Lecture 16. *Friday 6th December, 2019. Compiled: Saturday 21st December, 2019.*

0.1 Cubic term and first transition

Let us consider more general forms of the Landay free energy. For example, in the case in which the symmetry is not violated, one can consider also odd temrs such as the cubic one. In fact, we want to eneralize to include multicritical points, or phase transitions. The phase transitions can be obtained by introducing a cubic term in the Landau expansion. Remember that in the Ising model we have phase transition derived by symmetry breaking. Now, we have another type of phase transition.

The simplest Landau free energy that depends on a particular field is:

$$\mathcal{L}(\eta, t, h) = at\eta^2 - w\eta^3 + \frac{b}{4}\eta^4 - h\eta \tag{1}$$

where $t \equiv \frac{T-T^*}{2}$ and w is an additional parameter that we fix to be positive, $w > 0$.

Remark. For $w < 0$ the results are the same, but in the $\eta < 0$ diagram.

To satisfy thermodynamic stability we require $b > 0$, while

$$at = \frac{a}{2}(T - T^*) \quad \text{if} \begin{cases} > 0 & T > T^* \\ < 0 & T < T^* \end{cases} \tag{2}$$

The equation of state for $h \neq 0$ is:

$$\frac{\partial \mathcal{L}_G}{\partial \eta} = 0 \quad \Rightarrow h = 2at\eta - 3w\eta^2 + b\eta^3 \tag{3}$$

Let us consider the equilibrium states when $h = 0$:

$$h = 0 \quad \Rightarrow 0 = \eta(2at - 3w\eta + \beta\eta^2) \tag{4}$$

The possible solutions are

$$\begin{cases} \bar{\eta} = 0 & \text{disordered phase} \\ \bar{\eta} = \frac{1}{4b}\left(3w \pm \sqrt{qw^2 - 16abt}\right) & \text{ordered phases} \end{cases} \tag{5}$$

Let us rewrite the 'ordered' solutions as

$$\bar{\eta}_\pm = c \pm \sqrt{c^2 - \frac{at}{b}} \tag{6}$$

where

$$c = \frac{3w}{4b} \tag{7}$$

Note that

$$\bar{\eta}_\pm \in \mathbb{R} \iff c^2 > \frac{at}{b} \quad \Rightarrow \frac{T - T^*}{2} < \frac{c^2 b}{a} \equiv t^{**} \equiv \frac{T^{**} - T^*}{2} \tag{8}$$

It implies:

$$T^{**} = T^* + \frac{2c^2 b}{a} \tag{9}$$

- If $t > t^{**}$ ($\iff T > T^{**}$), we have $\bar{\eta}_\pm \notin \mathbb{R}$. The only real solution is $\bar{\eta} = 0$ that is also the absolute minimum of $\mathcal{L}$. The plot is shown in Figure 1.
- If $t \leq t^{**}$ ($\iff T \leq T^{**}$), we have $\bar{\eta}_\pm = c \pm \sqrt{c^2 - \frac{at}{b}} \in \mathbb{R}$ are both possible solutions. One will be a local maximum and the other a local minimum.

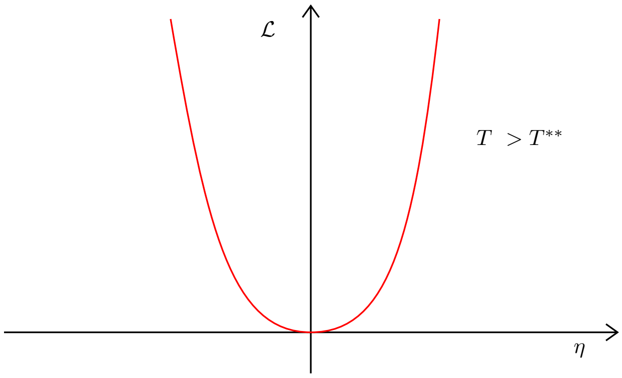

Figure 1: Description.

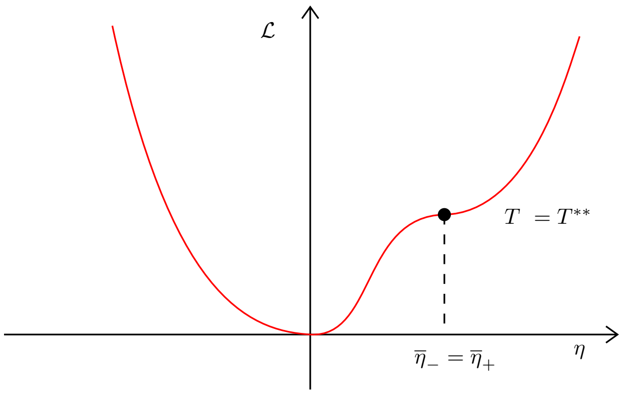

Figure 2: Description.

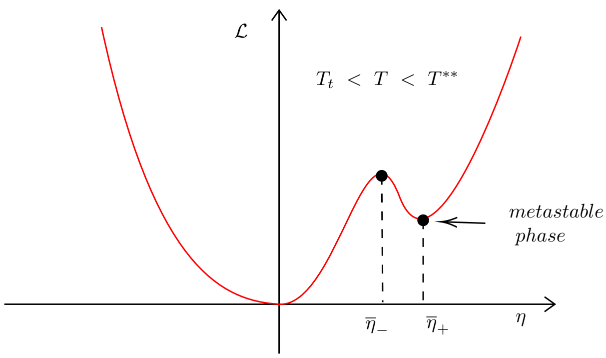

Figure 3: Description.

- At $T = T^{**}$, $\bar{\eta}_- = \bar{\eta}_+$ (flex point), as shown in Figure 2.
- For $T_t < T < T^{**}$, $\mathcal{L}(\bar{\eta}_+) > 0$. Since $\mathcal{L}(\bar{\eta} = 0)$, the solution $\bar{\eta}_+$ is a local minimum, as shown in Figure 3.
- By decreasing T firther one eventually reaches the value $T = T_t$ at which the local minimum $\mathcal{L}(\bar{\eta}_+)$ becomes zero, as in Figure 4. T_t is given by the coexistence condition

$$\mathcal{L}(\bar{\eta}_+) = \mathcal{L}(0) \tag{10}$$

  that is the coexistence between the disordered and ordered phases!

  In the plot of Figure 4 we see that there are two minima in the same line, this is a first order transition. At $T = T_t$ the system undergoes a first

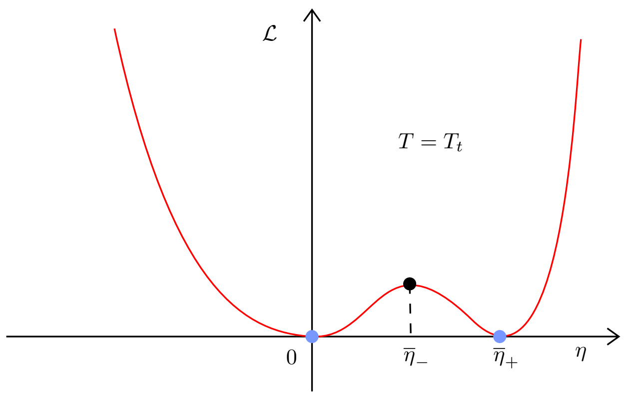

Figure 4: Description.

order transition. To determine T_t we consider

$$\begin{cases} \frac{\partial\mathcal{L}}{\partial\eta} = 0 = \eta\big(2at - 3w\eta + 2b\eta^2\big) & \text{extreme condition} \\ \mathcal{L}(0) = \mathcal{L}(\eta_+) & \text{coexistence condition} \end{cases} \tag{11}$$

$$\Rightarrow \begin{cases} 2at - 3w\eta + 2b\eta^2 = 0 \\ at - w\eta + \frac{b}{2}\eta^2 = 0 \end{cases} \tag{12}$$

Solving with respect to η and t we get

$$\begin{cases} \bar{\eta}_{+t} = +\frac{w}{b} > 0 \\ t_t = \frac{w^2}{2ba} \equiv \frac{1}{2}(T_t - T^*) \end{cases} \tag{13}$$

$$T_t = \frac{w^2}{ba} + T^* \tag{14}$$

Remark. Note that $T_t > T^*$.

Since at $T = T_t$ there is a first order transition does the system display latent heat?

$$s = -\frac{\partial\mathcal{L}}{\partial T}\bigg|_{\eta_t} = -\frac{1}{2}a\bar{\eta}_t^2 = -\frac{a}{2}\left(\frac{w}{b}\right)^2 \tag{15}$$

Remark. There is an entropy jump.

The latent heat adsorbed to go from the ordered to the disordred phase is

$$q = -T_t s = \frac{a}{2}T_t\left(\frac{w}{b}\right)^2 \tag{16}$$

– Finally for $T^* < T < T_t$, $\eta = \bar{\eta}_+$ becomes the global minimum ordered phase is the only stable one (Figure 5).

0.2 Phase stability and behaviour of $\chi_T \equiv \frac{\partial\eta}{\partial h}$

Let us derive the equation of state with respect to h

$$\frac{\partial}{\partial h}\left(\frac{\partial\mathcal{L}_G}{\partial\eta} = 0\right) = \frac{\partial}{\partial h}\big(2at\eta - 3w\eta^2 + 2b\eta^3 = h\big) \tag{17}$$

$$\Rightarrow \chi\big(2at - 6w\eta + 6b\eta^2\big) = 1 \tag{18}$$

The results is

$$\chi_T = \frac{1}{2at - 6w\eta + 6b\eta^2} \tag{19}$$

We now make use of equation (19) to compute the limit of stability of the phases we have found.

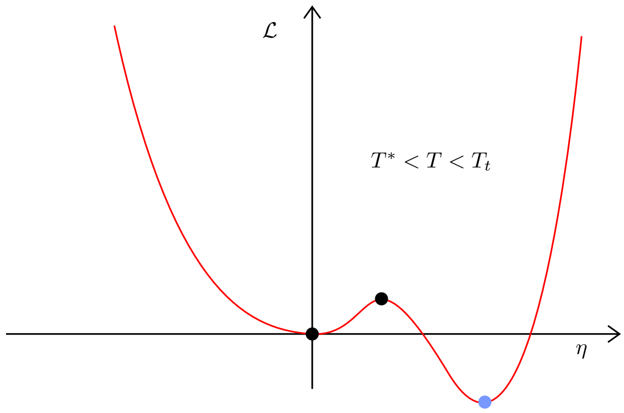

Figure 5: Description.

0.3 lesson

Another possibility is studying multicritical point.

$$\mathcal{L}_h(T, \Delta, \eta) = \frac{a(t, \Delta)}{2}\eta^2 + \frac{b(t, \Delta)}{4}\eta^4 + c\eta^6 - h\eta \tag{20}$$

Consider Δ (Δ_c is a critical value):

- $\Delta < \Delta_c$: as T decreases, it will reach a value, we have a that decreases.

$$T = T_c(\Delta) \Rightarrow \begin{cases} a(T_c, \Delta) = 0 \\ b(T_c, \Delta) > 0 \end{cases} \tag{21}$$

- $\Delta > \Delta_c$: as T decreases, we will have a and b that will decrease too. At that point:

$$b(\bar{T}, \Delta) = 0 \tag{22}$$

  The free energy now is

$$\mathcal{L} = \frac{a}{2}\eta^2 + c\eta^6 \tag{23}$$

  The plot of the free energy is in figure 2. We have the coexistence of three lines.

Tricritical point:

$$\Delta = \Delta_t, \quad T = T_t \tag{24}$$

$$a(\Delta_t, T_t) = b(\Delta_t, T_t) = 0 \tag{25}$$

$$\mathcal{L}_t = c\eta^6 - h\eta \tag{26}$$

As we approach the critical point $T \to T_c$, the correlation length $\xi \sim |T - T_c|^{-\nu}$ diverges.

Maybe mean field is not a very good approximation in proximity of the critical point. Question: how bad is the mean field approximation in proximity of the critical point?

$$\langle S_i S_j \rangle \overset{MF}{\to} \langle S_i \rangle \langle S_j \rangle \tag{27}$$

Calculate the error:

$$E_{ij} = \frac{|\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle|}{\langle S_i \rangle \langle S_j \rangle} \tag{28}$$

Define

$$G_c(i,j) \equiv \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle = \langle (S_i - \langle S_i \rangle)(S_j - \langle S_j \rangle) \rangle \tag{29}$$

If we want to compute the error in the mean field, is always zero. So, if we want calculate the average with respect to fluctuations it does not work. We can either look at the variation in which the field is the internal one, or we can somehow try to make a variation not because of thermal fluctuations but because we control it. We do this by using an external field. This is the response theory with a variation of the field.

In order to do that, instead using an H we use an H_i.

$$Z = \mathrm{Tr}_{\{S\}} \left(e^{-\beta\left(-J\sum_{\langle ij \rangle} S_i S_j - \sum_i H_i S_i\right)} \right) \tag{30}$$

The definition of the thermal average is

$$\langle S_i \rangle = \frac{\mathrm{Tr}_{\{S\}} \left(S_i e^{-\beta\left(-J\sum_{\langle ij \rangle} S_i S_j - \sum_i H_i S_i\right)} \right)}{Z} = \beta^{-1} \frac{\partial \ln Z}{\partial H_i} = -\frac{\partial F}{\partial H_i} \tag{31}$$

$$\langle S_i S_j \rangle = \frac{\beta^{-1}}{Z} \frac{\partial^2 Z}{\partial H_i \partial H_j} \tag{32}$$

$$G_c(i,j) = \beta^{-1} \frac{\partial^2 \ln Z}{\partial H_i \partial H_j} = -\frac{\partial^2 F(\{H_i\})}{\partial H_i \partial H_j} \tag{33}$$

$$\frac{\partial}{\partial H_j} \langle S_i \rangle = \frac{\partial}{\partial H_j} \left[-\frac{\partial F}{\partial H_i} \right] = G_c(i,j) \tag{34}$$

$$M = \sum_i \langle S_i \rangle \tag{35}$$

$$\frac{\partial M}{\partial H_j} = \sum_i \frac{\partial \langle S_i \rangle}{\partial H_j} = \sum_i G_c(i,j) \tag{36}$$

$$H_j = H_j(H) \tag{37}$$

$$\frac{\partial M}{\partial H} = \sum_j \frac{\partial M}{\partial H_j} \frac{\partial H_j}{\partial H} = \beta \sum_{ij} G_c(i,j) \tag{38}$$

the last one is the susceptibility χ_T. Therefore,

$$\chi_T = \beta \sum_{i,j} G_c(i,j) \tag{39}$$

$$G_c(i,j) \to G_c(|i-j|) \sim G(|\vec{\mathbf{r}}|) \tag{40}$$

More or less, we want to compute the total relative error

$$E_{TT} = \frac{\int_{V_\xi} \mathrm{d}^D \vec{\mathbf{r}}\, G_c(r)}{\int_{V_\xi} \mathrm{d}^D \vec{\mathbf{r}}\, \eta^2} \ll 1 \tag{41}$$

This quantity is related to χ_T. Because of the fluctutations we can say that the quantity above is

$$\sim \frac{\beta^{-1} \chi_T}{\int_{V_\xi} \mathrm{d}^D \vec{\mathbf{r}}\, \eta^2} \tag{42}$$

where $\chi_T \sim t^{-\gamma}$ and the denominator it is $\sim t^{2\beta} \xi^D$.

$$\frac{t^{-\gamma}}{t^{2\beta} t^{-\nu D}} \tag{43}$$

$$E \overset{t\to 0}{\sim}{}^{-\gamma-2\beta+\nu D} \ll 1 \tag{44}$$

$$-\gamma - 2\beta + \nu D \geq 0 \Rightarrow D > \frac{\gamma + 2\beta}{\nu} \tag{45}$$

this is called the *Ginzburg criterium*.

In the mean field we have: $\gamma = 1$, $\beta = 1/2$. We obtain:

$$D > \frac{2}{\nu} \tag{46}$$

We have $\nu_{MF} = 1/2$. THerefore the dimension is $D > 4$ for the mean field. The

$$D_c = \frac{\gamma + 2\beta}{2} \tag{47}$$

is called *upper critical dimension*.

Now we have a lower critical dimension (remember the last lessons!!) and an upper one.