Theory of Phase Transitions

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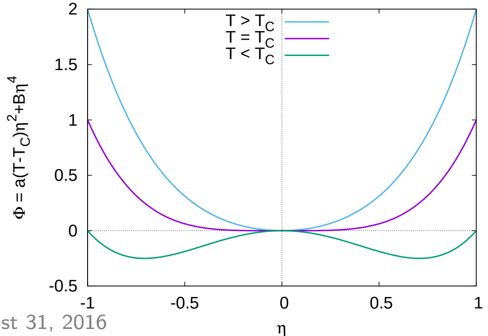
Content

- Phase transitions (e.g. van der Waals)
- Macroscopic/microscopic description
- Symmetry breaking and Phase transitions
- Mean-Field theory for the Ising model
- (Ginzburg-)Landau approach
  - Second order
  - weakly first order
  - coupled order parameters
- Limitations of mean-field theory
- Excitations
- Quantum Phase transitions and order without symmetry breaking

Equilibrium

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



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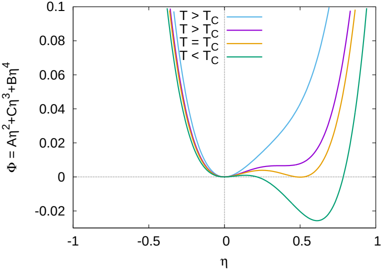
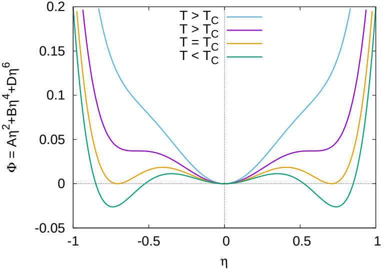
Weakly first order



$C\eta^3$



$B < 0, D\eta^6$

$$\Phi(\eta, T, p, \dots) = \Phi_0(T, p, \dots) + A(T, p, \dots)\eta^2 + \\ + C(T, p, \dots)\eta^3 + B(T, p, \dots)\eta^4 + \\ + F(T, p, \dots)\eta^5 + D(T, p, \dots)\eta^6 + \dots \quad (1)$$

More degrees of freedom

e.g. magnetism + lattice deformation

- magnetic order parameter η
- 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: $\frac{\partial\Phi}{\partial u} = bu + \lambda\eta^2 = 0, \quad u = -\frac{\lambda\eta^2}{b}$
- Re-insert into Φ:

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

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

Critical Fluctuations close to T_C

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

$$g(\vec{r}, \vec{r}') = \langle x(\vec{r}) x(\vec{r}') \rangle - \langle x(\vec{r}) \rangle \langle x(\vec{r}') \rangle \tag{3}$$

- no correlation $\Rightarrow \quad \langle x(\vec{r}) x(\vec{r}') \rangle = \langle x(\vec{r}) \rangle \langle x(\vec{r}') \rangle$
- Mean-field theory not applicable
- 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:

$$\langle(\Delta\eta)^2\rangle \approx \eta^2 \tag{4}$$

- Regime:

$$\tau = \frac{|T - T_C|}{T_C} \approx \frac{B^2}{9\pi^2 a^4 T_C^2 \xi_0^6} \approx \frac{B^2 T_C}{8\pi^2 a G^3} \tag{5}$$

- ξ_0: correlation length at $T = 0$
- outide τ, 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 ξ_o and small τ: superconductor

Critical Scaling and Universaity Classes

short-range interactions (e.g. magnetic) $\Rightarrow$ small ξ_0 $\Rightarrow$ large τ
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

$$G(\lambda^b B_0) = \lambda G(B_0) \tag{6}$$

- 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

Spatial variation: Ginzburg-Landau

$\Phi = \int d^3r\, \phi(\vec{r})$, e.g.: surface of a finite system, variation of η costs energy. Parameter G fixes length scale of 'acceptable' variation:

$$\Phi = \int d^3r\, \left(A\eta^2(\vec{r}) + B\eta^4(\vec{r}) + G(\nabla\eta(\vec{r}))^2\right) \tag{7}$$

(superconductivity) What if $G < 0$? Similar to $B < 0$, we need

higher-order terms like $E(\nabla^2\eta(\vec{r}))^2$.

Example: spirals

Relevant terms $Gq^2\eta^2 + Eq^4\eta^2$

$$\frac{\partial\Phi}{\partial q^2} = G\eta^2 + 2Eq^2\eta^2 = 0 \quad \Rightarrow \quad q^2_{\text{min}} = -\frac{G}{2E} > 0 \tag{8}$$

Topological defects

- available topological defects determined by symmetry class (homotopy group)
- point defects: vortices (e.g. superconductors)
- line defects: domain walls
- very stable
- Lifshitz invariants
  - lack of inversion symmetry
  - free energy can cotnain terms linear in gradient
  - system likes variation even for $G > 0$
  - allow 'particle-like' solutions to GL equation: defects (e.g. skyrmions)

Superconductivity: GL I

- Order parameter: complex scalar (or $2d$ vector)
- Quite a bit known about spatial dependence (magnetic field) $\Rightarrow$ Ginzburg-Landau equation

$$\Phi = \int \mathrm{d}^2 r \, \left(A|\psi(\vec{r})|^2 + B|\psi(\vec{r})|^4 + G|\nabla\psi(\vec{r})|^2 + \ldots \right) = $$
$$= \int \mathrm{d}^2 r \, \left(a\frac{T - T_C}{T_C}|\psi(\vec{r})|^2 + \frac{b}{2}|\psi(\vec{r})|^4 + \frac{1}{2m}|\nabla\psi(\vec{r})|^2 + \ldots \right) \tag{9}$$

- Known symmetries: gauge invariance; consistent ‘trick’ $-i\hbar\nabla \to -i\hbar\nabla - \frac{e^*}{c}\vec{A}$
- Need functional derivative w.r.t. $\psi(\vec{r})$ and w.r.t. $\vec{A}$: charged electrons modify electromagnetic field.

Superconductivity: GL II

- Minimisation w.r.t. $\vec{A}(\vec{r})$ give equation defining a current:

$$\frac{1}{4\pi}\vec{\nabla}\times\vec{B} = \frac{\hbar e^*}{2mc}\left(\psi^*\left(-i\vec{\nabla}-\frac{e^*}{\hbar c}\vec{A}\right)\psi-\psi\left(i\vec{\nabla}-\frac{e^*}{\hbar c}\vec{A}\right)\psi^*\right) \quad (10)$$

With $\vec{\nabla}\times\vec{B} = \frac{4\pi}{c}\vec{j}$, one gets

$$\vec{j} = \frac{\hbar e^*}{2m}\left(\psi^*\left(-i\vec{\nabla}-\frac{e^*}{\hbar c}\vec{A}\right)\psi-\psi\left(i\vec{\nabla}-\frac{e^*}{\hbar c}\vec{A}\right)\psi^*\right), \quad (11)$$

where $e^* = 2e$.

- Minimisation w.r.t. $\psi(\vec{r})$ and $\psi^*(\vec{r})$ determine order parameter:

$$\frac{1}{2m}\left(-i\hbar\vec{\nabla}-\frac{e^*}{c}\vec{A}\right)^2\psi(\vec{r})+a\frac{T-T_C}{T_C}\psi(\vec{r})+b|\psi(\vec{r})|^2\psi(\vec{r}) = 0 \quad (12)$$

Looks like Schrödinger equation: 'wave function of the condensate'

Microscopic variant and BCS theory

- Some attractive elecron-electron interaction
- (via phonons, see isotope effect; also note that this is long-range ⇒ mean-field good)
- Attraction only between electrons close to Fermi level, but let's simplify.

$$H = \sum_{\vec{k},\sigma} (\epsilon_{\vec{k}} - \mu) c^{\dagger}_{\vec{k},\sigma} c_{\vec{k},\sigma} + \frac{1}{2} \sum_{\substack{\vec{k},\vec{k}' \\ \sigma,\sigma'}} V_{\vec{k},\vec{k}'} c^{\dagger}_{\vec{k},\sigma} c^{\dagger}_{-\vec{k},\sigma'} c_{-\vec{k}',\sigma'} c_{\vec{k}',\sigma} \quad . \qquad (13)$$

- Perturbation theory in $V_{\vec{k},\vec{k}'}$ does not work: preserves a Fermi-liquid at all orders, which is not the ground state
- try mean-field theory

BCS theory I

- Possible mean-field decoupling with terms $\langle c^\dagger_{\vec{k},\sigma} c_{\vec{k}',\sigma}\rangle c^\dagger_{-\vec{k},\sigma'} c_{-\vec{k}',\sigma'}$ can describe magnetic order
- alternative mean-field decoupling:

$$\begin{aligned} c^\dagger_{\vec{k},\sigma} c^\dagger_{-\vec{k},\sigma'} c_{-\vec{k}',\sigma'} c_{\vec{k}',\sigma} \to & \langle c^\dagger_{\vec{k},\sigma} c^\dagger_{-\vec{k},\sigma'}\rangle c_{-\vec{k}',\sigma'} c_{\vec{k}',\sigma} \\ & + c^\dagger_{\vec{k},\sigma} c^\dagger_{-\vec{k},\sigma'} \langle c_{-\vec{k}',\sigma'} c_{\vec{k}',\sigma}\rangle \\ & - \langle c^\dagger_{\vec{k},\sigma} c^\dagger_{-\vec{k},\sigma'}\rangle \langle c_{-\vec{k}',\sigma'} c_{\vec{k}',\sigma}\rangle \ . \end{aligned} \tag{14}$$

- For $V(\vec{k},\vec{k}') = V_0$ and singlet pairing:

$$H_{\mathrm{MF}} = \sum_{\vec{k},\sigma} (\epsilon_{\vec{k}} - \mu) c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma} - \Delta^* \sum_{\vec{k}} c_{-\vec{k},\downarrow} c_{\vec{k},\uparrow} - \Delta \sum_{\vec{k}} c^\dagger_{\vec{k},\uparrow} c^\dagger_{-\vec{k},\downarrow} - \frac{|\Delta|^2}{V_0} \ . \tag{15}$$

BCS theory II

- biquadratic, almost there!
- Particle-hole transformation for ↓ electrons → Nambu spinor

$$H_{\mathrm{MF}} = \sum_{\vec{k}} (c^\dagger_{\vec{k},\uparrow}, h^\dagger_{\vec{k},\downarrow}) \begin{pmatrix} \epsilon_{\vec{k}} - \mu & -\Delta^* \\ -\Delta & -(\epsilon_{-\vec{k}} - \mu) \end{pmatrix} \begin{pmatrix} c_{\vec{k},\uparrow} \\ h_{\vec{k},\downarrow} \end{pmatrix} - \frac{|\Delta|^2}{V_0} \tag{16}$$

- Diagonalize:

$$\begin{pmatrix} \gamma_{\vec{k},\uparrow} \\ \gamma^\dagger_{-\vec{k},\downarrow} \end{pmatrix} = U \begin{pmatrix} c_{\vec{k},\uparrow} \\ c^\dagger_{-\vec{k},\downarrow} \end{pmatrix} = \begin{pmatrix} u^*_{\vec{k}} & v_{\vec{k}} \\ -v^*_{\vec{k}} & u_{\vec{k}} \end{pmatrix} \begin{pmatrix} c_{\vec{k},\uparrow} \\ c^\dagger_{-\vec{k},\downarrow} \end{pmatrix} \tag{17}$$

BCS theory III

- $$H = \sum_{\vec{k},\sigma} E_{\vec{k}} n_{\vec{k},\sigma} + E_0 \quad \text{with} \quad E_{\vec{k}} = \sqrt{(\epsilon_{\vec{k}} - \mu)^2 + |\Delta|^2} \qquad (18)$$
- n is the number operator for γ: ground state has none
- ground state:

$$|\psi_{\text{BCS}}\rangle \propto \prod_{\vec{k},\sigma} \gamma_{\vec{k},\sigma}|0\rangle \propto \prod_{\vec{k}} \left(u^*_{\vec{k}} + v_{\vec{k}} c^\dagger_{-\vec{k},\downarrow} c^\dagger_{\vec{k},\uparrow}\right)|0\rangle \,. \qquad (19)$$

$u_{\vec{k}} = \cos\theta_{\vec{k}}$ and $u_{\vec{k}} = \sin\theta_{\vec{k}}$ for real Δ

Gap = order parameter

- Self-consistency equation:

$$\Delta = \frac{V_0}{2} \sum_{\vec{k}} \frac{-\Delta}{E_{\vec{k}}} \,. \tag{20}$$

- $\Delta = 0$ one possible solution: no superconductivity
- For $V_0 < 0$ (attraction!), more solutions $\frac{2}{|V_0|} = \sum_{\vec{k}} \frac{1}{E_{\vec{k}}}$ possible
- $\Delta_{\sigma,\sigma'}(\vec{k}) = \sum_{\vec{k}'} V_{\vec{k},\vec{k}'} \langle c_{-\vec{k}',\sigma'} c_{\vec{k}',\sigma} \rangle$ complex number
- See also: complex order parameter from before
- BCS ground state is coherent state: has defined phase
- Broken symmetry: gauge invariance

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

- Method:
  - Start with some (e.g. random) configuration, energy E_0
  - Change it a bit ⇒ 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 have not much of an idea
  - Flexible
- Disadvantages:
  - ‘Long enough’ can be prohibitive
  - Especially hard near phase transitions, for many quantum problems
  - 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.’

Quantum Phase Transitions

- Phase transitions driven by T, entropy, thermal fluctuations
- Phase transition may also be driven by other parameter
- Different Hamiltonian $\Rightarrow$ different ground state
- Transition can be first order, i.e., 'the same' for finite T
- Or *at* $T = 0$
- Quantum fluctuations dominate
- signatures seen at higher T

Spin liquids and Topological Phase transitions

- So far: Interactions ⇒ ordered phase, chracterized by order parameter
- Other possibility: interactions, but no pattern
- Example: Frustration
- Additional ingredient: Quantum mechanics
- New concept: ‘topological order’
- Example: fractional Quantum Hall
- ‘Non-local’ order