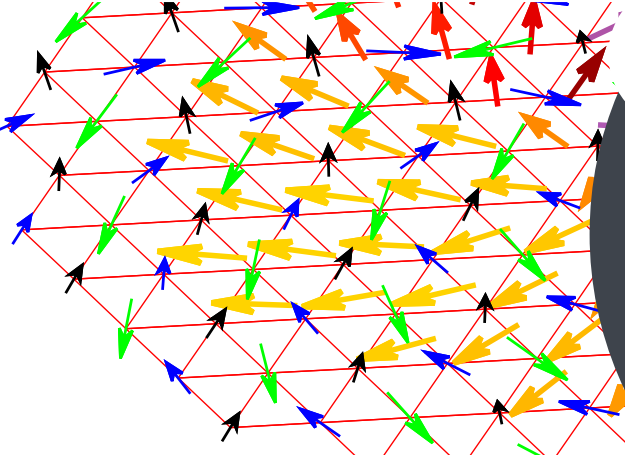
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# Phase Transitions

# Content

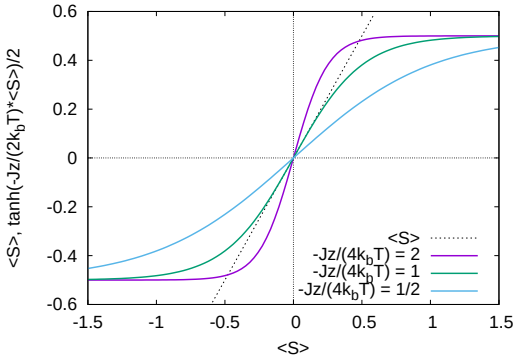
- first example: condensation
  - Macroscopic/microscopic description
  - relevance of interactions
  - classical/quantum
- second example: symmetry breaking
  - mean-field theory for the Ising model
  - (Ginzburg-)Landau approach
- Limitations of mean-field theory
- Excitations

# Summary Condensation

- van-der-Waals gas
  - interactions allow condensation
  - used classical thermodynamics
- Bose-Einstein condensation
  - used statistical physics
  - both Boltzmann and Bose particles in ground state at $T = 0$
  - appreciable fraction in ground state
    - Boltzmann particles: $k_B T_{\mathrm{Cl}} \ll \epsilon_1 - \epsilon_0$
    - much larger $T$ for Bose particles!
    - transition temperature for Boltzmann particles tends to 0 for large systems
    - condensation survives thermodynamic limit for bosons
  - quantum statistics allows phase transition for bosons

# Summary: Ising model

$$H = \sum_{i,j} J_{i,j} S_i S_j - \frac{g\mu_B}{2} \vec{B} \sum_i S_i \quad \rightarrow \quad H = -|J| \sum_{\langle i,j \rangle} S_i S_j - \frac{g\mu_B}{2} \vec{B} \sum_i S_i \qquad (1)$$




(plot for $S_i = \pm\frac{1}{2}$)

$$\langle S \rangle = \tanh \frac{2zJ\langle S \rangle}{2k_B T} \; . \qquad (2)$$

Criterion for more solutions:

- slope of $\tanh > 1$
- $1 \lesseqgtr \frac{-2zJ}{2k_B T} = \frac{z|J|}{k_B T}$
- $\Rightarrow \quad T_C = \frac{z|J|}{k_B}$

# Heisenberg Spins: continuous Symmetry

$S_i = \pm 1$ becomes $\vec{S}_i$ that can point anywhere

- Mean-Field theory essentially unchanged ($Z$ integral rather than sum)
- $\vec{B}$ serves to formally create 'special' direction
  - limit $\vec{B} \to 0$ can be done
  - (first thermodynamic limit, then $\vec{B} \to 0$)
  - for $T < T_C$, system chooses one direction
  - breaking of continuous symmetry
- However, excitations are different!

# Ginzburg-Landau Theory

Needs:

- Symmetry information
- Idea about plausible order parameter (scalar, vector, tensor, real/complex $dots$)
- No microscopic model/Hamiltonian

One can learn a lot even without a microscopic model!
Is a mean-field theory.

e.g. see Phys. Rep. **572**, 1 (2015) resp. arXiv:1410.7285

# Landau Approach

Assumptions made here:

- Homogeneous system
- Scalar real order parameter $\eta$ (e.g. $\langle S^z \rangle$)
- $\eta = 0$ at high $T$
- $\eta \neq 0$ possibly at low $T < T_C$
- $|\eta|$ small for $T \lesssim T_C$

Free energy expansion:

$$\Phi(\eta, T, p, \dots) = \Phi_0(T, p, \dots) + \alpha(T, p, \dots)\eta + A(T, p, \dots)\eta^2 + C(T, p, \dots)\eta^3 + \\ + B(T, p, \dots)\eta^4 + F(T, p, \dots)\eta^5 + D(T, p, \dots)\eta^6 + \dots \tag{3}$$

- equilibrium = minimum

$$\left.\frac{\partial \Phi(\eta, T, p, \dots)}{\partial \eta}\right|_{T,p,\cdots=\text{const.}} = \alpha(T, p, \dots) + 2A(T, p, \dots)\eta + \\ + 3C(T, p, \dots)\eta^2 + 4B(T, p, \dots)\eta^3 + \dots = 0 \tag{4}$$

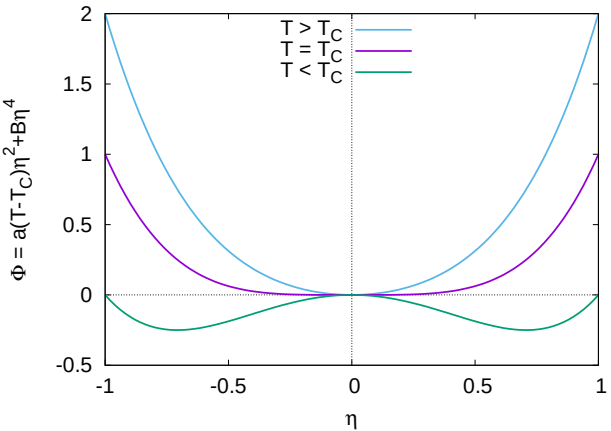
- $\eta = 0$ at $T > T_C \quad \Rightarrow \quad \alpha = 0$

# Symmetry breaking

If $\eta > 0$ and $\eta < 0$ are equivalent (inversion symmetry): only even powers of $\eta$.

$$\Phi(\eta, T, p, \dots) = \Phi_0(T, p, \dots) + A(T, p, \dots)\eta^2 + B(T, p, \dots)\eta^4 \tag{5}$$

- $\eta = 0$ always solution
- $\eta = \pm\sqrt{-\frac{A(T)}{2B(T)}} = \pm\sqrt{\frac{|A(T)|}{2B(T)}}$ solution for $A < 0$
- $A(T, p, \dots)$ must change sign at $T_C$.
- Simplest case: $A(T) = a(T - T_C)$
- $\eta = \pm\sqrt{\frac{a \cdot (T_C - T)}{2B}}$



# Second order

$$\Phi_{\min} = \Phi_0 + A\eta_{\min}^2 + \dots = \Phi_0 \begin{cases} +\,0 & \text{for } \eta_{\min}^2 = 0 \text{ at } T > T_C, \\ -\frac{a^2}{2B}(T - T_C)^2 + \dots & \text{for } \eta_{\min}^2 = \frac{a\cdot(T-T_C)}{2B} \text{ at } T \leq T_C, \end{cases} . \tag{6}$$

entropy

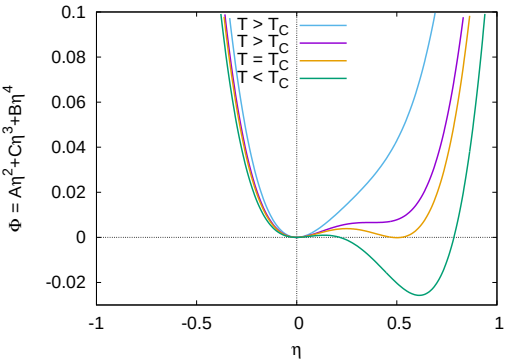
$$S = -\frac{\partial \Phi}{\partial T} = \underbrace{-\frac{\partial \Phi_0}{\partial T}}_{=S_0} + \begin{cases} 0 & \text{for } T > T_C, \\ \frac{a^2}{B}(T - T_C) + \dots & \text{for at } T \leq T_C \end{cases} , \tag{7}$$

specific heat

$$c_p = T\frac{\partial S}{\partial T} = T\frac{\partial S_0}{\partial T} + \begin{cases} 0 & \text{for } T > T_C, \\ T \cdot \frac{a^2}{B} + \dots & \text{for at } T \leq T_C \end{cases} , \tag{8}$$

# no inversion symmetry: weakly first order

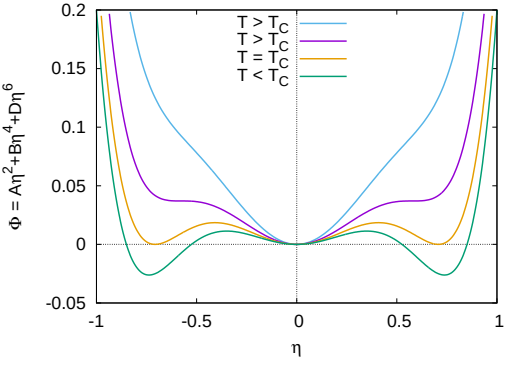
$$\Phi(\eta, T, p, \dots) = \Phi_0(T, p, \dots) + A(T, p, \dots)\eta^2 + C(T, p, \dots)\eta^3 + B(T, p, \dots)\eta^4 + \dots \quad (9)$$




- still no linear term $\propto \eta$ to allow disordered high-$T$ phase
- $\eta^3$ gives asymmetry
- Develops into a local minimum, which in turn finally dives below 0.
- Optimal $\eta$ jumps.

# Weakly first order with inversion symmetry

$$\Phi(\eta, T, p, \dots) = \Phi_0(T, p, \dots) + A\eta^2 - |B|\eta^4 + |D|\eta^6 + \dots \tag{10}$$




- $\phi$ symmetric in $\pm\eta$
- coefficient $B < 0$: 4th order favors large $\eta$
- $\Rightarrow$ 6th order becomes essential, assume $D > 0$
- Varying $A$ leads to Figure
- Local minima and finally sink below the $\eta = 0$ minimum.
- Order parameter jumps at $T_C$.

# More degrees of freedom: second vs. first order

e.g. magnetism + lattice deformation

- magnetic order parameter $\eta$
- lattice deformation $u$: $\pm u$ not equivalent $\Rightarrow$ odd powers allowed
- $\Phi = A\eta^2 + B\eta^4 + \frac{b}{2}u^2 + \lambda\eta^2 u$ ($b =$ 'bulk modulus')
- Minimize w.r.t. $u$:

$$\frac{\partial \Phi}{\partial u} = bu + \lambda\eta^2 = 0, \quad u = -\frac{\lambda\eta^2}{b} \tag{11}$$

- Re-insert into $\Phi$:

$$\Phi = A\eta^2 + B\eta^4 + \frac{\lambda^2\eta^4}{2b} - \frac{\lambda^2\eta^4}{b} = A\eta^2 + (B - \frac{\lambda^2}{2b})\eta^4 \tag{12}$$

- $\lambda$ large (strong coupling to lattice) and/or $b$ small (very compressible lattice) $\Rightarrow$ 'effective' $B < 0 \Rightarrow$ first order
- also: $u \propto \eta^2 \propto T_C - T$

# Ginzburg-Landau

- (not necessarily) homogeneous Hamiltonian
- potentially variable order parameter (superconductivity, magnetic spirals, vortices, ...)
- Free energy might depend on gradient of order parameter.
- In case of inversion symmetry: $\vec{r}$ equivalent to $-\vec{r} \Rightarrow$ no terms linear in gradient

plausible form of first few orders in the free energy:

$$\Phi = \int \mathrm{d}^2 r \ \left( A\eta^2(\vec{r}) + B\eta^4(\vec{r}) + G(\nabla\eta(\vec{r}))^2 + E(\nabla^2\eta(\vec{r}))^2 \right) \tag{13}$$

- $G > 0$ suppresses gradients $\Rightarrow$ homogeneous solution preferable $\Rightarrow$ use previous approach
- $G < 0$, gradients may be favorable, $E >$ prevents them from becoming too large

# Example: magnetic spiral

- homogeneous Hamiltonian $\Rightarrow$ go to momentum space

$$\Phi = \sum_{\vec{k}} \left( A\eta^2(\vec{k}) + B\eta^4(\vec{k}) + G(\nabla\eta(\vec{k}))^2 + E(\nabla^2\eta(\vec{k}))^2 \right) . \tag{14}$$

- assumption on order parameter: $M_x = M\cos\vec{q}\vec{r}$ and $M_y = M\sin\vec{q}\vec{r}$
- effective free energy with $\eta(\vec{k}) = \vec{M}\delta_{\vec{k},\vec{q}}$:

$$\Phi = AM^2 + BM^4 + Gq^2M^2 + Eq^4M^4 . \tag{15}$$

- direction of $\vec{q}$ does here not enter

# Example: magnetic spiral, II

optimal spiral via saddle point:

$$\frac{\partial \Phi}{\partial M} = 0 = M\left[(A + Gq^2) + (2B + 2Eq^4)M^2\right] \quad \text{and} \tag{16}$$

$$\frac{\partial \Phi}{\partial q} = 0 = qM^2\left[G + 2EM^2q^2\right] \ . \tag{17}$$

- $A > 0$: disordered $M = 0$ with arbitrary $q$
- $A > 0$ and $G > 0$: $M \neq 0$ and $q = 0$ (as $\eta$ before)
- $A > 0$ and $G < 0$: $M \neq 0$ and $q \neq 0$
  - special case (example) $q \approx 0$
  - $M$ mostly given by $A$ and $B$
  - $q$ determined by $GM^2$ and $EM^4$
  - improved values for $M$: $A \to A + Gq^2$ and $B \to B + Eq^4$

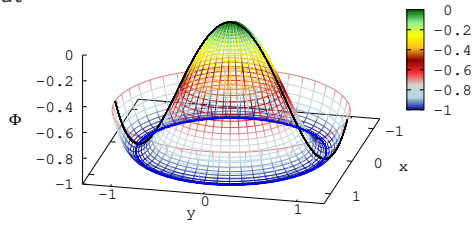
# Summary Ginzburg-Landau approach

- Also a kind of mean-field theory
- Starts from symmetry considerations rather than microscopic model
- Set up free energy consistent with symmetries
- valid fro small order parameters
- Gives second order for pure symmetry-breaking transition
- Applicable to weakly first-order transitions
- Applicable to more complicated situations (e.g. coupled order parameters)
- Can include spatial variations (e.g. spiral)

# Excitations for a continuous symmetry?

Heisenberg:

- Smallest excitation is slooooooow canting of spin.
- Locally, one is almost FM.
- Different directions, but always in valley of Mexican hat / wine bottle.
- Energy $\to 0$ for wavelength $\to \infty$.
- Impact on long-range order depends on
  - dispersion of excitation (linear vs. quadratic)
  - their density of states (dimensionality)
- Results:
  - $3d$: long-range order stable, $T_C > 0$
  - $2d$: no true long-range order at any $T > 0$
  - $1d$: AF ground state not even 'simple' alternating pattern




Ising: smallest excitation is spin flip, only dangerous in $d = 1$

# Formalized in quantum field theory

- 'normal' harmonic potential energy $U = \frac{1}{2}m^2\eta^2$
- $\Rightarrow$ Lagrangian

$$\mathcal{L} = T - U = \frac{1}{2}\partial^\mu\eta\partial_\mu\eta - \frac{1}{2}m^2\eta^2 = \frac{1}{2}(\partial_t\eta)^2 - \frac{1}{2}(\nabla\eta)^2 - \frac{1}{2}m^2\eta^2 \tag{18}$$

- Euler-Lagrange equations

$$\frac{\partial\mathcal{L}}{\partial\eta} - \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\eta)}\right) = 0 \quad \Rightarrow \quad (\partial_\mu\partial^\mu + m^2)\eta = 0 \tag{19}$$

- Solution: plane waves $\eta_{\vec{p}}(\vec{x},t) = a_{\vec{p}}\mathrm{e}^{-i(E_{\vec{p}}t - \vec{p}\vec{x})}$
- with dispersion $E_{\vec{p}} = \sqrt{m^2 + \vec{p}^2}$
- example: looks like acoustic phonons for $m = 0$

for example: 'Quantum Field Theory for the Gifted Amateur'

# Excitations cause deviations from order

- creation an annihilation operators

$$\eta(\vec{x}) = \frac{1}{\sqrt{2\pi}^3} \int \mathrm{d}^3k \frac{1}{\sqrt{2E_{\vec{k}}}} (a_{\vec{k}} \mathrm{e}^{i\vec{k}\vec{x}} + a^\dagger_{\vec{k}} \mathrm{e}^{-i\vec{k}\vec{x}}) \,. \tag{20}$$

- like $x$ and $p$ of harmonic oscillator expressed in $a^\dagger$ and $a$
- one kind of creator for each kind of excitations (e.g. Goldstone and amplitude modes, momenta)
- populate using bosonic statistics and $\mu = 0$
- single harmonic oscillator:

$$\langle x^2 \rangle = \frac{1}{M} \frac{\hbar}{2\omega} \Big( \underbrace{\langle a \; a \; \rangle}_{=\langle n-2|n\rangle = 0} + \underbrace{\langle a^\dagger a^\dagger \rangle}_{=0} + \underbrace{\langle a \; a^\dagger \rangle}_{=n+1} + \underbrace{\langle a^\dagger a \; \rangle}_{=n} \Big) = \frac{\hbar}{\omega M} \left( n + \frac{1}{2} \right) \,. \tag{21}$$

- with one kind of momentum-dependent excitations:

$$\langle \eta^2 \rangle \propto \int \mathrm{d}^d k \langle \eta^2(\vec{k}) \rangle = \int \mathrm{d}^d k \frac{1}{E_{\vec{k}}} \Big( \langle n(\vec{k}) \rangle + \frac{1}{2} \Big) = \int \mathrm{d}^d k \frac{1}{E_{\vec{k}}} \Big( \frac{1}{\mathrm{e}^{\beta E_{\vec{k}}} - 1} + \frac{1}{2} \Big) \,. \tag{22}$$

# Populate Goldstone excitations

$$E_{\vec{k}} = c|\vec{k}| \quad \Rightarrow \quad \langle u^2 \rangle \propto \int_0^{q_D} \mathrm{d}q \; q^{d-2} \Big( \frac{1}{\mathrm{e}^{\beta\hbar c q} - 1} + \frac{1}{2} \Big) \tag{23}$$

- $d = 1$: even zero-point fluctuations from $\frac{1}{2}$ diverges:

$$\int_0^{q_D} \frac{\mathrm{d}q}{q} \tag{24}$$

  $\Rightarrow$ order melts even at $T = 0$

- $T > 0$: focus on $c|\vec{k}| \ll k_B T \quad \Rightarrow \quad \beta c|\vec{k}| \ll 1$

$$\int_0^{k_D} \mathrm{d}k \; k^{d-2} \frac{1}{\mathrm{e}^{\beta\hbar c k} - 1} \approx \int_0^{k_D} \mathrm{d}k \; k^{d-2} \frac{1}{1 + \beta\hbar c k - 1} = \frac{1}{\beta\hbar c} \int_0^{k_D} \mathrm{d}k \; k^{d-3} \, . \tag{25}$$

  Diverges for $d \leq 2$.

# Mermin-Wagner Theorem

In $d = 2$, breaking of a continuous symmetry cannot lead to true long-range order at $T > 0$.

Why use Mean-Field theory, if it is so wrong?

- 'Strictly $2d$' and 'continuous symmetry' may not hold.
- With exceptions ($1d$ AF), mean-field gives good ground state.
- Usually reasonable starting point.
- There can be 'quasi' long-range order (Berezinskii-Kosterlitz-Thouless transition).

# Summary so far

## Condensation

- van-der-Waals gas
  - interactions allow condensation
  - used classical thermodynamics
- Bose-Einstein condensation
  - appreciable boson fraction in ground state at high $T$ and in thermodynamic limit
  - quantum statistics allows phase transition for bosons
  - used statistical physics

## Symmetry breaking in mean-field theory

- microscopic Ising model
  - statistical physics for model Hamiltonian
  - spontaneous symmetry breaking at low $T < T_C$
- Ginzburg-Landau approach
  - uses free energy
  - based on symmetry considerations

# Critical Fluctuations close to $T_C$

- Close to $T_C$, fluctuations are big and correlated
- Correlation between order parameter at different places:

$$g(\vec{r}, \vec{r}') = \langle x(\vec{r})x(\vec{r}')\rangle - \langle x(\vec{r})\rangle\langle x(\vec{r}')\rangle \tag{26}$$

- no correlation $\Rightarrow \quad \langle x(\vec{r})x(\vec{r}')\rangle = \langle x(\vec{r})\rangle\langle x(\vec{r}')\rangle$
- Important concept: 'correlation length' $\xi(T)$
- Susceptibility $\chi \propto \sum_{i,j} g_{i,j}$ diverges at phase transition
- $\xi(T)$ diverges at phase transition: this is how system learns everywhere what order to pick
- Long-range behavior much more important than short-range interactions

# Close to $T_C$: beyond mean-field

- How close is 'close'? How big is 'big'?
- Fluctuations comparable to order parameter:

$$\langle (\Delta\eta)^2 \rangle \approx \eta^2 \tag{27}$$

- Regime:

$$\tau = \frac{|T - T_C|}{T_C} \approx \frac{B^2}{9\pi^2 a^4 T_C^2 \xi_0^6} \approx \frac{B^2 T_C}{8\pi^2 a G^3} \tag{28}$$

- $\xi_0$: correlation length at $T = 0$
- outside $\tau$, Landau theory should work; $\frac{B^2 T_C}{8\pi^2 a G^3} \ll 1 \quad \Rightarrow \quad \tau$ negligible
- Good example for large $\xi_0$ and small $\tau$: superconductor

# Critical Scaling and Universality Classes

short-range interactions (e.g. magnetic) $\Rightarrow$ small $\xi_0 \Rightarrow$ large $\tau$
quantities typically behave like $|T - T_C|^\lambda$:

- $c \propto \tau^{-\alpha} = (\frac{|T_C - T}{T_C})^{-\alpha}$ (i.e. not a jump!)
- $\eta \propto \tau^{-\beta}$
- $\chi \propto \tau^{-\gamma}$
- $\xi \propto \tau^{-\nu}$
- Universal relations between them known, e.g., $\alpha + 2\beta + \gamma = 2$.
- Values depend on dimension $d$ and symmetry of order parameter $\Rightarrow$ 'universality class'

Knowledge about them from 'scaling theory'

# Scaling Theory

- Near $T_C$, correlation length diverges
- Making everything bigger by some factor should not 'essentially' change situation

$$G(\lambda^b B_0) = \lambda G(B_0) \tag{29}$$

- Indeed the case in second-order phase transitions: a few 'global features' more important than 'local details'
- idea applied to Ising model:
  - Collect spins into bigger 'block spin'
  - close enough to $T_C$, $\xi(T) \gg L_{\text{block}}$
  - block spin $S_b \approx \pm L_{\text{block}}^d$
  - Same model as before, but with modified parameters.
  - repeat

# Renormalization Group

More elaborate scheme based on scaling arguments:

- scheme:
  - go to larger scales/ lower energies/ ...
  - some couplings are going to get smaller ('irrelevant')
  - some get bigger ('relevant')
  - in between: 'marginal': maybe important, maybe not
- different microscopic models have similar phase transitions
- finds few relevant aspects out of many microscopic features

# ‘Brute-force’ numerics: Markov-chain Monte Carlo

- Method:
  - Start with some (e.g. random) configuration, energy $E_0$
  - Change it a bit $\Rightarrow$ $E_1$
  - Accept change with probability $\max(1, \mathrm{e}^{-\beta E_1}/\mathrm{e}^{-\beta E_0})$
  - Do this ‘long enough’
- Advantages:
  - ‘Unbiased’: Good when you do not have much of an idea
  - Flexible
- Disadvantages:
  - ‘Long enough’ can be prohibitive
  - Especially hard near phase transitions
  - Considerably more annoying for quantum systems
  - Finite systems can be misleading

Alan Sokal: ‘Monte Carlo is an extremely bad method, it should be used only when all alternative methods are worse.’