S\rangle + \mathcal{O}\Big(\overset{\frac{\langle S\rangle^3}{3}}{\cancel{\langle S\rangle^2}}\Big)$$

✓ wikipedia

$$\Rightarrow \mu h = k_B T \operatorname{artanh}\langle S\rangle - zJ\langle S\rangle$$

(self consistency equation)



$$\Rightarrow k_B T_c = zJ \overset{\text{cubic}}{=} 2dJ$$

higher d favour higher $T_c \Rightarrow$ order

$h=0$

$$\Rightarrow k_B T\left(1 + \frac{\langle S\rangle^2}{3}\right) = z\overset{T_c}{J} = k_B T_c$$

$T \to T_c$
$\Leftrightarrow \langle S\rangle \to 0$

$$\Rightarrow \langle S\rangle \approx \pm\sqrt{3}\,|\tau|^{1/2}$$

$\tau = \frac{T}{T_c} - 1$

$\langle m\rangle = \frac{\mu\langle S\rangle}{V_{uc}}$

$$\Rightarrow \langle m\rangle \sim |\tau|^\beta = \left(1 - \frac{T}{T_c}\right)^{1/2} , \quad \beta = 1/2$$

Domain Walls in 1-D Ising model

p. 362 Huang
p. 362 Ziman

A domain wall costs 2J in Energy. ($\mathcal{H} = -\frac{J}{2}\sum_{\langle ij\rangle} S_i S_j - \mu h \sum_i S_i$) $\left\{\begin{array}{ll} \uparrow\downarrow & J \\ \uparrow\uparrow & -J \end{array}\right\} 2J$

$F = U - Tk_B \log W \Rightarrow \quad F_{dw} = 2J - Tk_B \log(\overset{\swarrow \#\text{spacing}}{N-1})$

For $N \to \infty$, $F_{dw} < 0 \Rightarrow$ The creation of a domain wall (i.e. destroying the order) <u>decreases</u> the free energy.

The only state enabling order is $T=0$. Domain walls are topological ~~defects~~ objects or defects (dragging them into the system across its boundaries.

Solution via Transfermatrices

$$Z_N = \sum_{S_1}\sum_{S_2}\cdots\sum_{S_N} \exp\Big(\beta \sum_{k=1}^{N} \big[J S_k S_{k+1} + \frac{\mu h}{2}(S_k + S_{k+1})\big]\Big)$$

$$\langle S|T|S'\rangle = \exp\big(\beta\big[JSS' + \frac{\mu h}{2}(S+S')\big]\big), \quad T = \begin{pmatrix} e^{\beta[J+\mu h]} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta[J-\mu h]} \end{pmatrix}$$

$$\Rightarrow Z_N(T,h) = \sum_{S_1}\cdots\sum_{S_N} \langle S_1|T|S_2\rangle\langle S_2|T|S_3\rangle\ldots\langle S_N|T|S_1\rangle = \lambda_+^N + \lambda_-^N$$

$N \to \infty$

$$\Rightarrow g(T,h) \simeq -J - k_B T e^{-2J/k_BT} \underbrace{- \frac{\mu^2 h^2}{2k_BT} e^{2J/k_BT}}_{\text{Domain wall}}$$ (free energy per particle)

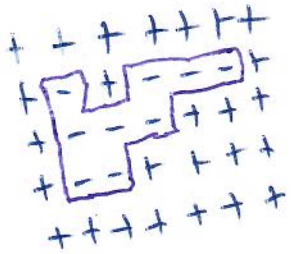
$$\langle m(T,h)\rangle = -\frac{\partial g}{V_{uc}\partial h} \cong \frac{\mu^2 h}{V_{uc} k_B T} e^{2J/k_BT} \xrightarrow[h\to 0]{} 0$$ no spontaneous magnetization

$$\chi = \frac{\partial m}{\partial h} = \frac{\mu^2}{V_{uc} k_B T} e^{2J/k_BT} \xrightarrow[T\to 0]{} \infty$$ T=0 phase transition

$$\xrightarrow[T\to\infty]{} \sim \frac{1}{(T-0)}$$ Curie-Weiss law with $T_c = 0$

Peierls Argument

p.350 Huang
p.364 Ziman (simple)



Energy of domain walls = $2JL$

$F = U - TS$, for small enough $T \Rightarrow$ order

dW

cost of domain $\sim \begin{cases} L^0 & 1D \\ L^1 & 2D \\ L^{d-1} & d\text{-}D \end{cases} \Rightarrow$ higher dimensions stabilize

$$p_- < \sum_L g(L) \underbrace{e^{-2JL/k_BT}}_{\text{cost in Energy of the loop}}$$

favours appearance of loops that flips the spin

Maximal surface

no crossings

$$g(L) \sim \left(\frac{L}{4}\right)^2 \cdot 4 \cdot 3^{L-1} \frac{1}{2L}$$

4direction

start at any point, go clock or anticlockwise

$$< \sum_{L=4,6,\dots}^{\infty} 3^L \frac{L}{24} e^{-2JL/k_BT} = \frac{1}{24} \sum_{L=4,5}^{\infty} -\frac{d}{d\alpha} e^{-\alpha L}$$

$$< \frac{5}{24} \frac{e^{-4\alpha}}{1-e^{-\alpha}} \quad , \quad \alpha = \frac{2J}{k_BT} - \log 3$$

$\Rightarrow$ for $k_BT < J$, $e^{-\alpha} < 0{,}41 \Rightarrow \langle s \rangle > 0{,}98$

$\Rightarrow$ below ~~for~~ $k_BT = J$ ~~then~~ the phase is ordered.

Onsager $\Rightarrow$ $k_BT_c \approx 2{,}27\,J$ depending on lattice

XY model in 2D

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j = -J \sum_{\langle i,j \rangle} \underbrace{\cos(\vartheta_i - \vartheta_j)}_{1 - \frac{(\vartheta_i - \vartheta_j)^2}{2} + \dots} \quad , \; h=0$$

Assume ϑ_0 for $T=0$, $z = 2d$

important

lattice spacing

$$\mathcal{H} \simeq -\frac{zNJ}{2} + \frac{1}{2} J \sum_{\langle i,j \rangle} (\vartheta_i - \vartheta_j)^2 = E_0 + \frac{Ja^2}{2} \int \frac{d^d r}{a^d} (\vec{\nabla}\vartheta)^2$$

$$\langle S_x^{\alpha} \rangle = \langle \cos\vartheta(\vec{r}) \rangle = \frac{\int \mathcal{D}[\vartheta(\vec{r})] e^{-\beta H_{el}} e^{i\vartheta(\vec{r})}}{\int \mathcal{D}[\vartheta(\vec{r})] e^{-\beta H_{el}}} = e^{-\langle \vartheta^2(\vec{r}) \rangle / 2}$$

$$\mathcal{H}_{el} = \frac{Ja^2}{2} \int \frac{d^d r}{a^d} [\vec{\nabla}\vartheta]^2 = \frac{Ja^2}{2} \sum_{\vec{k}} k^2 \vartheta_{\vec{k}} \vartheta_{-\vec{k}} \quad \text{(Gaussian Hamiltonian)}$$

Fourier

$$\langle \vartheta^2(\vec{r}) \rangle = \begin{cases} \frac{S^d}{(2\pi)^d} \frac{k_B T}{J} \frac{1}{d-2} & , d>2 \quad \text{short range reduce } \langle S_x \rangle \\ \infty \quad \text{for } k \to 0 & d \leq 2 \quad \langle S_x \rangle \to 0 \text{ , long range} \end{cases}$$

Remember:

$$C(\vec{r},0) = \langle \vec{S}(\vec{r}) \cdot \vec{S}(0) \rangle = \mathrm{Re} \langle \exp[i(\vartheta(\vec{r}) - \vartheta(0))] \rangle$$

$$= \exp(- \langle [\vartheta(\vec{r}) - \vartheta(0)]^2 \rangle / 2)$$

3D: $C(\vec{r},0) \xrightarrow{r \to \infty} \text{const}$ LRO

BKT makes it SRO

2D: $C(\vec{R},0) \xrightarrow{R \to \infty} \left(\frac{a}{R}\right)^{k_B T / 2\pi J} \xrightarrow[\text{alg.}]{\vec{R} \to \infty} 0$ QLRO

1D: $C(x,0) \xrightarrow{x \to \infty} \exp(-\frac{k_B T x}{2Ja}) \xrightarrow[\text{exp}]{x \to \infty} 0$ SRO

Hohenberg - Mermin - Wagner Theorem

p. 410 Huang

In systems with continuous symmetry every long range ordered phase is destroyed by fluctuations in one or two dimensions.

XY-model, Heisemberg, superfluids

Continuous symmetry broken ⇒ low energy excitation: fluctuations around one direction.

p. 407 Huang

Goldstone modes ~~are~~ have low ~~energy modes~~ have long wavelengths and only cost little deformation energy. ~~Lead~~ Lead to destruction of ordered phases in d=1, 2.

$$\langle \phi^2 \rangle \sim \int d^dk \frac{k_BT}{ck^2} \sim T \int dk k^{d-3} \sim \frac{T}{d-2} k^{d-2} \Big|_0 \xrightarrow{d=1,2} \infty$$

equipartition Theorem

Destruction of quasi-long-range order

p.496 Chaikin

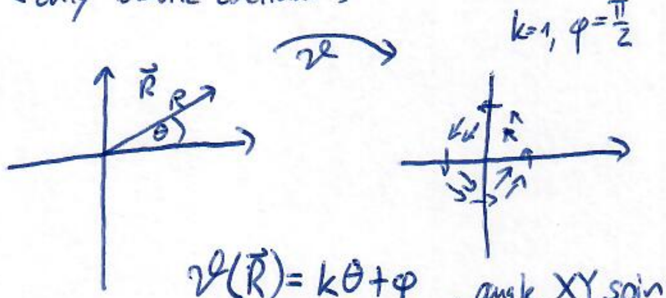
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \cos(\vartheta_i - \vartheta_j) \approx E_0 + \frac{Ja^2}{2} \int \frac{d^q r}{a^d} (\vec{\nabla}\vartheta)^2 \rightsquigarrow \text{QLRO}$$

Berezinskii phase

ϑ compact
topological excitations
lost

only elastic excitations

$$\Rightarrow C(\vec{R},0) \sim \exp[-R/\xi(T)]$$



$\vartheta(\vec{R}) = k\theta + \varphi$, angle XY spin

winding number

const

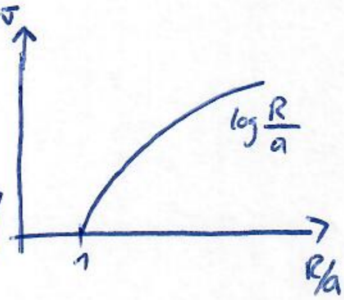
system size

$$E \approx \frac{J}{2} \int_a^L d^2R\, (\vec{\nabla}\vartheta)^2 = \pi J \log \frac{R_\infty}{R_0}$$

$R_\infty \sim L$, $R_0 \sim a$

lattice const

Some α constant specifying the shape of the vortex



vortex density

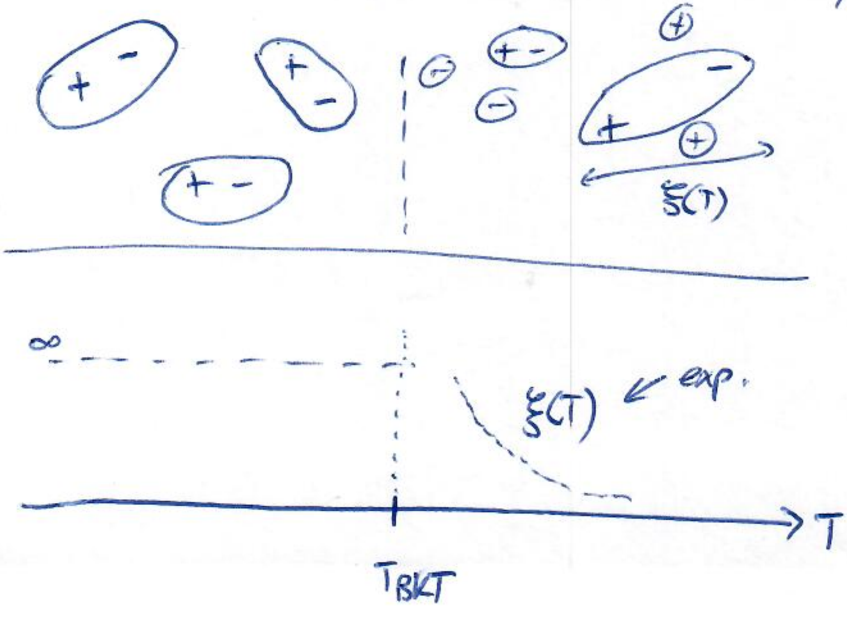
$$\mathcal{H}_\beta^{d=2} = \frac{J}{2} \int d^2R\, [\vec{\nabla}\vartheta_r]^2 - \pi J \underbrace{\int d^2R\, d^2R'\, n_v(\vec{R})\, n_v(\vec{R}')}_{\text{"neutral" Gas of vortices}} \cdot \left[\log \frac{|R-R'|}{a} - \log \frac{L}{a}\right]$$

leads to loss of QLRO

low temperature → vortices pairwise bound, do not destroy QLRO

more pairs appear

T_{BKT} → appearance of free vortices , destroy QLRO



unbind on scale $\xi(T)$
short range order

Berezinskii - Kosterlitz - Thouless transition

p. 496 chaikin

Estimation of T_{BKT}: A vortex cost an energy $\pi J \log\left(\frac{L}{a}\right)$. Possibility to place the vortex: $\left(\frac{L}{a}\right)^2 \Rightarrow S = k_B \log\left(\frac{L}{a}\right)^2$

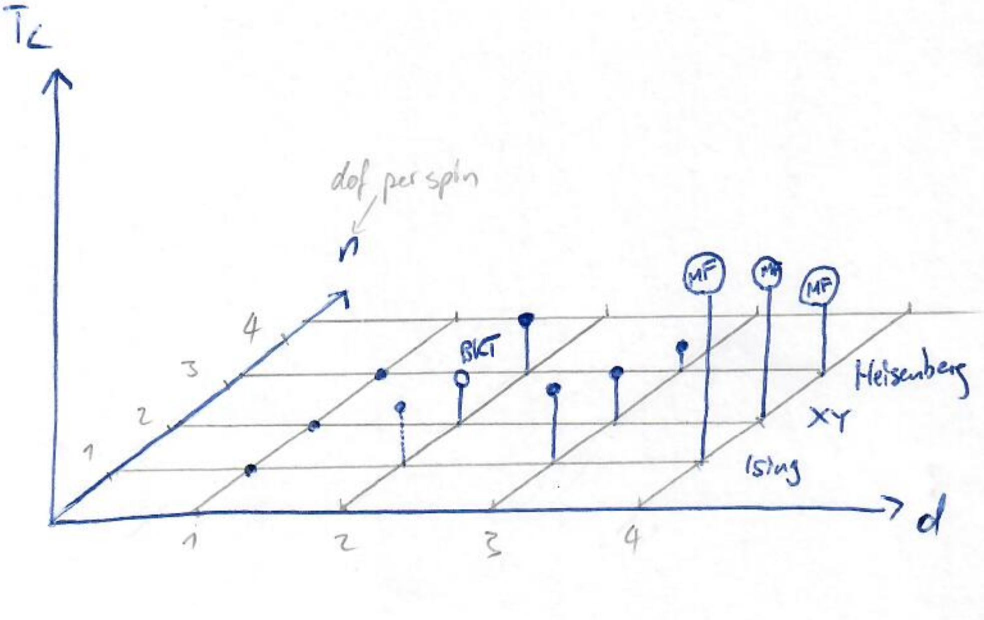
\# lattice points

$$\Rightarrow F = (\pi J - 2k_B T) \log \frac{L}{a}$$

$$\Rightarrow k_B T_{BKT} = \frac{\pi}{2} J$$

Heisenberg model [O(n) model]

$$k_B T_c \approx 2\pi J \frac{d-2}{n-2}$$



- Hohenberg - Mermin - Wagner
- Mean field ($\frac{1}{z}$ is small parameter)
- Ising 1D
- BKT
- $d=3$, symmetry$\nrightarrow$. T_c $\left(k_B T_c = J \frac{2d}{n}\right)$

Order

Correlator $C(\vec{r},\vec{r}') = \underbrace{\langle \vec{m}(\vec{r}) \cdot \vec{m}(\vec{r}') \rangle}_{\text{magnetisation}} = \mu^2 \underbrace{\langle \vec{S}(\vec{r}) \cdot \vec{S}(\vec{r}') \rangle}_{\text{Spin}}$

$$C(\vec{r},\vec{r}') \xrightarrow{|\vec{r}-\vec{r}'| \to \infty}$$

$\nearrow \langle \vec{m}(T) \rangle^2 \neq 0$ LRO, δ-Bragg peaks

$\searrow 0$

$\quad \nearrow \frac{1}{|\vec{r}-\vec{r}'|^{\alpha}2}$ algebraic, Quasi LRO, algebraic Bragg peaks

$\quad \searrow e^{-|\vec{r}-\vec{r}'|/\xi}$ exponential, SRO

Susceptibility and correlations

Space dependant drive $\vec{h}(\vec{r})$, response $\vec{m}(\vec{r})$

$$\chi_{ij}(\vec{r},\vec{r}\,') \overset{\text{def.}}{=} \frac{\delta \langle m_i(\vec{r})\rangle}{\delta h_j(\vec{r}\,')} = \frac{1}{k_B T}\langle \delta m_i(\vec{r})\delta m_j(\vec{r}\,')\rangle = \frac{1}{k_B T} G_{ij}(\vec{r},\vec{r}\,')$$

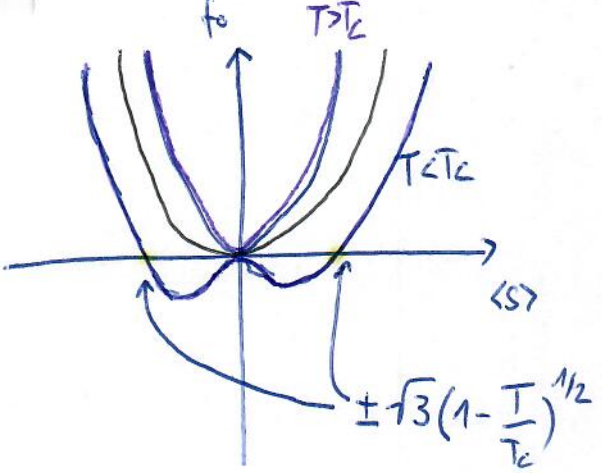
Bragg and Williams

$$\langle s\rangle \overset{\text{def.}}{:=} \frac{N_\uparrow - N_\downarrow}{N}\ ,\ S = k_B \log \binom{N}{N_\uparrow} = k_B \log \binom{N}{N\left(\frac{1+\langle s\rangle}{2}\right)} = \begin{cases} 0\ , & \langle s\rangle = \pm 1 \\ N k_B \log 2\ , & \langle s\rangle = 0 \end{cases}$$

$$U_h = -\frac{1}{2} N z J \langle s\rangle^2 - N \mu h \langle s\rangle$$ from mean field approximation

For $h=0$ and $\langle s\rangle$ small we get

$$f_0(T,\langle s\rangle) = \frac{U_0 - TS}{N} \simeq \frac{1}{2}(k_B T - \underbrace{Jz}_{k_B T_c})\langle s\rangle^2 + \frac{k_B T}{12}\langle s\rangle^4 \overbrace{- k_B T \log 2}^{\text{shift}}$$



The O(n) model

$$\mu \vec{h}' = \mu \vec{h} + zJ\langle \vec{S}\rangle \quad , \quad \langle S\rangle = \frac{\int d\Omega\, e^{\beta\mu\vec{h}'\cdot\vec{S}}\, \vec{S}}{\int d\Omega\, e^{\beta\mu\vec{h}'\cdot\vec{S}}}$$

XY-model

$$S^x = \cos\varphi \, , \quad \langle S^x\rangle = \frac{\int d\varphi\, e^{\beta\mu h'_x \cos\varphi} \cos\varphi}{\int d\varphi\, e^{\beta\mu h'_x \cos\varphi}} = \frac{I_1[\beta\mu h_x + \beta zJ\langle S^x\rangle]}{I_0[\beta\mu h_x + \beta zJ\langle S^x\rangle]}$$

Heisenberg

$$S^x = \cos\vartheta \, , \quad \langle S^x\rangle = \frac{\int d\varphi \int d\cos\vartheta\, e^{\beta\mu h'_x \cos\vartheta} \cos\vartheta}{\int d\varphi \int d\cos\vartheta\, e^{\beta\mu h'_x \cos\vartheta}} = \coth[\beta\mu h_x + \beta zJ\langle S^x\rangle] - \frac{1}{\beta\mu h_x + \beta zJ\langle S^x\rangle}$$

$$k_B T_c = \begin{cases} \frac{zJ}{1} , & \text{Ising} \\ \frac{zJ}{2} , & XY \\ \frac{zJ}{3} , & \text{Heisenberg} \end{cases} \qquad \begin{aligned} \langle S\rangle &= \sqrt{3}\sqrt{1-t} \\ \langle S\rangle &= \sqrt{2}\sqrt{1-t} \\ \langle S\rangle &= \sqrt{5/3}\sqrt{1-t} \end{aligned}$$

The qualitative behaviour of the order parameter with mean field theory is independant of the d and n.

$$f = \frac{r}{2}\langle S\rangle^2 + u\langle S\rangle^4 + \text{const} \quad , \quad r = r_0\left(1 - \frac{T}{T_c}\right)$$

f gives a universal behaviour independant from n and d. The differences are in r_0, u. and T_c. $k_B T_c = J\frac{zd}{n}$, fluctuations are missing!

Landau Theory (Overview)

Small parameter ϕ

$F(T,\Phi)$ described as taylor series in the $\overbrace{\text{order parameter}}$ used to describe the phenomenon in the proximity of a phase transition.

second order　　　stabilise　　　symmetries

$$f(T,\phi) = \frac{r}{2}\phi^2 - w\phi^{\cancel{4}3} + u\phi^4 + u'\phi^6 + \frac{c}{2}|\vec{\nabla}\phi|^2$$

no linear due to　　　first order (Symmetry?)　　　non local effects, spatial correlations

$g(T,h) = f - h\phi$

$$Z = \int \mathcal{D}[\phi(\vec{r})]\, \mathrm{Tr}_{\phi_\mu} \prod_{\vec{r}} \delta[\phi(\vec{r}) - \Sigma(\phi_\mu(\vec{r}))]\, e^{-\beta\mathcal{H}[\phi_\mu(\vec{r})]}$$

$$= \int \mathcal{D}[\phi(\vec{r})]\, e^{-\beta F[T,\phi(\vec{r})]}$$

and ϕ describe correct long wave and low energy physics

$Z_{MF} = e^{-\beta F_{MF}(T)}$, + Gaussian/quadratic fluctuations → Gauss model

$$\text{Gauss} \xleftrightarrow[\text{criterion}]{\text{Ginzburg}} \text{critical/large}$$

→ Mean field, $\frac{1}{z}$ small parameter, interaction must extend ~~to~~ over many degrees of freedom → high dimension or interaction long range

→ Landau theory, near T_c, order parameter small, jump must be small,

→ ~~Small~~ Gauss theory, small fluctuations

→ RG treatment, large fluctuations, near T_c

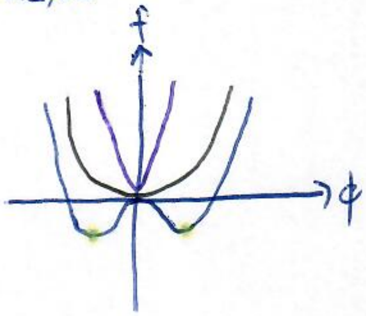
F must be consistent with the symmetries of the underlying Hamiltonian.

Second-order phase transitions

p. 422 Huang

$$f(T,\phi) = \underbrace{\frac{r}{2}\phi^2 + u\phi^4}_{u>0} \quad , \quad \xrightarrow[r(T<T_c)<0]{r(T>T_c)>0} r(T) = r_0(T-T_c)$$

$$\Rightarrow \phi_{min} = \begin{cases} 0 & T > T_c \\ \pm\left(\frac{-r}{4u}\right)^{1/2} & T < T_c \end{cases}$$



$$\Rightarrow \phi = \left(\frac{r_0}{4u}\right)^{1/2} (T_c - T)^{\beta} \quad , \quad \beta = 1/2 \quad , \quad \beta = 1/3 \text{ due to fluctuations in 3D}$$

$$h = \frac{\partial F}{\partial \phi} = r\phi + 4u\phi^3 \underset{\substack{T=T_c \\ \Leftrightarrow r=0}}{\Rightarrow} \phi = \left(\frac{h}{4u}\right)^{1/3} \Rightarrow \delta = 3$$

∂_h ϕ_{min}

use inverse

$$\chi = \frac{\partial \phi}{\partial h}\Big|_{h=0} = \begin{cases} 1/r & T > T_c \\ \frac{1}{2}\frac{1}{|r|} & T < T_c \end{cases} \Rightarrow \chi \sim \frac{1}{|T-T_c|^{\gamma}} \Rightarrow \gamma = 1$$

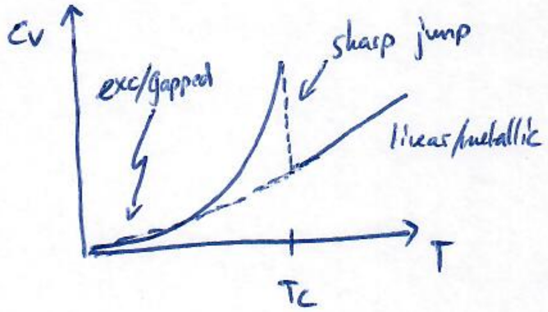
Fluctuations ⇝ $\gamma = \frac{4}{3}$ in 3D

$$\overset{\phi_{min}}{\Rightarrow} f = \begin{cases} 0 & T > T_c \\ -\frac{r^2}{16u} & T < T_c \end{cases} \quad , \quad C_V = -T\frac{\partial^2 f}{\partial T^2} = \begin{cases} 0 & T > T_c \\ \frac{T r_0^2}{8u} & T < T_c \end{cases}$$

at ϕ_{min}

$$C_V * \sim \frac{1}{|T-T_c|^{\alpha}} \quad , \quad \alpha = 0$$

its a jump
not a continuous transition
eventhough linear after



Typical for meanfield like

Superconductivity	bosonic superfluid
$n\xi_0^3 \gg 1$ ⇝ MF like	$n\xi_0 \sim 1$
$\Delta \sim \tau^{1/2}$ at T_c	λ transition

Non-local susceptibility and correlation length

(p. 425 Huang)
→ p. 154 Chaikin

$$\chi^{-1}(\vec{r},\vec{r}') = \frac{\delta^2 F}{\delta\phi(\vec{r})\,\delta\phi(\vec{r}')} = k_B T\, G^{-1}(\vec{r},\vec{r}') \quad , \quad F = \frac{r}{2}\phi(\vec{r})^2 + u\phi(\vec{r})^4 + \frac{c}{2}|\vec{\nabla}\phi|^2$$

$$\frac{\delta F}{\delta\phi(\vec{r})} = \frac{\partial f}{\partial \phi}(\vec{r}) - \vec{\nabla}\cdot\frac{\partial f}{\partial(\nabla\phi)}(r)$$

$$\chi^{-1}(\vec{r},\vec{r}') = (r + 12u\phi^2 - c\nabla^2)\,\delta(\vec{r}-\vec{r}')$$

Fourier

$$\chi(\vec{q}) = \frac{1}{r + 12u\phi^2 + cq^2}$$

divide the whole by $r+12u\phi$

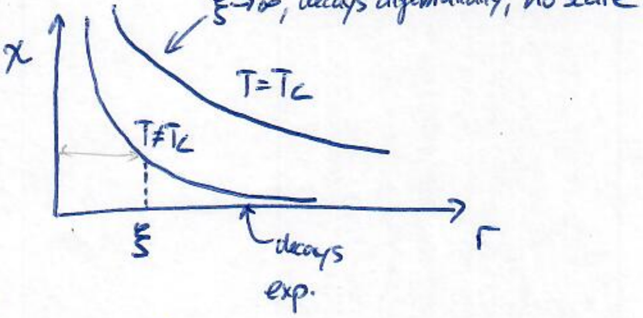
Orstein-Zernicke

$$\chi(q) = \frac{1}{c}\,\frac{\xi^2}{1+q^2\xi^2} \quad , \quad \xi(T) = \left(\frac{c}{r+12u\phi^2}\right)^{1/2} = \begin{cases} \sqrt{c/r} & T > T_c \\ \sqrt{-c/2r} & T < T_c \end{cases}$$

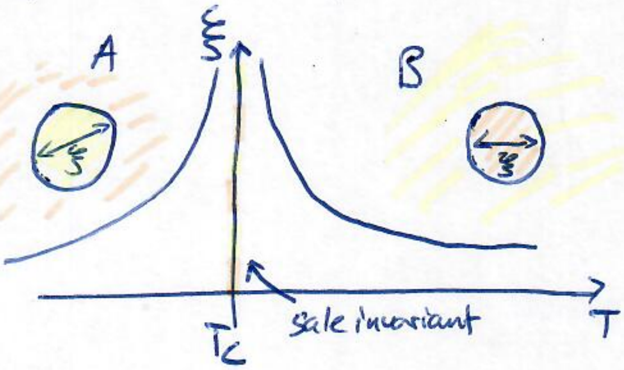
From $\xi(T) \sim \frac{1}{|T-T_c|^{\nu}} \Rightarrow \nu = 1/2$ ← Fluctuations: $\nu \approx 2/3$ in 3D

"Microscopic" correlation length, $T=0 \Rightarrow \xi_0 \approx \sqrt{\frac{c}{r_0 T_c}}$

inverse Fourier $\Rightarrow$ $\chi(r) = \frac{1}{cr^{d-2}}\,Y(r/\xi)$



The length ξ describes the distance over which a perturbation in the order parameter will recover, or over which a perturbation stretches.



$$\chi(r) \propto \frac{1}{r^{d-2+\eta}} \quad , \quad \eta = \frac{1}{4} \text{ for Kosterlitz-Thouless}$$

$\eta_{MF} = 0$

η anomalous dimension

Longitudinal and transverse response

p. 406 Huang
⇒ p 156. Chaikin

$\chi_{\parallel}$ and $\chi_{\perp}$ directed longitudinally and transverse to the direction of order.

$$\chi_{ij}^{-1}(\vec{q}) = (r + 4u\phi^2 + cq^2)\delta_{ij} + 8u\,\phi_i\phi_j$$

$$\phi^4 = \phi_i^2\phi_j^2 \begin{cases} 4\phi_i\phi_j \\ 4 \end{cases}$$

Assume symmetry broken along $\vec{\phi}$

$$\Rightarrow \quad P_{ij}^{\parallel} = \frac{\phi_i\phi_j}{\phi^2} \quad , \quad P_{ij}^{\perp} = \delta_{ij} - \frac{\phi_i\phi_j}{\phi^2}$$

$$\chi_{ij}^{-1}(\vec{q}) = \chi_{\parallel}^{-1}(\vec{q})\,P_{ij}^{\parallel} + \chi_{\perp}^{-1}(\vec{q})\,P_{ij}^{\perp}$$

same

$$\chi_{\parallel}(\vec{q}) = \frac{1}{r + 12u\phi^2 + cq^2} \quad , \qquad \chi_{\perp}(\vec{q}) = \frac{1}{r + 4u\phi^2 + cq^2} = \begin{cases} \underbrace{\dfrac{1}{r + cq^2}}_{} & T > T_c \\ \dfrac{1}{cq^2} & T < T_c \end{cases}$$

mass

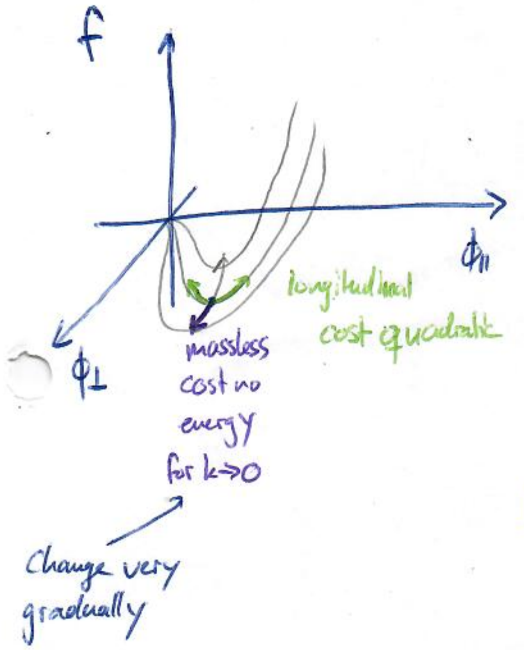
$\phi = 0$

$\phi_{min} = \sqrt{\frac{-r}{4u}}$

massless

$$\overset{r \neq 0}{\Rightarrow} \quad G_{\perp}(\vec{r}) \sim \frac{1}{r^{d-2}}$$

$|\vec{r}|$

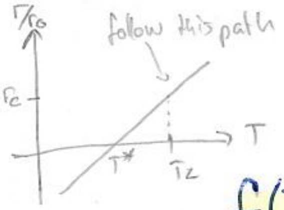


The softness of transverse fluctuations destroys the long-range order in lower dimensions d=1 and d=2, Hohenberg-Mermin-Wagner

longitudinal → change in amplitude in ϕ

transverse → change in "phase" or direction of ϕ.
spin waves

Only exists when a continuous symmetry is broken.



First-order phase transitions   p. 170 Chaikin

$$f(T,\phi) = \frac{r}{2}\phi^2 - w\phi^3 + u\phi^4 \, ,$$

w, u: >0 and constant

$$r = r_0(T-T^*)$$ only negative if for sure!!! phase transition

$$r_c = r_0(T_c - T^*)$$

at T_c
$$\begin{cases} \frac{\partial f}{\partial \phi} = (r - 3w\phi + 4u\phi^2)\phi \overset{!}{=} 0 \\ f = (\frac{r}{2} - w\phi + u\phi^2)\phi^2 \overset{!}{=} 0 \end{cases}$$

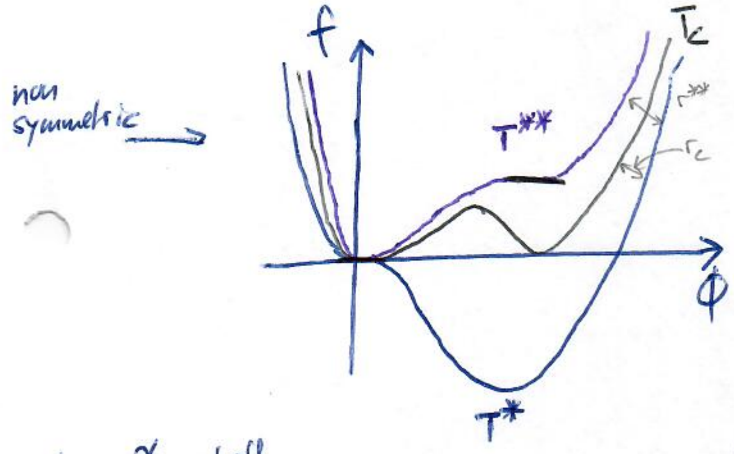
eliminate r

divide by ϕ

$$\Rightarrow \phi_{min} = \frac{w}{2u} \, , \, r_c = r_0(T_c - T^*) = \frac{w^2}{2u} > 0$$

where touchdown on $f=0$

insert in $f(\phi_{min}) = 0$



T^* and T^{**} define the spinodals (meta → un)

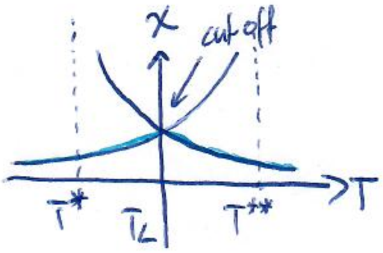
T^*: supercooling, T^{**}: superheating — hysteretic effects

$$f = \begin{cases} 0 & T > T_c \\ \underbrace{(r - r_c)}_{\text{yields } r_0(T-T_c)} \phi_{min}^2/2 & T < T_c \end{cases}$$

to lowest order, take ϕ^2 only, ϕ is small, $O(\phi^3)$

insert ϕ_{min}

$$\Rightarrow S_{\phi_{min}} - S_0 = -\frac{r_0 w^2}{8u^2}$$



$$\Rightarrow L = \frac{r_0 w^2 T_c}{8u^2} \, ,$$ vanishes with $w \to 0$

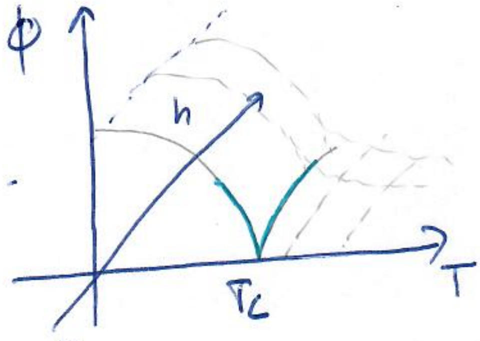
$$\chi = \frac{\partial \phi}{\partial h} = \begin{cases} \frac{1}{r_0(T-T^*)} & T > T_c \\ & \end{cases}$$

First-order phase transition shows no scaling laws and we cannot define any critical exponents.

Beware: First order transitions can also be obtained via ϕ^6 Theory including even powers ($u<0$).

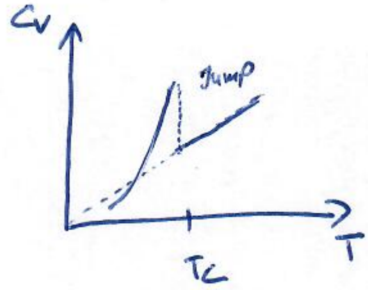
Landau mean field theory, second and first-order Assp.

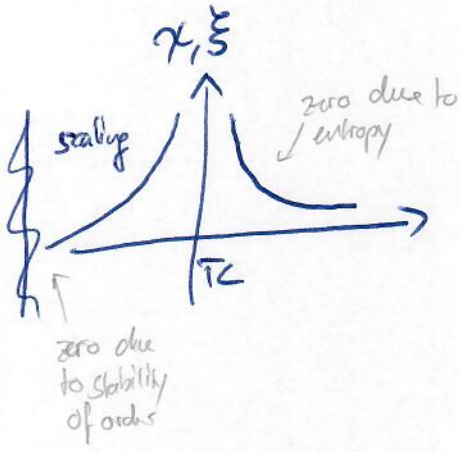
second



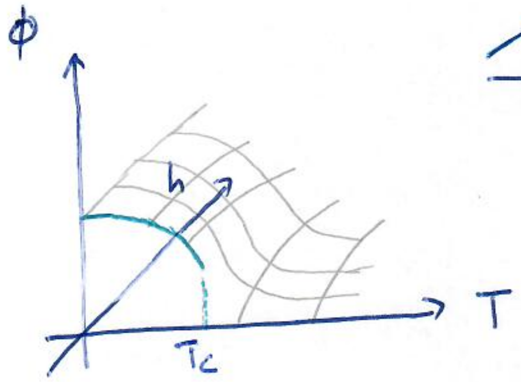
scaling

in supercond, h=0

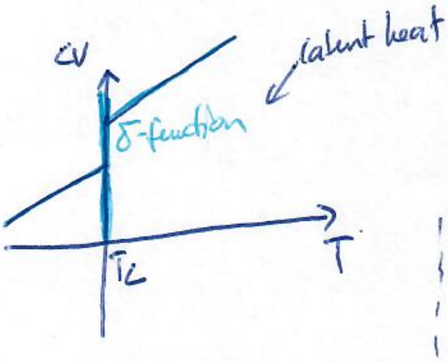


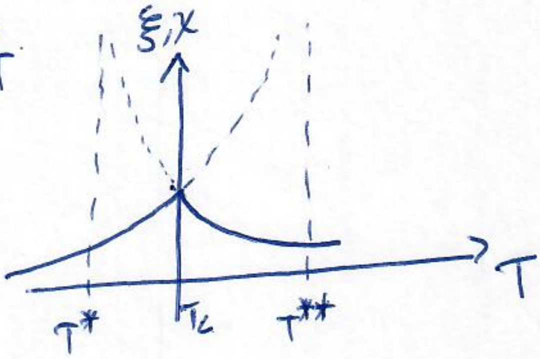


First



Jump





Multicritical points

p. 172 Chaikin

energy gap

$$f(T,\Delta,\phi) = \frac{1}{2} r(T,\Delta)\phi^2 + u(T,\Delta)\phi^4 + u'\phi^6$$

$r_0(T-T^*)$

$u' > 0$, Stability

for $u<0 \Rightarrow$ first order transitions

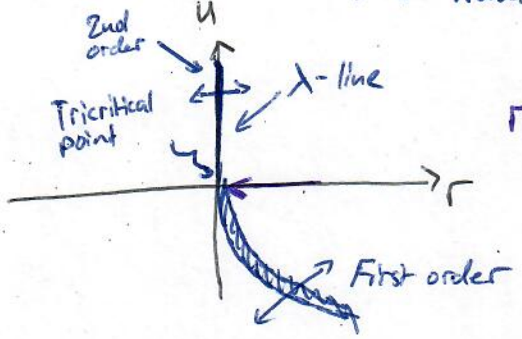
$u>0 \Rightarrow r(T,\Delta) \overset{=0}{}$ line of second-order phase transition

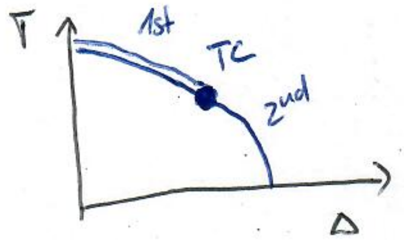
$f = \frac{\partial f}{\partial \phi} = 0$

$\phi \neq 0$

$$\Rightarrow r_c = r_0(T_c - T^*) = \frac{u^2}{2u'}$$

$r = r_0 T_{TC} Z$





The conjugate variables S and x jump on the first order line, and are related throug Clapeyron equations.

$$\Delta S = -\frac{\partial f}{\partial T} \approx -\frac{r_T}{4}\frac{|u|}{u'} \longrightarrow 0 \text{ at TC}$$

For the path $(u=0) \Rightarrow f = \frac{1}{2} r\phi^2 + u'\phi^6$

$$\Rightarrow \frac{\partial f}{\partial \phi} \overset{!}{=} 0 = r\phi + 6u'\phi^5 \Rightarrow \phi = \pm\left(\frac{-r}{6u'}\right)^{1/4} \sim Z^{\beta}$$

$$\Rightarrow \beta = 1/4$$

Generally, $h = r\phi + 4u\phi^3 + 6u'\phi^5$, and the critical isotherm at $r=0, u=0$, TC

$$\Rightarrow \phi = \left(\frac{h}{6u'}\right)^{1/\delta}, \quad \delta = 5$$

? maybe First order and hence $\phi \ll 1$?

For $u=0$, $h = \frac{\partial f}{\partial \phi}$

$$\Rightarrow \chi = \frac{\partial \phi}{\partial h} = \frac{1}{r + 30u'\phi^4} = \begin{cases} 1/r & T > T_{TC} \\ -1/4r & T < T_{TC} \end{cases} \sim |Z|^{\gamma} \Rightarrow \gamma = 1$$

$$f = \begin{cases} 0, & T > T_{TC} \\ \frac{r}{2}\sqrt{-r/6u'}, & T < T_{TC} \end{cases} \Rightarrow f \sim |\tau|^{3/2} \Rightarrow c_V = -T\frac{\partial^2 f}{\partial T^2} \sim |Z|^{-\alpha} \Rightarrow \alpha = \frac{1}{2}$$

Critical behaviour at the critical point

	α	β	γ	δ	ν	η
C	0	1/2	1	3	1/2	0
TC	1/2	1/4	1	5	1/2	0

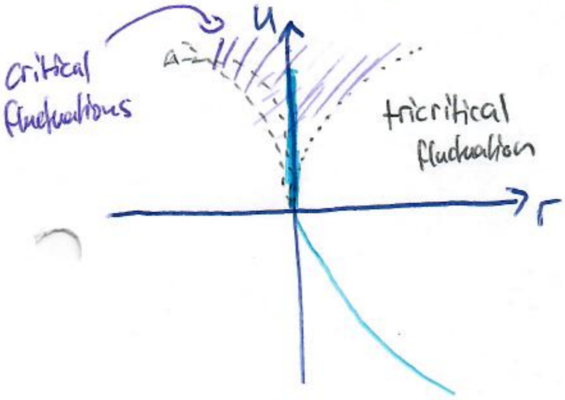
$f \approx \frac{r}{2}\phi^2 + u\phi^4$, $u'\phi^6$ small

$\updownarrow$

$f \approx \frac{r}{2}\phi^2 + u'\phi^6$, $u\phi^4$ small

↗ see sketch

$\Rightarrow u'\phi^2 \sim u$, $\left(\frac{r}{2}\phi^2 \sim u\phi^4 \Rightarrow \phi^2 \sim \frac{r}{2u}\right) \Rightarrow r \sim \frac{u^2}{u'}$



Lattice field theory and continuum limit

$$\mathcal{H}[\phi_\nu] = \underbrace{\sum_\nu \frac{r}{2}\phi_\nu^2 + u\phi_\nu^4}_{\downarrow} + \underbrace{\frac{1}{2}\sum_{\nu,\nu'} c_{\nu\nu'}(\phi_\nu - \phi_{\nu'})^2}_{\downarrow}$$

continuum limit

$$\int \frac{d^d r}{v} f[\phi(\vec{r})] \qquad \frac{1}{2}\int \frac{d^d r}{v} c[\vec{\nabla}\phi]^2$$

ϕ_ν^2-Term:

$$Z = \underbrace{\int D[\phi(\vec{r})]}_{\text{continuum limit}} e^{-\beta F[T,\phi(\vec{r})]} = \prod_\nu^N \int_{-\infty}^{\infty} d\phi_\nu\, e^{-(r/2k_BT)\phi_\nu^2} = \underbrace{\sqrt{\frac{2\pi k_B T}{r}}^{\,N}}_{\text{important result}}$$

drop quastic and elastic

$$\xrightarrow{\text{continuum limit}} \lim_{v\to 0} \prod_\nu \int_{-\infty}^{\infty} d\phi_\nu$$

$\phi\in\mathbb{R} \Rightarrow \phi_{-k} = \phi_k^*$

ϕ_ν^2, elastic Term:

$$\mathcal{H} = \underbrace{\frac{1}{2N}\sum_{\vec{k}}(r+ck^2)\phi_{\vec{k}}\phi_{-\vec{k}}}_{\mathcal{H}_G = \frac{1}{N}\sum_{\vec{k}}'(r+ck^2)|\phi_{\vec{k}}|^2} + \frac{u}{N^3}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3} \phi_{\vec{k}_1}\phi_{\vec{k}_2}\phi_{\vec{k}_3}\phi_{-\vec{k}_1-\vec{k}_2-\vec{k}_3}$$

$$\int D[\phi(\vec{r})] \longrightarrow \int \prod_{k<\Lambda}' d\phi_k\, d\phi_k^*/N \longrightarrow \int \prod_{k<\Lambda}' \frac{2}{N}\, d\,\Re\phi_{\vec{k}}\, d\,\Im\phi_{\vec{k}}$$

Gaussian model

$$\mathcal{H}_G = \frac{1}{2}\int \frac{d^d r}{V}\left[r\phi^2(\vec r) + c|\vec\nabla\phi(\vec r)|^2\right] \overset{\text{F.T.}}{=} \frac{1}{N}\sum_{\vec k}{}' \left[r+ck^2\right]|\phi_{\vec k}|^2 =: \frac{1}{N\beta}\sum_{\vec k}{}' \phi^*_{\vec k}\, G_0^{-1}(\vec k)\,\phi_{\vec k}$$

$$Z_N = \int \mathcal{D}[\phi(\vec r)]\, e^{-\beta\mathcal{H}[\phi(\vec r)]} = \int \prod_k^{\Lambda}{}' d\phi_k\, d\phi_k^*$$

$$G_0(\vec k) = \frac{k_B T}{r+ck^2}$$

$$\Rightarrow Z_G = e^{-\beta F_G} = \prod_{\vec k}^{\Lambda}\sqrt{\frac{2\pi k_B T}{r+ck^2}}\,, \quad 0<|\vec k|<\Lambda$$

$$\Longrightarrow F = F_{MF} - \underbrace{\frac{k_B T}{2}\sum_{|\vec k|<\Lambda}\log\frac{2\pi k_B T}{r+ck^2}}_{F_G}$$

$\log T$

$$\Rightarrow \frac{F_G}{V} = -\frac{k_B T}{2}\int\frac{d^d k}{(2\pi)^d} \approx \frac{S_{d-1}}{d}\frac{k_B T}{a^d}\log\Lambda + \frac{S_{d-1}}{d(2\pi)^d}\frac{k_B T}{\xi^d}\log\xi = F_a + F_{sing}$$

$$\xi = \sqrt{\frac{c}{r_0(T-T_c)}}$$

$$c_V = -T\frac{\partial^2 F}{\partial T^2}$$

$$\Longrightarrow c_V \sim k_B\int\frac{d^d k}{(2\pi)^d}\frac{(T\partial_T r)^2}{(r+ck^2)^2} \sim k_B\,\xi^{4-d}\underbrace{\int_0^{\Lambda\xi} dx\,\frac{x^{d-1}}{(1+x^2)^2}}_{<\infty \text{ for } 1<d<4}\,, \quad x = k\xi$$

$$\Longrightarrow c_V \sim \text{const}\,\xi^{4-d} \xrightarrow{\tau\to 0^+} \infty \quad \text{for } 1<d<4$$

$$\Longrightarrow c_V \sim \tau^{-(4-d)/2} \sim \tau^{-\alpha} \Rightarrow \alpha = 2 - \frac{d}{2}$$

From above: $c_V \sim \int_{\xi^{-1}} d^d k\, \frac{1}{k^4} \Rightarrow \begin{cases} \text{diverging for small } k\text{, infrared divergence} & 1<d<4 \\ \text{diverging but prefactor} \to 0\text{, regular result} & d>4 \\ \text{remains finite, fluctuations do not provide a correction} & \\ \text{logarithm} & d=4 \end{cases}$

Gaussian approximation of a Hamiltonian

$$\left.\frac{\delta \mathcal{H}}{\delta \phi(\vec{r})}\right|_{\phi_{saddle}} = 0 \quad , \quad \mathcal{H}_{saddle} = \mathcal{H}(\phi_{saddle})$$

↖ any extremum of $\mathcal{H}$

The mean-field approximation of a theory corresponds to a saddle point approximation where the saddle is a minimum

$$Z_{MF} = e^{-\mathcal{H}(\phi_{min})/k_BT} \quad , \quad \left.\frac{\delta \mathcal{H}}{\delta \phi(\vec{r})}\right|_{\phi_{min}(\vec{r})} = h(\vec{r})$$

$$\mathcal{H}_G = \underbrace{\mathcal{H}(\langle\phi(\vec{r})\rangle)}_{\text{not } \phi_{min}} + \frac{1}{2}\int d^d r\, d^d r'\, \delta\phi(\vec{r}) \underbrace{\left.\frac{\delta^2 \mathcal{H}}{\delta\phi(\vec{r})\,\delta\phi(\vec{r}')}\right|_{\langle\phi(\vec{r})\rangle}}_{\mathcal{H}_2 \text{ (operator)}} \delta\phi(\vec{r}')$$

fluctuations can change the mean value of ϕ

$$\Rightarrow \mathcal{H}_2\, \delta\phi_\lambda(\vec{r}) = \varepsilon_\lambda\, \delta\phi_\lambda(\vec{r})$$

$$\{\delta\phi_\lambda\} \quad \delta\phi(\vec{r}) = \sum_\lambda c_\lambda\, \delta\phi_\lambda(\vec{r})$$

$$\Rightarrow \mathcal{H}_G = \mathcal{H}(\langle\phi(\vec{r})\rangle) + \frac{1}{2}\sum_\lambda \varepsilon_\lambda c_\lambda^2$$

Example ϕ^4-Theory

$$\Rightarrow r\phi_{min} + 4u\phi_{min}^3 = h$$

$$\Rightarrow (r + 12u\langle\phi\rangle^2 - c\nabla^2)\,\delta(\vec{r}-\vec{r}') = \mathcal{H}_2$$

$$\overset{FT}{\Rightarrow} \varepsilon_{\lambda=k} = r + 12u\langle\phi\rangle^2 + ck^2$$

$$\Longrightarrow \mathcal{H}_G^{\phi^4} = \mathcal{H}(\langle\phi\rangle) + \frac{1}{2V}\sum_{\vec{k}\neq 0} \phi_{\vec{k}}^*(r + 12u\langle\phi\rangle^2 + ck^2)\,\phi_{\vec{k}}$$

Susceptibility and correlator, Gauss vs. Meanfield

$$\chi_0 = G_0/k_BT \quad , \quad \chi_0 = \frac{\partial\langle\phi\rangle}{\partial h} \quad , \quad G_0 = \langle\delta\phi\,\delta\phi\rangle$$

$$\chi^{-1}(\vec{r},\vec{r}') \overset{def}{=} \frac{V^2\delta^2\mathcal{H}_G}{\delta\phi(\vec{r})\,\delta\phi(\vec{r}')} \underset{\substack{ex.9\\(4)}}{\overset{\frac{\delta H}{\delta h(\vec{r})}}{=}} V(r - c\nabla^2)\,\delta(\vec{r}-\vec{r}') \overset{FT}{\rightsquigarrow} \chi_0(\vec{q}) = \frac{1}{r+cq^2}$$

$$\langle\delta\phi(\vec{r})\,\delta\phi(\vec{r}')\rangle \overset{def.}{=} \langle\phi(\vec{r})\phi(\vec{r}')\rangle - \cancelto{0}{\langle\phi(\vec{r})\rangle\langle\phi(\vec{r}')\rangle}$$

$$\overset{FT}{=} \frac{1}{N^2}\sum_{\vec{k},\vec{k}'} e^{i\vec{k}\cdot\vec{r}} e^{i\vec{k}'\cdot\vec{r}'} \langle\phi_{\vec{k}}\phi_{\vec{k}'}\rangle$$

$$\Rightarrow \langle\phi_k\phi_{k'}\rangle \underset{\substack{S.11\\ex.9}}{\overset{def.}{=}} \frac{1}{Z_G}\int\prod_{\vec{q}}{}' \frac{d\phi_q\,d\phi_q^*}{N}\,\phi_k\,\phi_{k'}\,e^{-\beta H_G} = \begin{cases} 0 & \vec{k}\neq\vec{k}' \\ 0 & \vec{k}=\vec{k}' \end{cases}$$

$$\langle\phi_{\vec{k}}\phi_{\vec{k}}\rangle \overset{\text{integration}}{=} \frac{Nk_BT}{r+ck^2} \qquad \text{(Equipartition Theorem)}$$

$$\Rightarrow \langle\phi_k\phi_{k'}\rangle = \delta_{\vec{k},-k'}\frac{Nk_BT}{r+ck^2} = N\delta_{k,-k}\,G_0(k) = N\delta_{k,-k}\,k_BT\,\chi_0(\vec{k})$$

$$\Rightarrow \gamma = 1, \quad \nu = 1/2, \quad \eta = 0$$

rewrite in $\frac{q_1\xi^2}{c(1+\xi^2k^2)}$ form, coefficient comparison, $\xi^2 = \frac{c}{r}$

$$\int\frac{d^dr}{V}G(\vec{r}) = G(\vec{k}=0) = k_BT\,\chi(T) = \frac{k_BT}{r(T)}$$

The Ginzburg criterion   p. 214 Chaikin

The Ginzburg criterion defines the region around T_c, where the fluctuations are important – this region is called critical.

in use definition

$$\frac{r_0^2 T_c}{8u} \overset{\downarrow}{=} \Delta c_V =: c_V(T-T_c)|_{T_G}$$

ϕ vs. $\delta\phi$

$V_\xi = \xi^d$

$$\overline{\delta\phi} = \frac{1}{V_\xi}\int d^d r\, \delta\phi(\vec{r}) \longrightarrow \langle \overline{\delta\phi}^2 \rangle$$

Fluctuations become relevant when $\langle \overline{\delta\phi}^2 \rangle > \langle \phi \rangle^2$

$$\Rightarrow \langle \overline{\delta\phi}^2 \rangle = \langle \phi \rangle^2 |_{T_G}$$

$$\langle \overline{\delta\phi}^2 \rangle = \frac{A_d k_B T \xi_0^2}{2c\,\xi^d |1-t|}\ , \qquad \langle \phi \rangle^2 = \frac{2\Delta c_V T_c}{c}\xi_0^2 |1-t|$$

Using $\Delta c_V \lesssim \frac{k_B}{dof}$

$$\Rightarrow \quad 1-t_G \sim \left(\frac{1}{\#dof \text{ in } \xi_0^d}\right)^{2/4-d} \qquad (I)$$

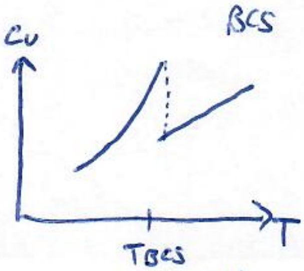
For $d>4$

$$\left(\frac{\xi}{\xi_0}\right)^{d-4} > \frac{A_d k_B}{\Delta c_V \xi_0^d} = G_i$$

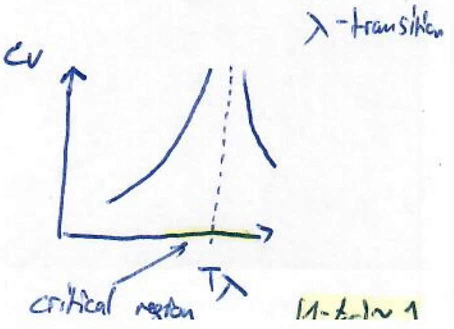
$d_u = 4$ above which mean field theory describes well the transition

For $d<4$

The critical range $\overset{(I)}{T_G} < T < T_c$ inside which the fluctuations dominate



$|1-t_G| \sim 10^{-16}$



$|1-t_G| \sim 1$

Critical fluctuations and scaling laws

$$\mathcal{H} = \int d^d r \left\{ \frac{r}{2}\phi^2 + \frac{c}{2}(\vec{\nabla}\phi)^2 + u\phi^4 \right\}$$

$$\tilde{r} := \frac{r}{c} \qquad \tilde{\phi} := \sqrt{\beta c}\,\phi \qquad \tilde{u} := \frac{u}{\beta c^2}$$

rescaled parameters

$$\tilde{\mathcal{H}} = \beta\mathcal{H} = \int d^d r \left\{ \frac{\tilde{r}}{2}\tilde{\phi}^2 + \frac{1}{2}(\vec{\nabla}\tilde{\phi})^2 + \tilde{u}\tilde{\phi}^4 \right\}$$

dimensionless Hamiltonian

all in lengths → $\overset{\nabla\tilde{\phi}}{[\tilde{\phi}] = L^{1-d/2}}$, $[\tilde{r}] = \frac{1}{L^2}$, $[\tilde{u}] = L^{d-4}$, $\xi^2 \sim \frac{c}{r}$

lengthscale

divided by lengths → $\varphi := \frac{\hat{\phi}}{\xi^{1-d/2}}$, $\tilde{r} \to 1$, $u_0 := \frac{\hat{u}}{\xi^{d-4}}$, $\vec{x} = \frac{\vec{r}}{\xi}$ all dimensionless

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{int} = \int d^d x \left\{ \frac{1}{2}[\varphi^2 + (\vec{\nabla}\varphi)^2] + \underbrace{u_0\varphi^4}_{\mathcal{H}_{int}} \right\}$$

$Z = \int \mathcal{D}[\varphi]\, e^{-\mathcal{H}[\varphi]}$ is solved trivially for $u_0 = 0$

For $u_0 \neq 0$ but small $\Rightarrow$

$$Z \simeq \int \mathcal{D}[\varphi]\, e^{-\mathcal{H}_0[\varphi]} \left(1 - \mathcal{H}_{int} + \frac{1}{2!}\mathcal{H}_{int}^2 - \dots\right) \begin{cases} d < d_u & \text{diverges term by term} \\ d > d_u & \text{no guarantee for convergence} \end{cases}$$

$$u_0 \overset{\text{def above}}{=} \frac{u}{\beta c^2}\,\xi^{4-d}\Big|_{T \to T_c} \longrightarrow \begin{cases} 0 & d > 4 \\ \infty & d < 4 \end{cases}$$

$d > 4$ ⇒ perturbation breaks down

$d < 4$ ⇒ ~~perturbation breaks dow~~

$$u_0 = \frac{k_B T u}{c^2}\,\xi^{4-d} \overset{\text{erweitern}}{\sim} \frac{k_B}{r_0^2 T_c/u}\,\frac{T_c^{\,2}}{c^2/r_0^2}\,\xi^{4-d} \underset{\frac{c}{r_0} = \xi_0^2}{\overset{\Delta c_V \sim \frac{r_0^2 T_c}{u}}{\sim}} \frac{k_B}{\Delta c_V\, \xi_0^4}\,\xi^{4-d} \sim Gi\left(\frac{\xi}{\xi_0}\right)^{4-d} \underset{T = T_G}{\sim} 1$$

Scaling laws (Overview)

(p. 400 Huang)
(p. 230 Chaikin)
(p. 483 Landau)

$$L \sim \xi \overset{\text{def.}}{\sim} \frac{1}{|\tau|^\nu}, \quad \nu = \frac{1}{2} - \theta$$

There are two scales packed into L

Assumption that $\eta \neq 0$ is also a scale.

$$[\beta f] = L^{-d}$$

dimension analysis 2 length scales

$$[G] = L^{2-d-\eta}$$

$$[m] = [\phi] = L^{1-\frac{d}{2}-\frac{\eta}{2}}$$

$$[\underbrace{k_B T \chi}_{\int d^d r\, G}] = L^{2-\eta}$$

$$[h] = [\beta H] = L^{-1-\frac{d}{2}+\frac{\eta}{2}}$$

$\beta \int d^d r\, H\phi = 1$
$\Leftrightarrow \phi = -\partial_H f$

β included

$$c_v \sim |\tau|^{-\alpha}$$
$$\chi \sim |\tau|^{-\gamma}$$
$$\phi \sim |\tau|^{\beta}$$
$$\phi \sim h^{1/\delta}$$

$$|\tau|^{-\alpha} \overset{\text{def.}}{\sim} c_v \sim T\partial_T^2 f \sim T\partial_T^2 \xi^{-d} \sim |\tau|^{d\nu - 2}$$

$$\Rightarrow \nu d = 2 - \alpha \quad \text{(Josephson)} \qquad (I)$$

$$|\tau|^{\beta} \overset{\text{def.}}{\sim} \phi \sim |\tau|^{-\nu(2-d-\eta)/2} \Rightarrow \beta = -\nu(2-d-\eta)/2 \qquad (II)$$

$$|\tau|^{-\gamma} \overset{\text{def.}}{\sim} \chi \sim |\tau|^{-\nu(2-\eta)} \Rightarrow \gamma = \nu(2-\eta) \quad \text{(Fisher)} \qquad (III)$$

$$|\tau|^{\beta\delta} \sim h \sim |\tau|^{\nu(2+d-\eta)/2} \Rightarrow \beta\delta = \nu(2+d-\eta)/2 \qquad (IV)$$

II & III and III & IV

$-$ $\beta(\delta - 1) = \gamma$ (Widom)

$+$ $\alpha + 2\beta + \gamma = 2$ (Rushbrooke)

Dimensional analysis with two length scales

There are two length scales, ξ and Λ^{-1}, the latter influences the fluctuations in the critical region.

Example. $a = \Lambda^{-1}$

$$\hat{G}(\vec{k}, T_c) \sim a^2 k^{-2+\eta}$$

$$G'(k', T_c) \sim a'^2 k'^{-2+\eta}, \quad \text{again } L' = \varepsilon L$$

$$\sim \left(\frac{a}{\varepsilon}\right)^2 (\varepsilon k)^{-2+\eta} \sim \frac{1}{\varepsilon^2} a^2 k^{-2+\eta} \sim \frac{1}{\varepsilon^2} G(k, T_c)$$

Similarly,

$$\xi = \frac{1}{\sqrt{\tilde{r}}} f(\tilde{r} a^2) \xrightarrow[\text{"}]{f(x \to 0)} \begin{cases} \text{reguler} \Rightarrow \nu = 1/2 \\ x^\theta \Rightarrow \nu = \underset{\text{canonical}}{1/2} - \underset{\text{anomalous dimension}}{\theta} \end{cases}$$

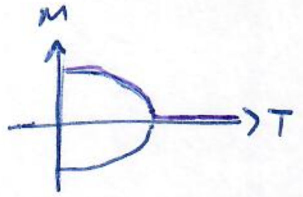
$\Rightarrow$ The critical exponents can assume non trivial values away from the results of Landau mean field Theory.

$$\tilde{\phi} \sim L^{1 - \frac{d}{2} - \eta/2}$$

Widom scaling p. 403 Huang

Assume magnetic system, $\tau = \frac{T}{T_c} - 1$, $\beta H = h$. Consider $m(\tau, h)$

$$m(\tau,0) \sim \begin{cases} 0 , & \tau > 0 \\ \pm|\tau|^{\beta} , & \tau < 0 \end{cases}$$



$$m(0,h) \sim \pm |h|^{1/\delta} , \quad \tau = 0$$

$$\Rightarrow \quad m(\tau,h) \sim |\tau|^{\beta} \mathcal{M}_{\pm}\left(\frac{h}{|\tau|^{\Delta}}\right)$$

β ← ~~Gap~~ exponent (universal)

Δ ← Gap exponent (universal)

$\mathcal{M}_{\pm}$ ↑ two scaling functions, + and − ; $+$: $\tau > 0$; $-$: $\tau < 0$

By choosing 3 parameters correctly, reduce all curves to two, above and below T_c.

→ reduces data to two curves

→ able to find T_c and the critical exponent as the data reduction only works ~~for~~ if β, Δ and T_c are correct.

$$M_{\pm}(-x) = -M_{\pm}(x) ; \quad \chi(h=0) = \frac{\partial m}{\partial h} = \beta \frac{\partial m}{\partial H} \sim \frac{|\tau|^{\beta}}{\tau^{\Delta}} M_{\pm}'(0) \sim |\tau|^{\gamma}$$

$$\Rightarrow \Delta = \beta + \gamma$$

Assume the Ansatz: $M_{\pm}(x \to \infty) \sim x^{\lambda}$, for $h \neq 0, \Delta > 0, |\tau| \to 0$

$$M(0,h) = |\tau|^{\beta} M_{\pm}\left(\frac{h}{|\tau|^{\beta+\gamma}}\right) \sim |\tau|^{\beta}\left(\frac{h}{|\tau|^{\beta+\gamma}}\right)^{\lambda} \sim h^{\lambda} |\tau|^{\beta(1-\lambda)-\lambda\gamma} \sim h^{1/\delta}$$

close to zero ↗

$$\xRightarrow{M \text{ finite}} \beta(1-\lambda) = \gamma\lambda \Rightarrow \beta(\delta-1) = \gamma \quad \text{(Widom)}$$

Free energy density

At $h=0$ $$\beta f(\tau) \sim \xi^{-d} \sim |\tau|^{\nu d} \sim |\tau|^{2-\alpha}$$

see scaling overview

Josephson

Scaling ansatz for $h\neq 0$, $$f(\tau,h) = |\tau|^{2-\alpha}\, \mathcal{F}_{\pm}\left(\frac{h}{|\tau|^{\Delta}}\right)$$

$$m \sim \partial_h f \sim |\tau|^{2-\alpha-\Delta}\, \mathcal{F}_{\pm}'\left(\frac{h}{|\tau|^{\Delta}}\right) \overset{h\to 0}{\sim} |\tau|^{\beta}$$

$$\Rightarrow 2-\alpha-\Delta = \beta \qquad (I)$$

$$\chi = \frac{\partial^2 f}{\partial h^2} \sim |\tau|^{2-\alpha-2\Delta}\, \mathcal{F}_{\pm}''\left(\frac{h}{|\tau|^{\Delta}}\right) \overset{h\to 0}{\sim} |\tau|^{-\gamma}$$

$$\Rightarrow 2-\alpha-2\Delta = -\gamma \qquad (II)$$

(I)&(II) $$\Rightarrow \quad \alpha + 2\beta + \gamma = 2 \qquad \text{(Rushbrooke)}$$

Another scaling Ansatz: $$f(\tau,h) = b^{-d} f(b^{\lambda_\tau}\tau, b^{\lambda_h} h)$$

choosing: $b \sim |\tau|^{-1/\lambda_T}$ $\Rightarrow$ makes $f(1, b^{\lambda_h} h)$ and $b \sim \xi$

$\Rightarrow f \sim \xi^{-d} \sim |\tau|^{\nu d}$ for $h=0$ if $\lambda_\tau = \frac{1}{\nu}$

overview

Kadanoff's block spin transformation p. 237 chaikin

Ising model:
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i$$

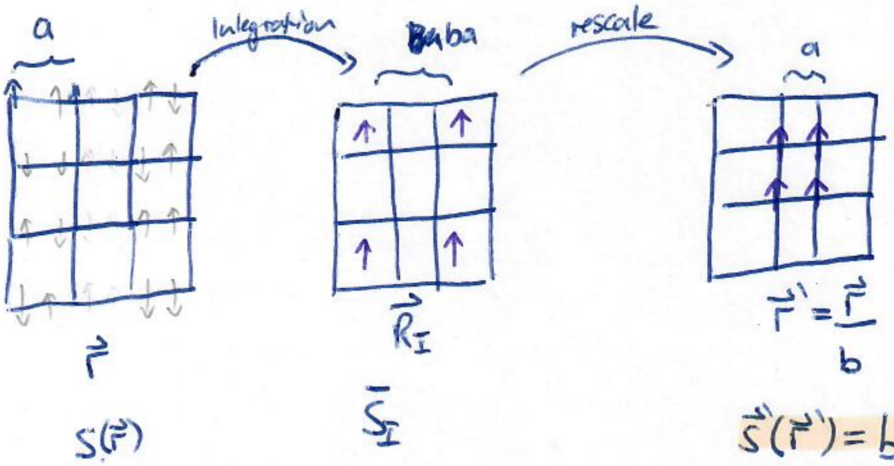
Near T_c, $\xi \to \infty \Rightarrow$ spins are strongly correlated $\rightsquigarrow$ coarse grained description

$$\bar{S}_I = b^{-d} \sum_{i \in B_I} S_i \qquad , \; B_I \text{ a block containing } b^d \text{ spins}$$

$\Rightarrow$ $\vec{R}_I$ has lattice constant ba, $b^{-d}N$ particles and $\xi \to \xi/b$

$\Rightarrow$ further away from the critical point.

The transition to Blockspins is an integration over small-scale or high energy degrees of freedom, which ~~does~~ shall not change the form of the theory, the Hamiltonian or other quantities.



$$\vec{s}'(\vec{r}') = b^{\lambda_s} s(\vec{r})$$

$$G(\vec{R}_I, \vec{R}_J) = b^{-2d} \sum_{i \in B_I} \sum_{j \in B_J} \langle S_i S_j \rangle = \overset{[\text{correlator}]}{\langle \bar{S}_I \bar{S}_J \rangle} \sim |\vec{R}_I - \vec{R}_J|^{-(d-2+\eta)}$$

Similarly, $\quad G(\vec{r}_1, \vec{r}_2) \sim |\vec{r}_1 - \vec{r}_2|^{-(d-2+\eta)}$

$$G'(\vec{r}_1{}', \vec{r}_2{}') = \langle s'(\vec{r}_1{}') s'(\vec{r}_2{}') \rangle = b^{2\lambda_s} \langle s(\vec{r}_1) s(\vec{r}_2) \rangle \sim b^{2\lambda_s} |\vec{r}_1 - \vec{r}_2|^{-(d-2+\eta)}$$

$$\overset{!}{\sim} \left| \frac{\vec{r}_1}{b} - \frac{\vec{r}_2}{b} \right|^{-(d-2+\eta)} \Rightarrow \lambda_s = \frac{(d-2+\eta)}{2}$$

Reduced Hamiltonian

p. 240 chaikin

$$\mathcal{K}_J = \mathcal{H}_J / T \overset{\substack{\text{expansion}\\ \text{critical}\\ \text{point}}}{\approx} \mathcal{K}_{\cancel{J}c} + \tau \overset{J/T_c}{K_c} \sum_{\vec r, \vec d} s(\vec r)\, s(\vec r + \vec d)$$

$$= \mathcal{K}_c + K_c \sum_{\vec r} \tau\, \underbrace{\varepsilon(\vec r)}$$

local energy density

$$\varepsilon(\vec r) = \sum_{\vec d} s(\vec r) s(\vec r + \vec d)$$

nearest neighbourgh
~~do~~ double count?

$\Rightarrow$ ε assumes the role of the field conjugate to τ.

Ansatz:

$$\boxed{\begin{aligned} \varepsilon'(\vec r') &= b^{\lambda_\varepsilon} \varepsilon(\vec r) \\ \tau' &= b^{\lambda_\tau} \tau \end{aligned}}$$

From analysis (see page before): $\lambda_\varepsilon = d - \lambda_\tau = \dfrac{d\nu - 1}{\nu}$, $\lambda_\tau = \dfrac{1}{\nu}$

$$f(\tau, h, x, \dots) = b^{-d} f(b^{\lambda_\tau}\tau, b^{\lambda_h} h, b^{\lambda_x} x, \dots) \quad , \forall b$$

Choosing $b = |\tau|^{-\nu} = \xi$

Δ_x

$$\Rightarrow f(\tau, h, x, \dots) = \xi^{-d} f_0\left(h/|\tau|^{\Delta_h}, x/|\tau|^{\Delta_x}, \dots \right) \quad , \quad \Delta = \lambda \underset{\substack{\uparrow \\ \nu > 0}}{\nu}$$

from def. $b = |\tau|^{-\nu}$

lets say Δ is the gap exponent of v

$$\Rightarrow \quad v \longmapsto b^{\lambda} v \longrightarrow \begin{cases} 0 & \lambda < 0 \quad \text{irrelevant} \\ & \lambda = 0 \quad \text{marginally relevant} \\ & \lambda > 0 \quad \text{relevant} \end{cases}$$

Universality

Once a Hamiltonian approaches the same form under rescaling they describe the same physics.

Renormalization group equations (p.446 Huang)

Consider the most general Hamiltonian $\mathcal{H}[\{K\}]$ that depends on a complete set of coupling constant $\{K\}$. New terms may be generated in the step of renormalization, therefore the set $\{K\}$ shall be complete.

Example. Ising spin system

$$\mathcal{H}[\{K\}] = \sum_{\alpha} K_{\alpha} S_{\alpha}$$, K is a vector in coupling space

with

$$S_{\alpha} = \prod_{i \in I_{\alpha}} S_i$$

arbitrary set of site labels

We call this operation of coarse graining a renormalization group transformation R_b, where the index b tells that we have combined b^d original degrees of freedom into a new one. Bsp. cell with b^d spins is averaged to a single spin with a tiebreaker.

$$K' = R_b[K]$$ (RG equation)

The operator R_b can create entries where there were none before. R_b defines a semi-group; $R_{b_1} R_{b_2} = R_{b_1 b_2}$

Idea

dimensionless

I: $\bar{K} = -\mathcal{H}/T \;, \Rightarrow \quad Z_N[K] = \mathrm{Tr}_{\{S_i\}} \exp(\bar{K}[K, \{S_i\}]) \Rightarrow F = -\log Z_N$

II: $S_i \overset{B_I}{\rightsquigarrow} \bar{S}_i := S_i' \;, N \rightarrow N' = \frac{N}{b^d}$ $\quad \Rightarrow f = \frac{1}{N} \log Z_N$

III: $$e^{\mathcal{K}[K', \{S_I'\}]} = \mathrm{Tr}_{\{S_i\}} \underbrace{P(\{S_i\}, \{S_I'\})}_{\geq 0} e^{\bar{K}[K, \{S_i\}]} =$$

$= \begin{cases} 1 & \text{if } \{S_i\} \text{ leads to } \{S_I'\} \\ 0 & \text{else} \end{cases}$

$$\sum P(\{S_i\}, \{S_I'\}) = 1$$

Fixed points and exponents

p.449 Huang
p.252 Chaikin
26:00 15.12. Lecture

Let $b \to 1$, continuous flow

$$K^* = R_b[K^*] \qquad (\text{fixed points})$$

RG generally takes the system away from a critical point as

$$\xi' = \xi[K'] = \xi[K]/b = \xi/b$$

At a fixed point however, ξ hat to remain invariant

trivial (phase)

$$\Rightarrow \xi[K^*] = \frac{\xi[K^*]}{b} \Leftrightarrow \xi^* = \begin{cases} 0 \text{ or} \\ \infty \end{cases}$$

critical (phase transition)

Basin of attraction.

A point K is in the basin of attraction ~~of~~ of K^* if

$$\lim_{n\to\infty} R_b^n[K] \to K^*$$

These points are characterized by (for critical fixed point)

assumption?

$$0 \neq \xi[K] = b\,\xi[R_b[K]] = \ldots = b^n \xi[R_b^n[K]] \longrightarrow \lim_{n\to\infty} b^n \xi[K^*] = \infty$$

otherwise already K^* (trivial)

They define the critical manifold, associated with the fixed point.

All the different Hamiltonians in the basin of attraction of a given critical fixed point exhibit the same critical behaviour characterized by the same exponents.

Flow in the vicinity

$$K_n = K_n^* + \delta K_n \quad , \qquad n\text{-th component}$$

RG

$$K_n' = K_n^* + \delta K_n'$$

linearized RG equation ⟶

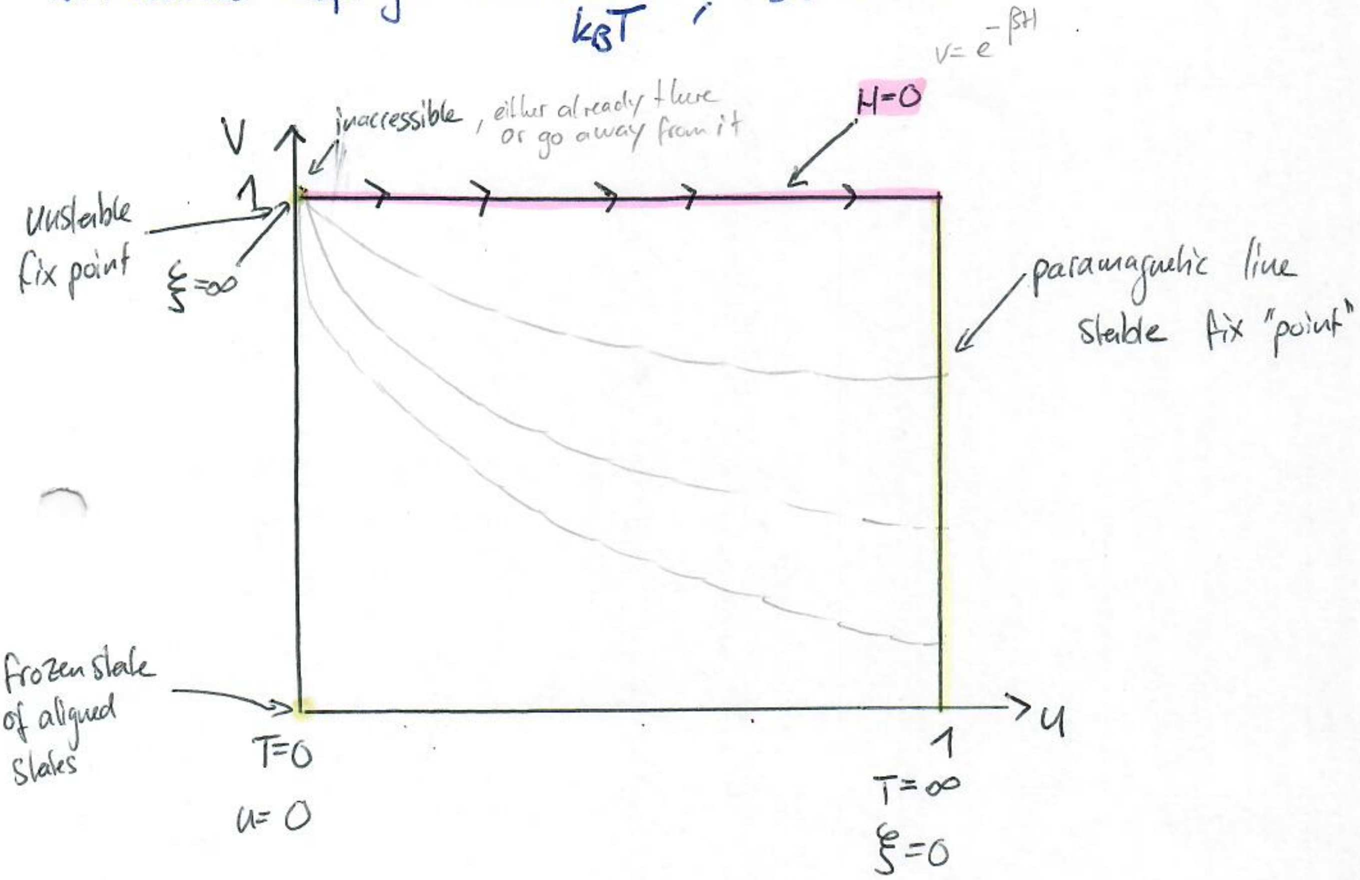
$$\delta K_n' = \sum_m \frac{\partial K_n'}{\partial K_m}\Big|_{K=K^*} \delta K_m = \sum_m R_{nm}[K^*]\,\delta K_m$$

Real space normalization of spin models

p. 444 ~~Chaikin~~ Huang
p. 242 Chaikin

1D Ising model

Dimensionless coupling: $K = \frac{J}{k_B T}$, set $h=0$



$$\tanh(K') = \tanh(K)^b \quad \text{RG equation}$$