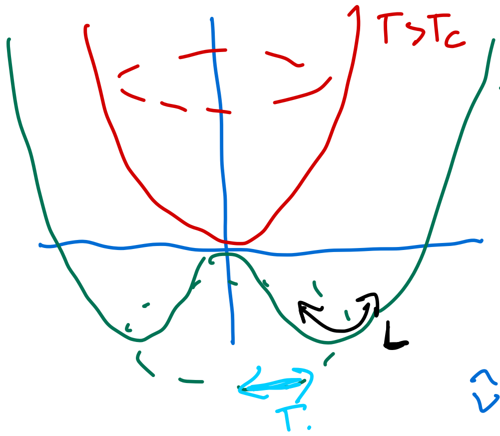
Lecture 7: The Berezinskii-Kosterlitz-Thouless transition.

In last lecture, we discussed correlation functions for spontaneously broken continuous symmetries.

Example: $O(N)$ model.



In other words; if order parameter is $\vec{\phi}$:

$$\langle \delta\vec{\phi}(\vec{r})\delta\vec{\phi}(\vec{r}\,')\rangle =: \underline{\underline{G}}(\vec{r}-\vec{r}\,')$$

and we found within the Landau-Ginzburg model:

$$\underline{\underline{G}}(\vec{r}) = \underbrace{G_T(\vec{r})\,(\underline{\underline{I}}-\hat{\nu}\hat{\nu})}_{\substack{\text{Transverse part}\\ \Leftrightarrow \text{Goldstones}}} + \underbrace{G_L(\vec{r})\,\hat{\nu}\hat{\nu}}_{\text{Longitudinal part}}$$

$$\hat{\nu} = \frac{\langle\vec{\phi}(\vec{r})\rangle}{|\langle\vec{\phi}(\vec{r})\rangle|}$$

The longitudinal part behaves the same as in the discrete case, modes behaved as massive particles. The transverse modes, however, behaved as massless modes, i.e.

$$G_T(\vec{r}) = \frac{k_B T}{K}\int_{|\vec{k}|<\Lambda}\frac{d^d\vec{k}}{(2\pi)^d}\frac{e^{i\vec{k}\cdot\vec{r}}}{\vec{k}^2} \sim \begin{cases}\Lambda^{d-2} - r^{2-d} & d>2\\ \log \Lambda r & d=2\\ r-\Lambda^{-1} & d=1\end{cases}$$

Λ: microscopic cutoff

We learn that for $d>2$, most correlations are dominated by the Goldstones! (Longitudinal decay of correlations is exponentially damped, whereas transverse part decays algebraically!)

Note that $G_T(\vec{r})$ quantifies the angular fluctuations in the order parameter $\vec{\phi}$! For $d\leq 2$ these angular fluctuations become larger and larger for increasing separation $\Rightarrow$ destruction of long-range order!

$d\leq d_\ell = 2$ is called the lower critical dimension of this model.

$G_T(\vec{r})$ describes the so-called would-be Goldstone modes (if there is no underlying order, there are also no Goldstones! In $\langle\delta\vec{\phi}(\vec{r})\delta\vec{\phi}(\vec{r}\,')\rangle$ we looked at small transverse fluctuations, so what about arbitrary transverse fluctuations? We want a model for the Goldstones.

$O(N)$ model: $$F_L[\vec{\phi}] = \int d^d\vec{r}\left[\frac{K}{2}|\nabla\vec{\phi}|^2 + V(|\vec{\phi}|)\right]$$

Below T_c: $\langle \vec{\phi} \rangle = \phi_0 \hat{n} \Rightarrow V(|\vec{\phi}|) = V(\phi_0)$ and $|\nabla \vec{\phi}|^2 = \phi_0^2 |\nabla \hat{n}|^2$

So we get $F_L[\hat{n}] = \int d^d\vec{r}\, \underbrace{\frac{K}{2}\phi_0^2}_{:= \frac{\rho_s}{2}\text{ (stiffness)}} [\nabla \hat{n}]^2$ + terms dependent on ϕ_0

Note that $|\hat{n}|^2 = 1$!

$$\Rightarrow Z = \int \mathcal{D}\hat{n}(\vec{r})\, e^{-\beta F_L[\hat{n}]}\, \delta(\hat{n}^2(\vec{r}) - 1)$$

This is called the non linear sigma model (NLSM)

(Name comes from HE physics for pion-pion interactions).

This is generally speaking an interacting field theory!

Suppose ground state is $\hat{n}_0 = (1, 0, 0, \dots, 0)$ then:

Write: $\hat{n}(\vec{r}) = (\sigma(\vec{r}), \vec{\pi}(\vec{r})) \Rightarrow \sigma(\vec{r})^2 = 1 - \vec{\pi}(\vec{r}) \cdot \vec{\pi}(\vec{r})$ with $\sigma \neq 0$

Therefore:

from continuum limit

$$F_L[\vec{\pi}] = \int d^d\vec{r} \left[\frac{\rho_s}{2} |\nabla \vec{\pi}|^2 + \frac{\rho_s}{2} \frac{(\vec{\pi} \cdot \nabla \vec{\pi})^2}{1 - \vec{\pi}^2} + \underbrace{\frac{C'}{2} \ln(1 - \vec{\pi}^2)}_{\text{from } \delta} \right].$$

and $Z = \int \mathcal{D}\vec{\pi}\, e^{-\beta F_L[\vec{\pi}]}$

Note that in this parametrization only an $O(N-1)$ symmetry is manifest due to an implicit choice of a ground state!

Note that for $N > 2$, the NLSM describes an interacting theory of Goldstones! If we analyse the would-be Goldstones using e.g. RG methods, we find that they acquire a mass $\Rightarrow$ An ordered is unstable due to the presence of transverse fluctuations. Something special happens for $N = 2$: Then we can write $\hat{n} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$

Then NLSM: $Z = \int \mathcal{D}\theta(\vec{r})\, e^{-\beta F_L[\theta]}$ with $F_L[\theta] = \int d^d\vec{r}\, \frac{\rho_s}{2} |\nabla \theta|^2$.

Free theory!

We find $\langle \theta(\vec{r})\,\theta(\vec{r}\,')\rangle = \frac{1}{\rho_s}\int \frac{d^d \vec{k}}{(2\pi)^d}\,\frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}}{k^2}$ (we already analysed this)

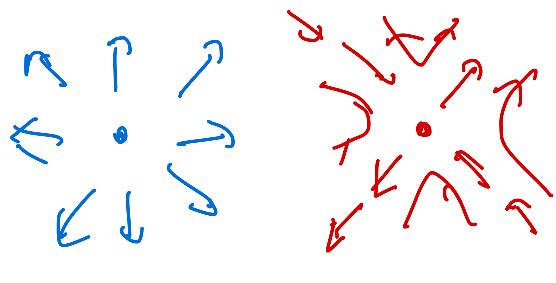
$\sim \log(\Lambda r)$. and

But $\langle \hat{n}(\vec{r})\cdot\hat{n}(\vec{r}\,')\rangle \sim \frac{1}{|\vec{r}-\vec{r}\,'|^{\eta}}$ with $\eta = \frac{1}{2\pi\rho_s}$ (*)

$\Rightarrow$ Order parameter correlations decay algebraically at low temperatures. Note that it has the same form as the longitudinal correlations at the critical point, so here it is as if we have a "critical line".

(*) describes the low temperature behaviour and is called quasi long-range order (QLRO). The high-temperature behaviour is not captured by $Z = \int \mathcal{D}\theta(\vec{r})\, e^{-\beta F_L[\theta]}$. (**)

You have seen in Tutorial 6, that (**) follows from the continuum limit of the XY model $H = -J\sum_{\langle ij\rangle} \vec{s}_i\cdot\vec{s}_j$. Here it was assumed that angles vary slowly from site to site. So configurations like



vortex
$n=1$

antivortex.
$n=-1$

were not included.

(we have not included that θ is periodic field)

These are examples of topological defects. Note that θ is not defined in the center and that topological defects are described by winding number n:

$$\oint \nabla\theta\cdot d\vec{\ell} = 2\pi n.$$

One such configuration is

$$\nabla\theta = \frac{n}{r^2}(y, -x).$$

With this, we can estimate the free energy of a vortex:

$$F_{vortex} = \frac{\rho_s}{2} \int d^2\vec{r}\, (\nabla\theta)^2 = \pi n^2 \rho_s \log\left(\frac{L}{a}\right) + F_{core}$$

So let us take $n=1$. (higher order windings are more costly)

$$P_{vortex} \propto \left(\frac{L}{a}\right)^2 \frac{e^{-\beta F_{vortex}}}{Z} = \frac{e^{-\beta F_{core}}}{Z} \left(\frac{L}{a}\right)^{2-\beta\pi\rho_s}$$

vortex can sit anywhere.

So for $2-\beta\pi\rho_s > 0$ no suppression of vortices.

$$\frac{2}{\pi\rho_s} > \frac{1}{k_B T_{BKT}} \Rightarrow k_B T_{BKT} > \frac{\pi\rho_s}{2}.$$

(and actually accurate analysis shows that it is an infinite-order phase transition)

So the mental image one should have is the following.

- $T < T_{BKT}$: gas of bound vortex-antivortex pairs (spin-wave, i.e. topological trivial theory is sufficient) $\Rightarrow$ QLRO.
- $T > T_{BKT}$: Vortex-antivortex pairs unbind and one gets disordered gas of defects. $\Rightarrow$ disordered state.

Up until now in this course, we have looked at mesoscopic physics using field theory. It was motivated using the continuum limit of lattice models (long wave-length physics). We can ask now the question

* What about microscopically resolved correlations?
* What about more realistic models than lattice models?

More realistic Hamiltonian (not confined to lattice

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \Phi(\hat{\vec{r}}_1, \ldots \hat{\vec{r}}_N)$$

Quantum systems $\rightsquigarrow$ later

(no internal degrees of freedom)

Classical systems: degrees of freedom $\{\vec{p}^N, \vec{r}^N\}$, so we expect

$$Z(N,V,T) = C \underbrace{\int d\vec{p}^N \int d\vec{r}^N}_{(\text{angular momentum})^{3N}} e^{-\beta H(\vec{r}^N, \vec{p}^N)} \quad (*)$$

C → dimensionless ($\log(\ldots)$)

H ↳ classical Hamiltonian.

Previous courses: $\epsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$ $\quad \vec{k} = \left(\frac{2\pi}{L}\right)\vec{n}$

$\vec{n}$ ← quantum number. $n_i \in \mathbb{Z}$ (periodic boundary conditions)

Compute partition function in two ways: $Z = \mathrm{Tr}\left[e^{-\beta \hat{H}}\right]$ or with $(*)$ and compare.

But we can give more straightforward method.

For example, classical limit of $\hat{H} = \frac{\hat{\vec{p}}^2}{2m} + V(\hat{\vec{r}})$ (single particle in an external potential)

$\frac{\hat{\vec{p}}^2}{2m}$: kinetic energy; $V(\hat{\vec{r}})$: external potential

$[\hat{\vec{r}}, \hat{\vec{p}}] = i\hbar \mathbb{1}$.

Recall completeness relations: $\int d\vec{r}\, |\vec{r}\rangle\langle\vec{r}| = \mathbb{1}$ with $\hat{\vec{r}}|\vec{r}\rangle = \vec{r}|\vec{r}\rangle$ $(*)$

$\int d\vec{p}\, |\vec{p}\rangle\langle\vec{p}| = \mathbb{1}$. with $\hat{\vec{p}}|\vec{p}\rangle = \vec{p}|\vec{p}\rangle$

Note that this is position and momentum kets are a complete set of states!

Let us compute:

$$Z = \mathrm{Tr}\left[e^{-\beta\hat{H}}\right] = \sum_{\nu} \langle \nu | \overset{(*)}{\vphantom{|}} e^{-\beta \hat{H}} \overset{(*)}{\vphantom{|}} | \nu \rangle$$

$$= \sum_{\nu} \langle \nu | \int d\vec{r}\, |\vec{r}\rangle\langle \vec{r}| e^{-\beta \hat{H}} \int d\vec{r}\,' |\vec{r}\,'\rangle\langle \vec{r}\,'|\nu\rangle$$

$$\sum_{\nu} |\nu\rangle\langle\nu| = \mathbb{1}$$

$$\langle \vec{r}\,'|\vec{r}\rangle = \delta(\vec{r}-\vec{r}\,')$$

$$= \int d\vec{r} \int d\vec{r}\,' \langle \vec{r}|e^{-\beta\hat{H}}|\vec{r}\,'\rangle \sum_{\nu} \langle \vec{r}\,'|\nu\rangle\langle\nu|\vec{r}\rangle$$

$$= \int d\vec{r} \int d\vec{r}\,' \langle\vec{r}|e^{-\beta\hat{H}}|\vec{r}\,'\rangle\, \delta(\vec{r}-\vec{r}\,')$$

$$= \int d\vec{r}\, \langle \vec{r}|e^{-\beta \hat{H}}|\vec{r}\rangle. \quad (**)$$

Recall the operator identity $e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}+\frac{1}{2}[\hat{A},\hat{B}]+\dots}$

$$\Rightarrow e^{-\beta\hat{H}} = e^{-\beta\hat{\vec{p}}^2/2m}\, e^{-\beta V(\hat{\vec{r}})} + \mathcal{O}(\hbar)$$

$$(**) = \int d\vec{r}\, \langle \vec{r}|\, e^{-\beta \hat{\vec{p}}^2/2m}\, e^{-\beta V(\hat{\vec{r}})}|\vec{r}\rangle$$

$$= \int d\vec{r}\, e^{-\beta V(\vec{r})} \langle \vec{r}|e^{-\beta\hat{\vec{p}}^2/2m}|\vec{r}\rangle$$

$$\int d\vec{p}\, |\vec{p}\rangle\langle\vec{p}|$$

$$= \int d\vec{r}\, e^{-\beta V(\vec{r})}\int d\vec{p}\, e^{-\beta\vec{p}^2/2m}\langle\vec{r}|\vec{p}\rangle\langle\vec{p}|\vec{r}\rangle$$

Together with $\langle \vec{r}|\vec{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\, e^{i\vec{p}\cdot\vec{r}/\hbar}$

$$\langle\vec{p}|\vec{r}\rangle = \langle\vec{r}|\vec{p}\rangle^*$$

$\Rightarrow$

$$Z(N,V,T) = \frac{1}{h^3}\int d\vec{p}\int d\vec{r}\, e^{-\beta H(\vec{p},\vec{r})}$$

with $H(\vec{p},\vec{r})$ the classical Hamiltonian.

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

In many-body case, we need to use:

$$|\vec{r}_1,\dots\dots,\vec{r}_N\rangle = \frac{1}{\sqrt{N!}}\sum_{P\in S_N}\xi^P\, |\vec{r}_{P(1)}\rangle\cdots\cdots|\vec{r}_{P(N)}\rangle$$

where $\xi^P = \begin{cases}1 & \text{bosons}\\ \text{sgn}(P) & \text{fermions.}\end{cases}$

Then same can be repeated (see lecture notes):

$$Z(N,V,T) = \frac{1}{N!h^{3N}} \int d\vec{p}^{\,N} \int d\vec{r}^{\,N} e^{-\beta H(\vec{p}^{\,N},\vec{r}^{\,N})}$$

and therefore,

$$F(N,V,T) = -k_B T \log \Big[\underbrace{\frac{1}{N!h^{3N}} \int d\vec{r}^{\,N} \int d\vec{p}^{\,N} e^{-\beta H(\vec{r}^{\,N},\vec{p}^{\,N})}}_{\text{to be computed.}} \Big].$$

Note that in equilibrium we can introduce a (continuous) probability density on the classical phase space:

$$f_c(\vec{p}^{\,N},\vec{r}^{\,N}) = \frac{1}{Z} e^{-\beta H} \quad \text{(by definition of } Z: \frac{1}{N!h^{3N}}\int d\vec{r}^{\,N} \int d\vec{p}^{\,N} f(\vec{r}^{\,N},\vec{p}^{\,N}) = 1)$$

Suppose we have a function of phase space variables. $A(\vec{r}^{\,N},\vec{p}^{\,N})$

Then

$$\langle A(\vec{r}^{\,N},\vec{p}^{\,N})\rangle = \int d\vec{r}^{\,N} \int d\vec{p}^{\,N} A(\vec{r}^{\,N},\vec{p}^{\,N}) f_c(\vec{r}^{\,N},\vec{p}^{\,N})$$

$$= \frac{1}{Z} \int d\vec{r}^{\,N} \int d\vec{p}^{\,N} A(\vec{r}^{\,N},\vec{p}^{\,N}) e^{-\beta H(\vec{r}^{\,N},\vec{p}^{\,N})}$$

Ensemble average.

Suppose $(\vec{r}^{\,N}(t),\vec{p}^{\,N}(t))$ is a solution from Hamilton's equations:

$$\overline{A(\vec{r}^{\,N}(t),\vec{p}^{\,N}(t))} = \lim_{\tau\to\infty} \int_0^{\tau} dt\, A(\vec{p}^{\,N}(t),\vec{r}^{\,N}(t)) \quad \text{Time average.}$$

(e.g. obtained from molecular dynamics).

System is ergodic $\Leftrightarrow$ $\langle A(\vec{r}^{\,N},\vec{p}^{\,N})\rangle = \overline{A(\vec{r}^{\,N}(t),\vec{p}^{\,N}(t))}$.

Non-ergodic: glasses, ...

It is straightforward to write probability densities for other ensembles in classical limit.

For example, grand canonical ensemble:

$$\Xi(\mu,V,T) = \sum_{N\geq 0}^{\infty} e^{\beta\mu N} Z(N,V,T)$$ (grand-canonical partition function)

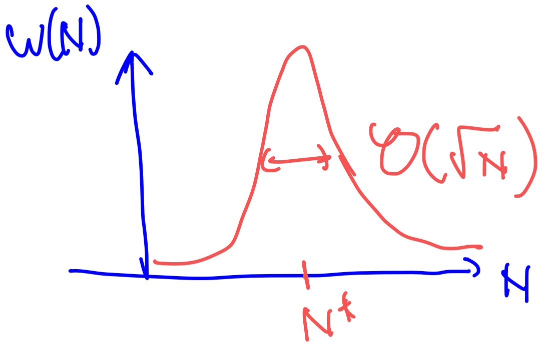
$$\Omega(\mu,V,T) = -k_B T \log \Xi$$ (grand potential)

$$f_g(\vec{r}^N,\vec{p}^N;N) = \frac{e^{-\beta(H-\mu N)}}{\Xi(\mu,V,T)}$$

Note that $\sum_{N\geq 0}^{\infty} \frac{1}{N!h^{3N}} \int d\vec{r}^N \int d\vec{p}^N f_g(\vec{r}^N,\vec{p}^N;N) = 1$

Marginal probability density: $W(N) = \frac{1}{N!h^{3N}} \int d\vec{r}^N \int d\vec{p}^N f_g(\vec{r}^N,\vec{p}^N;N)$

$$= \frac{e^{\beta\mu N}}{Z(N,V,T)}.$$



General classical Hamiltonians for particles without internal degrees of freedom

$$H(\vec{r}^N,\vec{p}^N) = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \Phi(\vec{r}^N).$$

N-body interaction potential $\qquad \vec{F}_i = -\frac{\partial\Phi}{\partial\vec{r}_i}.$

Simplest case: $\Phi = 0$ (ideal gas).

In this case: $$Z(N,V,T) = \frac{1}{N!h^{3N}} \prod_{i=1}^{N} \underbrace{\int d\vec{p}_i\, e^{-\beta\vec{p}_i^{\,2}/2m}}_{\text{Gaussian integral}} \cdot \int d\vec{r}^N$$

$$= \frac{V^N}{N!\Lambda^{3N}}$$

Here, $\Lambda = \frac{h}{\sqrt{2\pi m k_B T}}$ Thermal de Broglie wavelength.

From partition function thermodynamic properties can be inferred:

$$\beta f_{id}(\rho, T) := \frac{\beta F_{id}(N,V,T)}{V} = \rho\left[\log(\rho\Lambda^3) - 1\right]$$

where $\rho = \frac{N}{V}$ = constant.

From standard thermodynamic relations, we find: (Check!)

$\beta E = 3/2 N$; $\beta p = \rho$; $\beta\mu = \log(\rho\Lambda^3)$

$S/k_B = \frac{5}{2}N - N\ln\rho\Lambda^3$ (Sackur-Tetrode equation)

Note that above expressions are valid for $\rho\Lambda^3 \ll 1$.

Namely, for $\rho\Lambda^3 > \exp(5/2)$ $S < 0$

$\Rightarrow$ Quantum mechanical effects become important!

So a rough measure when quantum effects become important

$\rho\Lambda^3 \approx 1$

Then $\Lambda \sim \frac{h}{\sqrt{\langle \vec{p}^{\,2} \rangle}}$

Note that classical effects dominate when $m \uparrow$ $T \uparrow$ $\rho^{-1/3} \uparrow$

What systems behave classically?

microscopic | mesoscopic | macroscopic.

$\mathcal{O}(1\,nm)$ $\mathcal{O}(10\,nm)$

- Macroscopic objects
- Simple fluids (one-component, atomic, molecular, ...)
- Complex liquids (milk, blood, polymer melt, liquid crystals, proteins ....)

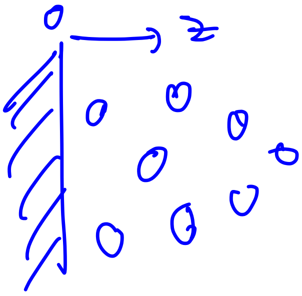
Interacting classical fluids. $(\Phi \neq 0)$

Generally, we can write.

$$\Phi(\vec{r}^N) = \underbrace{\sum_{i=1}^{N} V_{ext}(\vec{r}_i)}_{\substack{\text{one-body} \\ \text{(external potential)}}} + \underbrace{\sum_{i=1}^{N} \sum_{j<i} v(|\vec{r}_i - \vec{r}_j|)}_{\substack{\text{two-body interactions} \\ \text{(isotropic, translational invariance)}}} + \ldots\ldots$$

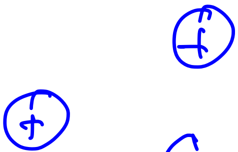
three-body
four-body etc.

Examples



hard wall.

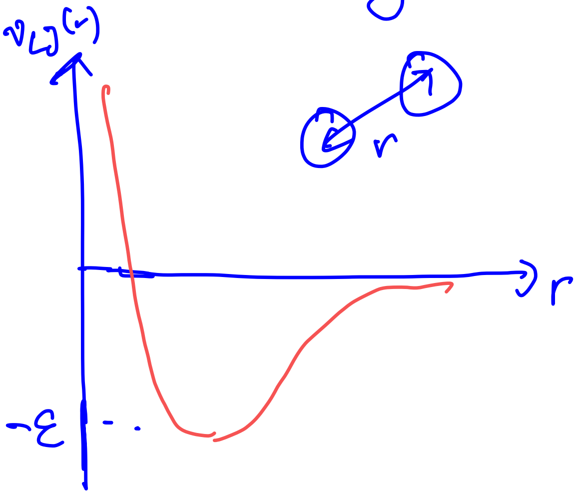
$$V_{ext}(z) = \begin{cases} \infty & z<0 \\ 0 & z>0 \end{cases}$$



Coulomb

$$v(r) = \frac{e^2}{4\pi\epsilon_0 r}$$

For classical systems, we often use various model potentials:

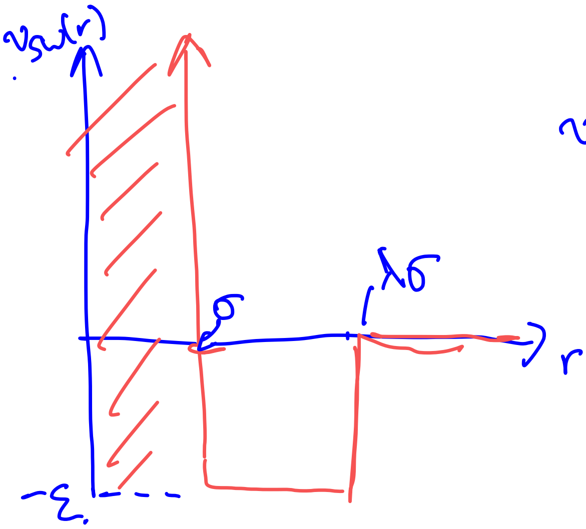


Lennard-Jones potential (empirical)

$$v_{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right]$$

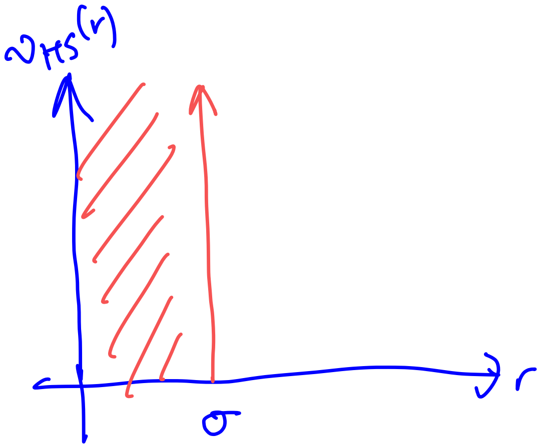
Pauli exclusion
+ Born repulsion.

Van der Waals
interaction.



$$v_{SW}(r) = \begin{cases} \infty & r<\sigma \\ -\varepsilon & \sigma<r<\lambda\sigma \quad (\lambda>1) \\ 0 & r>\lambda\sigma. \end{cases}$$

Square-well potential. When $\varepsilon > 0$
also called sticky hard spheres.



$$v_{HS}(r) = \begin{cases} \infty & r < \sigma \\ 0 & r > \sigma. \end{cases}$$

Hard-sphere potential.

Non-isotropic potentials:

$$v_{GB}(\vec{r}, \vec{u}_1, \vec{u}_2) = \epsilon(\hat{u}_1, \hat{u}_2, \hat{r}) \left[\left(\frac{\sigma_0}{r - \sigma(\hat{u}_1, \hat{u}_2, \hat{r}) + \sigma_0} \right)^{12} - \left(\frac{\sigma_0}{r - \sigma(\hat{u}_1, \hat{u}_2, \hat{r}) + \sigma_0} \right)^{6} \right].$$

Gay-berne potential.

Dipole-dipole interaction:

$$v(r, \vec{\mu}_1, \vec{\mu}_2) = \underbrace{\frac{1}{4\pi\epsilon_0 r^3}}_{\text{distance}} \underbrace{\left[\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\vec{\mu}_1 \cdot \hat{r})(\vec{\mu}_2 \cdot \hat{r}) \right]}_{\text{orientational part.}}$$

In general, all these model potential are so-called effective interaction potentials! (Integrated out degrees of freedom).

Note that for $H(\vec{r}^N, \vec{p}^N) = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \Phi(\vec{r}^N)$

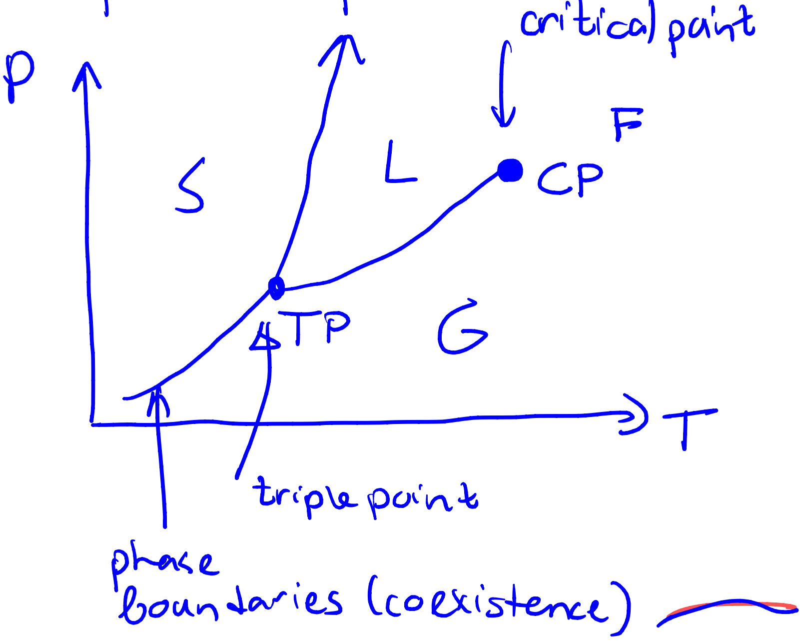
that $Z(N,V,T) = \dfrac{Q(N,V,T)}{\Lambda^{3N} N!}$ where $Q(N,V,T) = \underbrace{\int d\vec{r}^N e^{-\beta \Phi(\vec{r}^N)}}_{\text{configurational integral.}}$

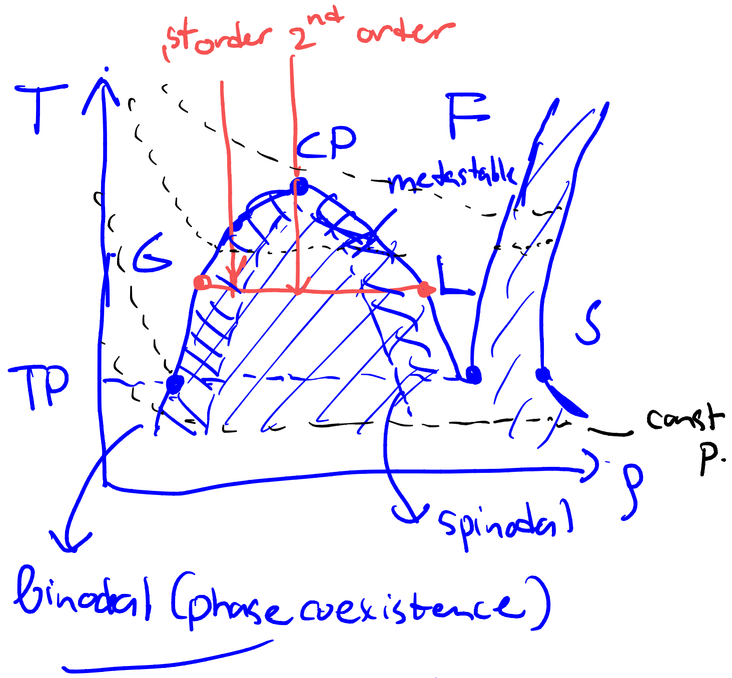
Note that for ideal gas $Q(N,V,T) = V^N$.

Interactions can lead to non-trivial phase behaviour

* Phase diagrams: Conditions under which phases coexist.

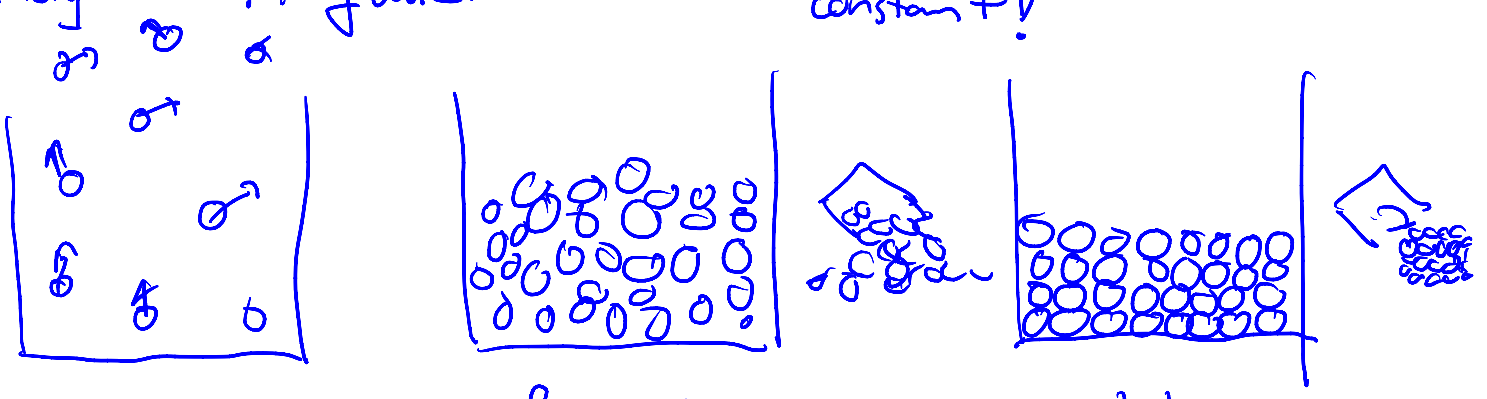
Simplest example:





in coexisting phases, all intensive thermodynamic variables are constant!

S: solid G: gas
L: liquid F: fluid.



gas	liquid	solid.
☐ volume not fixed	☐ fixed volume	☐ fixed volume
☐ low density	☐ high density	☐ high density
☐ non-fixed shape	☐ non-fixed shape	☐ fixed shape
☐ high compressibility	☐ low compressibility	☐ low compressibility
☐ translational inv.	☐ translational inv.	☐ Translational symmetry broken (crystal) or invariant (amorphous)
☐ potential energy $\langle K \rangle > \langle \Phi \rangle$ kinetic energy	☐ $\langle K \rangle \sim \langle \Phi \rangle$	$\langle \Phi \rangle > \langle K \rangle$

Phase diagrams can be very complicated (e.g. water...)