LECTURE 4
Thermal Fluctuations and Long Range Order. Criterion for the Mean Field Description. Upper Critical Dimension.

1. Landau Theory and Thermal Fluctuations

We have see that, in the frameworks of Landau Theory, Free energy F, as a function of uniform order parameter η, takes its canonical form

$$F = F_0 + \int d\mathbf{r} \left\{ \frac{\alpha}{2}\,\eta^2 + \frac{\gamma}{4}\,\eta^4 \right\}, \tag{1}$$

where the parameter $\alpha(T)$ vanishes at critical temperature $T = T_c$.

Statistical Mechanics of the system is determined by the partition function

$$Z = \int d\,\eta\ \exp\left[-\frac{F}{T}\right] \tag{2}$$

Since the Free energy F of a macroscopic system is proportional to its volume (or the number of particles), the integral in Eq (2) is determined by the value of the order parameter η, which corresponds to minimum of the free energy. The fluctuations around this value are small.

More realistic treatment allows to order parameter to vary in space and the free energy to become a functional of the function $\eta(\mathbf{r})$

$$F = F_0 + \int\ d\mathbf{r}\,\mathcal{F}\left\{\eta(\mathbf{r})\right\}, \quad \mathcal{F} = \frac{\alpha}{2}\,\eta^2 + \frac{s}{2}\,(\nabla\eta)^2 + \frac{\gamma}{4}\,\eta^4. \tag{3}$$

This form of free energy leads to expression for partition function Z in the form of a functional integral

$$Z = \int D\ \eta(\mathbf{r})\ \exp\left[-\frac{1}{T}\ \int d\mathbf{r}\ \mathcal{F}\left\{\eta(\mathbf{r})\right\}\right] \tag{4}$$

Condition of a minimum of the Free energy (3) forms a differential equation. We studies an equation of this kind discussing properties of superconductors.

As for significance of fluctuations, this question becomes now much more subtle because the minimum of the functional (3) is the minimum in a multi-dimensional space[1]. This means that, near the minimum, the order parameter takes the form

$$\eta(\mathbf{r}) = \eta_0 + \delta\eta(\mathbf{r}),$$

[1] Infinitely-dimensional in macroscopic limit.

and rigidity of the minimum with respect of different modes of deviations $\delta\eta(\mathbf{r})$ could be very different.

For instance, at $T > T_c$ the mean value of the order parameter η_0 vanishes, and the mean square of fluctuations is

$$\langle \eta(\mathbf{r})\ \eta(\mathbf{r}') \rangle_{\mathbf{k}} = \frac{T}{\alpha + s\ \mathbf{k}^2}, \qquad (5)$$

and, therefore, at $T \to T_c$, the fluctuations $\eta(\mathbf{k})$ of the order parameter with very small wave vectors are large even in a macroscopic system. Since the free energy functional is not quadratic in $\eta(\mathbf{r})$, the effect of large fluctuations leads to a significant deviations from the predictions of the mean field approximation. Such an effect of non-linear mode coupling of the soft modes will be a subject of the study in the rest of this course. Meanwhile, let us digress to one more mechanism, which leads to forming the soft modes.

2. Landau Theory and Goldstone Theorem

Consider an isotropic ferromagnet. The order parameter for this substance is magnetisation $\mathbf{m}(\mathbf{r})$. In presence of external magnetic field $\mathbf{H}$, the density $\mathcal{F}$ of free energy is presented by Landau expansion

$$\mathcal{F} = \frac{\alpha}{2}\ \mathbf{m}^2 + \frac{s}{2}\ (\nabla \mathbf{m})^2 + \frac{\gamma}{4}\ \mathbf{m}^4 - \mathbf{H}\ \mathbf{m}. \qquad (6)$$

The minimum of Free energy corresponds to uniform magnetisation $\mathbf{M}$ directed along externam magnetic field $\mathbf{H}$ and determined by equation

$$\alpha\,\mathbf{M} + \frac{\gamma}{4}\,\mathbf{M}\,\mathbf{M}^2 = \mathbf{H} \tag{7}$$

For longitudinal $\mathbf{m}_{\|}$ and transverse $\mathbf{m}_{\perp}$ fluctuations

$$\mathbf{m} = \mathbf{M} + \mathbf{m}_{\|} + \mathbf{m}_{\perp}, \qquad \mathbf{m}_{\|}\cdot\mathbf{m}_{\perp} = \mathbf{m}_{\perp}\cdot\mathbf{M} = 0 \tag{8}$$

the free energy functional takes the form

$$\mathcal{F} = \mathcal{F}(\mathbf{M}) + \frac{\alpha}{2}\,\left(\mathbf{m}_{\perp}^2 + \mathbf{m}_{\|}^2\right) + \frac{s}{2}\,\left[(\nabla\mathbf{m}_{\perp})^2 + (\nabla\mathbf{m}_{\|})^2\right]$$
$$+\frac{\gamma}{4}\,\left[\left(\mathbf{M} + \mathbf{m}_{\perp} + \mathbf{m}_{\|}\right)^4 - \mathbf{M}\right] - \mathbf{H}\mathbf{m}_{\|} \tag{9}$$

Using the condition (8), one can significantly simplify the expression (9). The further simplification occurs from an obvious fact that the lowest energy corresponds to conservation of the modulus

$$\mathbf{M}^2 = \left(\mathbf{M} + \mathbf{m}_{\|} + \mathbf{m}_{\perp}\right)^2 \to \mathbf{m}_{\|} = -\frac{\mathbf{M}}{2M^2}\,\mathbf{m}_{\perp}^2 \tag{10}$$

Using Eq (10) and obtaining quadratic in $\mathbf{m}_{\perp}$ free energy $\mathcal{F}_{\perp}$

$$\mathcal{F}_{\perp} = \frac{s}{2}\,(\nabla\mathbf{m}_{\perp})^2 + \frac{H}{2M}\mathbf{m}_{\perp}^2 \tag{11}$$

and the mean square of perpendicular fluctuation

$$\langle\mathbf{m}_{\perp}(\mathbf{r})\;\mathbf{m}_{\perp}(\mathbf{r}')\rangle_{\mathbf{k}} = \frac{T}{s\mathbf{k}^2 + H/2M} \tag{12}$$

Eqs (11) and (12) are expressing the Goldstone theorem. Therefore, spontaneous breaking of a continuous symmetry is accompanied by appearance of soft modes and enhancement of the amplitude of thermal fluctuations with the small wave vectors.

3. Continuous Symmetry Breaking, Fluctuations and Long Range Order

Consider the simplest case of spontaneous symmetry breaking: a one-dimensional periodic chain of atoms. The density $\rho(x)$ in such a chain is

$$\rho(x) = \frac{m}{a} \sum_{n=-\infty}^{+\infty} \delta(x - na - u_n), \qquad (13)$$

where m is the mass of an atom, a is the lattice constant and u_n denotes the displacement of the n-th atom from $x = na$. The density (13) corresponds to the symmetry breaking and, if the free energy $F\{u_n\}$ for displacements u_n independent on n is the same as for $u_n = 0$. Therefore, in the continuous limit[2], the free energy is equal to

$$F = F_0 + \frac{s^2}{2} \int dx \left(\frac{\partial u(x)}{\partial x} \right)^2 = F_0 + \int \frac{dk}{2\pi} \frac{s^2\ k^2}{2} |u(k)|^2 \quad (14)$$

We see here that the spontaneous breaking of symmetry, which fixes position of our chain in space, is accompanied by presence of soft mode of elastic deformation. Finite temperature T leads to thermal fluctuations. As the result, the relative displacements $u(x)$ and $u(0)$ of two distant atoms grows with their separation x:

$$\langle [u(x) - u(0)]^2 \rangle = \frac{\int \mathcal{D}u(z)\, [u(x) - u(0)]^2 \exp\{-F/T\}}{\int \mathcal{D}u(z) \exp\{-F/T\}} =$$

[2]In the continuous limit, $u(x)$ is the function, which takes values u_n at $x = na$.

$$\frac{T}{s^2}\int\frac{dk}{2\pi}\,\frac{1-\cos kx}{k^2}=\frac{T}{2s^2}\;|x|. \tag{15}$$

If an experiment with the X-ray scattering with wave vector transfer $b = 2\pi l/a$ is conducted in order to obtain the Bragg-type of diffraction pattern, the intensity of obtained patter is proportional to the square of the form-factor

$$f_b = \langle|\sum_n e^{ib(an+u_n)}|^2\rangle = \langle|\sum_n e^{ibu_n}|^2\rangle \tag{16}$$

The measure of the long range order is determined by the space dependent form-factor

$$\begin{aligned} f_b(x) &= \langle e^{ibu(x)}e^{-ibu(0)}\rangle = \exp\left\{-\frac{b^2\langle[u(x)-u(0)]^2\rangle}{2}\right\} \\ &= \exp\left\{-\frac{Tb^2}{4s^2}\;|x|\right\} \end{aligned} \tag{17}$$

Eq (17) shows that the termal fluctuation lead to destruction of the long range order in a one-dimensional chain and the correlation radius ξ - determined by taking $b = 2\pi/a$ - is

$$\xi(T)=\left(\frac{sa}{\pi}\right)^2\;\frac{1}{T} \tag{18}$$

One can repeat the consideration of the effect of thermal fluctuation on long range order in 2D and 3D solids, as well as in different systems with spontaneous symmetry breaking: cholesteric and smectic liquid crystals, ferromagnet and anti-ferromagnet at different dimensions, etc.

4. Effect of Fluctuations near Transition Point. Upper Critical Dimension

Let us return to the case, when the varying in space order parameter $\eta(x)$ is just a scalar function. In this case, at $T < T_c$ only the discrete symmetry $\eta \to -\eta$ is broken, and there is no soft modes at $T \ll T_c$. Nevertheless, as one could see from Eq (5), there is a soft mode small wave vectors $\mathbf{k}$ and $\alpha = \alpha' \ (T - T_c) \to 0$.

In the mean field approximation, at $T > T_c$, the free energy is a constant. Neglecting quartic term in η, obtain the contribution of fluctuations of the soft mode to free energy as

$$\begin{aligned} F &= F_0 - T \ln \int \mathcal{D}\eta(\mathbf{r}) \ \exp\left[-\frac{1}{2T}\int d\mathbf{r}\left(\alpha\eta^2 + s^2 \ (\nabla\eta)^2\right)\right] = \\ &= F_0 + T\int \frac{d^d\mathbf{k}}{(2\pi)^d}\ln\left(\alpha + s^2\mathbf{k}^2\right). \end{aligned} \tag{19}$$

BB Contribution δC of these fluctuation to specific heat

$$C = \frac{\partial}{\partial T} \ (TS) = -\frac{\partial}{\partial T}\left(T\frac{\partial F}{\partial T}\right)$$

is

$$\delta C(T) = T(\alpha')^2 \int \frac{d^d\mathbf{k}}{(2\pi)^d}\frac{1}{(\alpha + s^2\mathbf{k}^2)^2} \tag{20}$$

Eq (20) expresses the leading correction to specific heat beyond the limits of the mean field approximation. The integral in the right-hand side of this equation is taken not over infinite space but over the Brillouin zone of the crystal, i.e. at $k < 1/a$. At space dimensions $d \leq 4$, this integral diverges at $\alpha \to 0$, and

$$\delta C(T) = T(\alpha')^2 \begin{cases} \frac{T}{8\pi}\left(\frac{\alpha'}{s}\right)^{3/2} \frac{1}{\sqrt{T-T_c}}, & d = 3 \\ \frac{T}{16\pi^2}\left(\frac{\alpha'}{s}\right)^2 \ln\left[\frac{s^2}{a^2\alpha'(T-T_c)}\right], & d = 4 \end{cases} \tag{21}$$

It makes sense to compare the fluctuation correction (21) to specific heat with the jump ΔC in specific heat obtained in the frameworks of Landau Theory. This comparison gives

$$\Delta C > \delta C(T), \quad \begin{cases} T - T_c > \frac{1}{(4\pi)^2}\frac{\gamma^2}{\alpha' s^3}, & d = 3 \\ T - T_c > \frac{s^2}{\alpha' a^2} \exp\left[-\frac{\gamma}{8\pi^2 s^2}\right], & d = 4 \end{cases} \tag{22}$$

This means that the Landau theory (and the mean field approximation) are not working very close to the temperature of the phase transition T_c. Since both criteria of Eq (22) include the coefficient γ at the quartic term in Landau expansion, the theory, which gives description of thermodynamics close to transition point must include both dispersion and anharmonism. Dimension $d = 4$, at which the power law divergences of the integral, which determines the fluctuation correction to specific heat, changes from logarithmic, is called the *upper critical dimension* d_c. At $d > 4$, the integral in the right-hand side of Eq (20) converges even at $\alpha = 0$, and, therefore, the Landau theory remains valid up to transition temperature.

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PROBLEMS

P4.1. Long Range Order in Crystals Discuss stability of a Long Range order in:

- **P4.1.A. In 2D Crystal**
- **P4.1.B. in 3D Crystal**
- **P4.1.C. In a layered (Smectic) Crystal**[1]

P4.2. Longitudinal Fluctuation of Magnetisation in a Ferromagnet

[1]The density in a smectic crystal does not depend on two coordinates along the layer and periodically depends on the coordinate in third (perpendicular to the layers) direction

Using the principle of constant modulus, expressed by Eq (12), find the mean square $\langle \mathbf{m}_{\|}(\mathbf{r})\ \mathbf{m}_{\|}(\mathbf{r}')\rangle_{\mathbf{k}=0}$ of fluctuation of magnetisation parallel to magnetic field.
Hint Use the rule

$$\langle \mathbf{m}_{\perp}^2(\mathbf{r})\ \mathbf{m}_{\perp}^2(\mathbf{r}')\rangle_{\mathbf{k}} = 2\int \frac{d\mathbf{q}}{(2\pi)^3}\ \langle \mathbf{m}_{\perp}\ \mathbf{m}_{\perp}\rangle_{\mathbf{k}+\mathbf{q}}\ \langle \mathbf{m}_{\perp}\ \mathbf{m}_{\perp}\rangle_{-\mathbf{q}}$$

P4.3. Upper Critical Dimension at Tricritical Point
At Tricritical point, the density $\mathcal{F}$ of free energy is

$$\mathcal{F} = \frac{s}{2}\ (\nabla\eta)^2 + \frac{c}{3!}\ \eta^6$$

Find the upper critical dimension d_c.