LECTURE 2
Mean Field Approximation and Landau Theory of type II Phase Transitions

Lecture 1 was devoted to phenomenological thermodynamics of phases and phase transitions. In the rest of this course, we will analyse the criticality, i.e. thermodynamics at the temperatures close to that of the phase transition, by the means of statistical physics. Concentrating attention at universal features connected with criticality. Phenomenology appears yet many times during these lectures.

1. Structural Transitions Displacement Type and Order-Disorder Type.

We begin with a simple model of a structural transition in a crystal: each unit cell of a crystal forms a 'cage' for an atom with mass m. This atom is allowed to be displaced by the distance x_i from its position of equilibrium, all other atoms are fixed. The Lagrangian $\mathcal{L}$ of the crystal has the following form :

$$\mathcal{L} = \sum_i \left\{ \frac{m}{2} \dot{x}_i^2 - \frac{A}{4} \left(x_i^2 - a^2 \right)^2 \right\} - \sum_{i \neq j} V_{ij} \left(x_i - x_j \right)^2 \qquad (1)$$

The Lagrangian of Eq (1) shows that, at $A > 0$, within the unit cell, the position $x_i = 0$ corresponds to unstable equilibrium, and this instability is stabilised by the quartic (anharmonic) potential. Displacements x_i and x_j in different unit cells are interacting with each other and, at $V_{ij} > 0$, displacements in the same direction correspond to a lower energy.

Thermodynamic properties of the crystal are determined by the Free energy $F = -T \ln Z$, where partition function $Z(\beta)$, $(\beta = 1/T)$ is

$$Z = \int_{x(\beta) = x(0)} \prod_i \mathcal{D}\, x_i(\tau) \ \exp \left[- \int_0^\beta \tilde{\mathcal{L}} d\tau \right], \qquad (2)$$

where

$$\tilde{\mathcal{L}} = \sum_i \left\{ \frac{m}{2} \left(\frac{\partial x_i}{\partial \tau} \right)^2 + \frac{A}{4} \left(x_i^2 - a^2 \right)^2 \right\} + \sum_{i \neq j} V_{ij} \left(x_i - x_j \right)^2 . \qquad (3)$$

Eqs (2) and (3) contain the displacements $x_i(\tau)$ $(0 \leq \tau \leq \beta)$ as the functions of imaginary time $t = i\tau$. If a Fourier transform

$$x(\tau) = \sum_n x_n \, e^{i \omega_n \tau}, \quad \omega_n = 2\pi T n \qquad (4)$$

is made, then the Eq (2) could be rewritten as an integral

$$\int \mathcal{D}x(\tau) = \prod_{n=-\infty}^{+\infty} \int d\ x_n,$$

and the term with time derivatives in Eq (3) takes the form

$$\int_0^\beta d\tau \left(\frac{\partial x}{\partial \tau}\right)^2 = T \sum_{n=-\infty}^{+\infty} \ \omega_n^2 |x_n|^2.$$

If the temperature T is low, the sum over Matsubara frequencies ω_n can be replace by an integral over frequencies. In the opposite case of high temperatures, only one Fourier component x_n with $n = 0$ is essential, and Eqs (2) and (3) return us to Classical Statistical Mechanics. We will stick to this Classical case in the rest of these lectures.

Two limited cases occur if/when the interaction $V_{ij}\ a^2$ is either smaller, or larger, than the scale $A\ a^4$ of the potential within the unit cell.

Order-disorder Type Transition.

If $A\ a^2 \gg V$, then two scales of temperature $T_* \sim A\ a^4$ and $T_C \sim \mathcal{J} = 2\ V\ a^2$ $(T_* \gg T_C)$ naturally occur. At relatively high temperature $T \ll T_*$, displacements x_i in each unit cell correspond to energy minimum at $x_i = \pm a$. Under this condition, the energy $\mathcal{E}$ of the crystal is reduced to that of the *Ising model*

$$\mathcal{E} = \mathcal{E}_0 - \sum_{i,j} \mathcal{J}_{ij}\ \sigma_i\ \sigma_j, \quad \sigma_i = \frac{x_i}{a} = \pm 1,\ J_{ij} = 2\ a^2\ V_{ij}. \quad (5)$$

Thermodynamics of Ising model is well-studied. The crystal undergoes the second order phase transition: at $T \geq T_C = \sum_{j\neq i}\mathcal{J}_{ij}$ dynamical variables $\sigma_i = \pm 1$ are not ordered, i.e. $\langle\sigma_i\rangle = 0$. At lower temperatures $T < T_C$, a spontaneous symmetry breaking $s = \langle\sigma_i\rangle \neq 0$ occurs[1] .

Displacement Type Phase Transition.

If $A\ a^2 \ll V$, then the effective energy, associated with displacements x_i

$$\mathcal{E} = \mathcal{E}_0 + \mathcal{E}_2 + \mathcal{E}_4, \tag{6}$$

$$\mathcal{E}_2 = \frac{A\ a^2}{2}\ \sum_i x_i^2 + \sum_{ij} V_{ij}\ \left(x_i - x_j\right), \tag{7}$$

$$\mathcal{E}_4 = \frac{A}{4}\ \sum_i x_i^4. \tag{8}$$

corresponds to weak anharmonism and $\mathcal{E}_2 \gg \mathcal{E}_4$ at typical values of displacements x_i. Using the Fourier transform, obtain

$$\mathcal{E} = \mathcal{E}_0 + \sum_{\mathbf{k}} \frac{\omega^2(\mathbf{k})}{2}\ |x(\mathbf{k})|^2 + \frac{\gamma}{4} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} x(\mathbf{k}_1)x(\mathbf{k}_2)x(\mathbf{k}_3)x(\mathbf{k}_4)\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4) \tag{9}$$

Harmonic part $\mathcal{E}_2$ of effective potential energy of oscillations (9), at most of the values of quasi wave vectors $\mathbf{k}$ is larger,

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[1] In contrast with Displacement Type Phase Transition, in crystals, undergoing the Order-disorder Type Transition, even at $T \geq T_C$, when $s = \langle\sigma_i\rangle = 0$, in every unit cell, the atom in the "cage" is displaced from its center.

than its anharmonic part $\mathcal{E}_4$. The frequency $\omega(\mathbf{k})$ is mall only at very small values of $\mathbf{k}$, where

$$\omega^2(\mathbf{k}) = \omega^2(0) + s^2\ \mathbf{k}^2, \quad k\ a \ll 1. \tag{10}$$

The coefficient s has an usual order of magnitude $s \sim \omega_D a$, while $\omega^2(0)$ is small and could be even negative. If $\omega^2(0) = -\mu$ ($\omega_D^2 \gg \mu > 0$), then, at $T = 0$, the crystal is unstable with respect to uniform displacements $x(\mathbf{k} = 0)$. At finite temperature, effective frequency $\omega(\mathbf{k}, T)$ is a subject of renormalisation due to anharmonic interaction. In the leading approximation in small amplitude γ,

$$\omega^2(\mathbf{k}, T) = -\mu + \Sigma(\mathbf{k}, T),\ \ \Sigma(\mathbf{k}, T) = 6\,\gamma\ \sum_{\mathbf{k}} \langle |x(\mathbf{k})|^2 \rangle_T \tag{11}$$

Using renormalised harmonic energy, obtain

$$\mathcal{G}(\mathbf{k}, T) = \langle |x(\mathbf{k})|^2 \rangle_T = \frac{T}{\omega^2(\mathbf{k}, T)}, \tag{12}$$

$$\omega^2(0) = -\mu + 6\frac{\gamma T}{(2\pi)^3} \int \frac{d\mathbf{k}}{\omega^2(\mathbf{k})}. \tag{13}$$

The integral in the right hand side of Eq (13) is determined by large values of the quasi wave vectors $\mathbf{k}$ and, therefore, in the leading approximation, does not depend on temperature. Therefore, effective frequency $\omega(0)$ of soft phonons obeys the Curie-Weiss law

$$\omega^2(0) = \frac{T - T_c}{C}, \qquad T_c = \mu\ C. \tag{14}$$

Therefore, the crystal is stable at $T > T_c$ and loses stability at $T \leq T_c$[2].

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[2] Since the amplitude γ of an anharmonic interaction is small, the Curie-weiss constant C is large ($C \gg T_c$)

In view of the mentioned instability, at $T < T_c$, the displacement x_i must be viewed as a sum

$$x_i = \eta + \delta x_i, \quad x(\mathbf{k}) = \eta\delta(\mathbf{k}) + \delta x(\mathbf{k}) \tag{15}$$

of the uniform displacement η and the local displacement δx_i. Analogously the Fourier image $x(\mathbf{k})$ of a displacement could be presented (as done in Eq (15)) as a sum. Omitting the effect of thermal fluctuations of δx, obtain the free energy F as

$$F = F_0 + \frac{T - T_c}{2C}\,\eta^2 + \frac{\gamma}{4}\,\eta^4, \tag{16}$$

This form of Free energy is called in literature *Landau expansion* and the uniform displacement η bear the name the *order paramenter.*

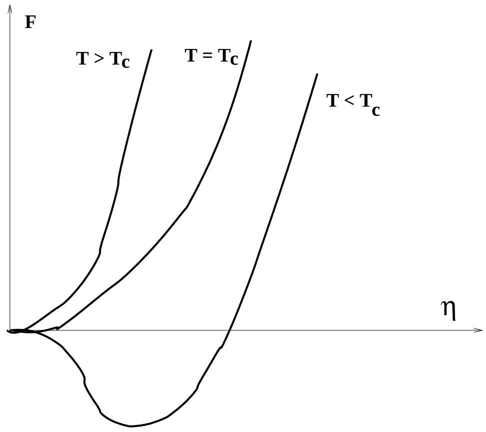

Figure 1: Free energy F in Landau Theory as a function of order parameter η

2. Landau Theory of Type II Phase Transitions.

Fig 1 presents dependence of Free energy $F(\eta)$ on order parameter η at different temperatures. At $T > T_c$, the free energy has minimum at $\eta = 0$. At $T < T_c$, the state with $eta = 0$ corresponds not to a minimum but to a maximum of Free energy. Taking derivative in eta from the Landau expansion (16), obtain the equilibrium value $\eta(T)$ and the free energy at $T < T_c$

$$\eta(T) = \pm\sqrt{\frac{T_c - T}{\gamma C}}, \quad F = F_0 - \frac{(T_c - T)^2}{4C^2\gamma}. \tag{17}$$

Eq (17) shows that not only free energy F is continuous at $T = T_c$, but its derivative in temperature, the entropy, has no jumps at the transition point. This means that there is no hidden heat of the type II transition. As for specific heat $C(T) = T(\partial S/\partial T) = -T(\partial^2 F/\partial T^2)$ it has a jump and

$$C(T - 0) = C(T + 0) + \Delta C, \quad \Delta C = \frac{T_c}{2C^2\gamma}. \tag{18}$$

We will see that this jump in specific heat is an artefact of the mean field approximation, underlying Landau theory.

Fig 2 presents - schematically - dependence on temperature T the order parameter η and the specific heat C in frameworks of Landau theory.

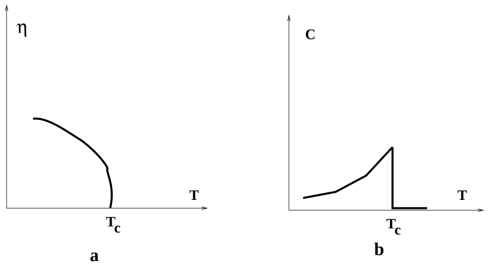

Figure 2: Temperature dependences of the order parameter η and the specific heat C in Landau Theory.

3. Landau Theory and Symmetry Breaking

We consider here how the concepts of symmetry and symmetry breaking are linked with Landau theory of type II phase transitions. Let, the symmetric phase (at high temperature $T \geq T_c$) has the symmetry group G. This means, for instance, that the density $\rho_0(\mathbf{r})$ at high temperature is invariant with respect to transformations $\hat{g} \in G$. This means that $\rho_0(\hat{g}\mathbf{r}) = \rho_0(\mathbf{r})$. At low temperature $T \leq T_c$ the density has lower symmetry:

$$\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \sum_{\alpha} \eta_\alpha \phi_\alpha(\mathbf{r}) \ , \tag{19}$$

where summation in Eq (19) is conducted over irreducible representations of the group G (excluding the trivial - scalar - representation). The eigenvectors of representation Γ_α are presented by the normalised functions $\phi_\alpha(\mathbf{r})$. Free energy

F at $T > T_c$ is

$$F = F_0 + \sum_\alpha \frac{a_\alpha}{2}\, \eta_\alpha^2, \quad a_\alpha > 0. \tag{20}$$

At $T = T_c$, one of rigidities a_α vanishes (say, for $\alpha = 1$). Therefore, at $T < T_c$ the rigidity $a_1 < 1$, which makes symmetric phase unstable with respect to developing the deformation η_1. In order to determine the amplitude of above mentioned deformation, the free energy (20) must be completed with higher power of η_1

$$F = F_0 + \frac{a_1}{2}\, \eta_1^2 + \frac{c}{3}\, \eta_1^3 + \frac{b}{4}\, \eta_1^4 + .. \tag{21}$$

In case the coefficient c is not vanishing, transition from $\eta_1 = 0$ to $\eta_1 \neq 0$ occurs discontinuously (first order phase transition). In order to find out whether c is finite, one must consider symmetrised cube $[\Gamma_1 \times [\Gamma_1 \times \Gamma_1]]$ of representation Γ_1. If the expansion of this symmetrised cube into sum of irreducible representations contains the scalar Γ_0, i.e. if

$$[\Gamma_1 \times [\Gamma_1 \times \Gamma_1]] = \Gamma_0 + ...,$$

then $c \neq 0$ and the transition is discontinuous. Otherwise, $c = 0$.

The quartic term (or terms) determines similar splitting of symmetrised fourth power $[\Gamma_1 \times [\Gamma_1 \times [\Gamma_1 \times \Gamma_1]]]$ of irreducible representation Γ_1. The symmetrised fourth power always contains the scalar. At least, one, but, sometimes several. If $c = 0,\ b > 0$[3], then we get a continuous (second order) transition.

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[3] Or, the quartic terms form a positively define polynomial

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PROBLEMS

P2.1. Bi-critical Point .
A system might undergo two phase transitions which lead to appearance of either order parameter ψ or order parameter ϕ. The free energy as the finction of two external parameters τ and h has the following form

$$F = F_0 + \frac{\tau + h}{2}\,\psi^2 + \frac{\tau - h}{2}\,\phi^2 + \frac{\beta_1}{4}\,\psi^4 + \frac{\beta_2}{4}\,\phi^4 + \frac{\beta_3}{4}\,\psi^2\phi^2 \quad (1)$$

Draw the phase diagram in plane (τ, h). How this phase diagram depends on relation between β_1, β_2 and β_3 ?

P2.2. Tricritical point
Landau expansion of free energy F in superfluid helium has the following form

$$F = F_0 + \frac{\alpha}{2}\,(T - T_\lambda)\,|\psi|^2 + \frac{b}{4}\,|\psi|^4 + \frac{c}{6}\,|\psi|^6, \quad c > 0. \quad (2)$$

In the mixture of isotopes ${}^3He_x\ {}^4He_{1-x}$ both T_λ and the coefficient b depend on concentration x. The dashed line in Fig 1 shows how the critical temperature $T_\lambda(x)$ decreases with increase of concentration x of isotope ${}^3He$. The dotted line in the same figure shows the temperature T and concentration x at which $b(x,T) = 0$. Above dotted line $b(x,T) > 0$, and below dotted line $b(x,T) < 0$. Analyse stability of superfluid and normal phases in such a mixture and finish the drawing the phase diagram[1].

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[1] The point at the phase diagram determined by two conditions $T = T_\lambda(x)$ and $b(x,T) = 0$ is called *Tricritical point*

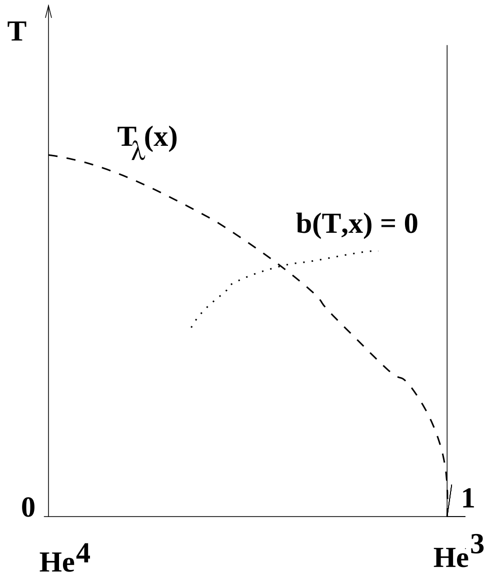

Figure 1: Phase diagram of the mixture ${}^3He_x\ {}^4He_{1-x}$ of the isotopes of liquid helium in variables (x,T).

P2.3. Cubic Ferromagnet

A ferromagnet in a crystal with cubic symmetry in presence of external magnetic field $\mathbf{H}$. Landau expansion of Gibbs free energy G in Magnetisation $\mathbf{M}$

$$G = G_0 + \frac{T - T_c}{2C}\,\mathbf{M}^2 + \frac{b}{4}\,\left(\mathbf{M}^2\right)^2 + \\ \frac{b_1}{4}\,\left(M_x^4 + M_y^4 + M_z^4\right) - \frac{\mathbf{H}\cdot\mathbf{M}}{4\pi} + \frac{\mathbf{H}^2}{8\pi} \qquad (3)$$

- Find dependence of the components M_x, M_y and M_z of magnetisation on temperature T at $\mathbf{H} = 0$ for different values of the coefficients b and b_1.

- For $b > 0$ and $b_1 > 0$, find temperature dpendences of the tensor of magnetic sucsessibility

  $$\chi_{\alpha\beta} = \left(\frac{\partial^2 G}{\partial H_\alpha \partial H_\beta}\right)_{\mathbf{H}\to 0}$$

  Pay attention to the difference in structure of the tensor $\chi_{\alpha\beta}$ at $T > T_c$ and at $T < T_c$.

- For given modulus of magnetic field $|\mathbf{H}|$, find dependence the modulus of magnetisation $|\mathbf{M}|$ on direction of magnetic field.

P2.4. Isolated Critical Point

- **P2.4.A.**

  Landau expansion of free energy F in order parameter η has the following form

  $$F = F_0 + \frac{\tau - h}{2}\,\eta^2 + \frac{\tau + h}{3}\,\eta^3 + \frac{b}{4}\,\eta^4\ , \qquad (4)$$

where τ and h are two thermodynamical parameters (for example, the temperature and the pressure). Draw the phase diagram in $(\tau,\ h)$ plane.

- **P2.4.B. Nematic Liquid Crytal**
  Nematic Liquid crystal is characterised by the order parameter $Q_{\alpha\beta},\ \mathrm{tr}\,\hat{Q}=0$, which determines the anysotropic part of dielectric constant

  $$\epsilon_{\alpha\beta}=\epsilon_0\ \delta_{\alpha\beta}+Q_{\alpha\beta}$$

  A liquid solution is characterised by the temperature T and concentration c of a solvant. Canonically conjugaed to concentration c is the chemical potential μ of the solvant. There is an isolated point (T_i,μ_i) in the plane of thermodynamic variables (T,μ), at which the transition from isotropic liquid to a liquid crystal is the type II phase transiion. Near such a point - at variables $T=T_i+\tau,\ \ \mu=\mu_i+\nu$ - the landau expansion for the grand canonical potential Ω has the following form

  $$\Omega=\Omega_0+\frac{\tau-\nu}{2}\ Q_{\alpha\beta}\ Q_{\beta\alpha}+\frac{\tau+\nu}{3}\ Q_{\alpha\beta}\ Q_{\beta\gamma}\ Q_{\gamma\alpha}+ \\ \frac{b}{4}\ \left(Q_{\alpha\beta}\ Q_{\beta\alpha}\right)^2+\frac{b_1}{4}\ Q_{\alpha\beta}\ Q_{\beta\gamma}\ Q_{\gamma\delta}\ Q_{\delta\alpha} \qquad (5)$$

  - Using the substitution

    $$Q_{\alpha\beta}=q\ \left(n_\alpha n_\beta-\frac{\delta_{\alpha\beta}}{3}\right)+q\ r\ \left(m_\alpha m_\beta-\frac{\delta_{\alpha\beta}}{3}\right) \\ \mathbf{n}^2=\mathbf{m}^2=1 \qquad \mathbf{n}\cdot\mathbf{m}=0,\quad 0\le r\le 1 \qquad (6)$$

draw the phase diagram in plane of variables τ and ν, indicating the phases with $q = 0$, $q \neq 0,\ r = 0$ and $q \neq 0,\ r \neq 0$[2] .

– Draw the phase diagram in the plane of temperature T and solvant's concentration c.

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[2] Parameter q determines anysotropy. In case $r = 0$, the anysotropy of dielectric constant $\hat{\epsilon}$ is uniaxial. In case $r = 1$, the of dielectric constant $\hat{\epsilon}$ is uniaxial as well (Inroduction of the vector $\mathbf{l} = [\mathbf{n} \times \mathbf{m}]$ allows to show that at $r = 1$, $\quad Q_{\alpha\beta} = -q\,(l_\alpha\, l_\beta - \delta_{\alpha\beta}/3)$). The case $0 < r < 1$ correspond to two-axial anysotropy of dielectric constant $\hat{\epsilon}$.