HH0034 Landau Theory of Phase Transitions

Landau constructed a systematic formulation to describe all sorts of phase transitions within mean-field approximation. The key is to introduce the notion of order parameter ξ, which can be magnetization in ferromagnetic transition, dielectric polarization in ferroelectric systems, fraction of superconducting electrons in a superconductor and so on.

⓪ Landau free energy function:

Consider a phase transition for the order parameter ξ with Z_2 symmetry (i.e. $\xi \leftrightarrow -\xi$ symmetry). The Landau free energy function is

$$F_L(\xi,\tau) \equiv U(\xi,\tau) - \tau\sigma(\xi,\tau)$$

The equilibrium value $\xi_0(\tau)$ minimizes F_L and the free energy is

$$\boxed{F(\tau) = F_L(\xi_0,\tau) \leq F_L(\xi,\tau)}$$

$F_L(\xi,\tau)$ can tell us $\xi_0(\tau)$ and $F(\tau)$!

OK, this sounds great but how can we get $F_L(\xi,\tau)$? Near the phase transition, Landau assumes $F_L(\xi,\tau)$ can be expanded,

$$\boxed{F_L(\xi,\tau) = F_0 + \frac{1}{2}a(\tau-\tau_0)\xi^2 + \frac{1}{4}b\xi^4 + \frac{1}{6}c\xi^6 + \cdots\cdots}$$

In general, f_0, a, b, c are smooth functions of temperature and can be treated as constant. The $(\tau-\tau_0)$ factor needs some physical insight.

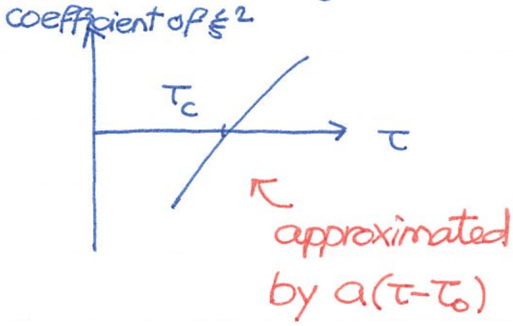
Think...

$$\begin{cases} \tau > \tau_c, & \text{we want } \xi_0 = 0 \\ \tau < \tau_c, & \text{we expect } \xi_0 \neq 0 \end{cases}$$

Coefficient of ξ^2 should be positive

coefficient of ξ^2 should be negative.

The previous argument means the coefficient of ξ^2 changes sign when crossing $\tau=\tau_c$. Although the motivation is justified and the critical temperature of the second-order phase transition is indeed $\tau_c=\tau_0$. But, for the first-order phase transition, the transition temperature $\tau_t \neq \tau_0$ in general.

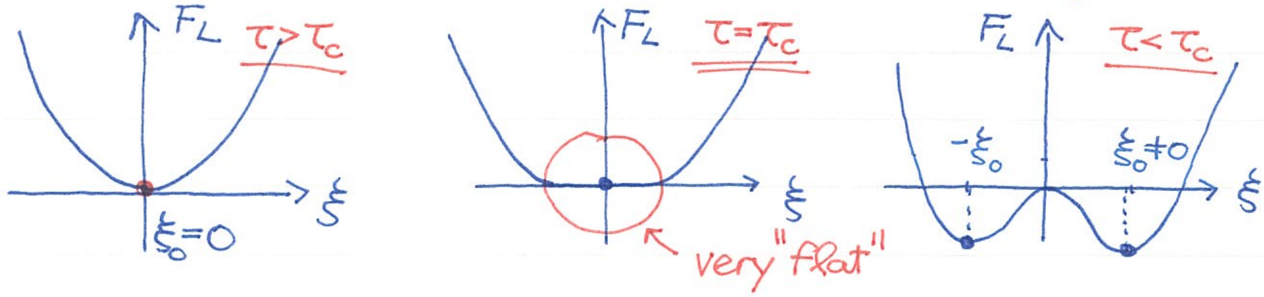


② 2^{nd}-order phase transition.

For $b>0$, it is not necessary to include higher-order terms,

$$\boxed{F_L(\xi,\tau) = F_0 + \frac{1}{2}a(\tau-\tau_0)\xi^2 + \frac{1}{4}b\xi^4}$$

introduce $\tau_c=\tau_0$



The profiles of $F_L(\xi,\tau)$ are shown above. For $\tau>\tau_c$, there is only one minimum $\xi_0=0$. For $\tau<\tau_c$, there are two minima $\pm\xi_0\neq 0$ (related by Z_2 symmetry). At the critical point, the ξ^2-term vanishes and the profile is very "flat".

$$\frac{\partial F_L}{\partial \xi}=0 \longrightarrow a(\tau-\tau_0)\xi_0+b\xi_0^3=0$$

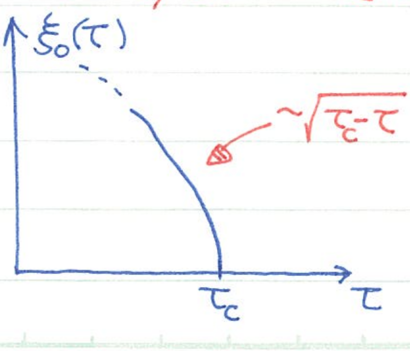
$$\boxed{\xi_0=\pm\sqrt{\frac{a(\tau_c-\tau)}{b}}}$$

only for $\tau<\tau_c$!

Substitute ξ_0 into F_L to get $F(\tau)$:

$$\boxed{F(\tau)=\begin{cases} F_0, & \tau>\tau_c \\ F_0-\dfrac{a^2}{4b}(\tau_c-\tau)^2, & \tau<\tau_c \end{cases}}$$

emergent order $\xi_0\neq 0$ stablize the system!



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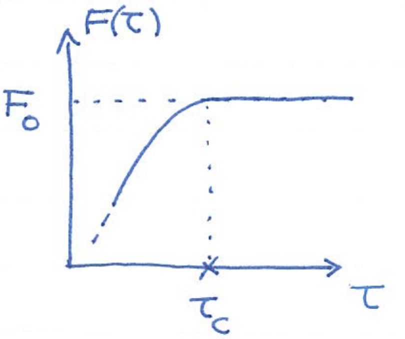


It's obvious that $F(\tau)$ is continuous. What about its derivatives?

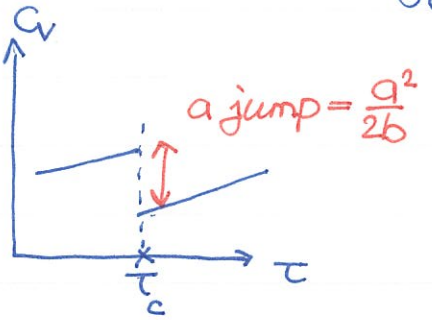
$$\frac{\partial F}{\partial \tau} = -\sigma = \begin{cases} 0 & \tau > \tau_c \\ \frac{a^2}{2b}(\tau_c - \tau) & \tau < \tau_c \end{cases}$$

The 1^{st} derivative is still continuous. It implies the latent heat is zero:

$$\boxed{L = \tau_c \Delta\sigma = \tau_c\left[\sigma(\tau_c^+) - \sigma(\tau_c^-)\right] = 0}$$

Let's compute the second derivative ☺

$$\frac{\partial^2 F}{\partial \tau^2} = -\frac{\partial \sigma}{\partial \tau} = -\frac{1}{\tau} C_V = \begin{cases} 0, & \tau > \tau_c \\ -a^2/2b, & \tau < \tau_c \end{cases}$$



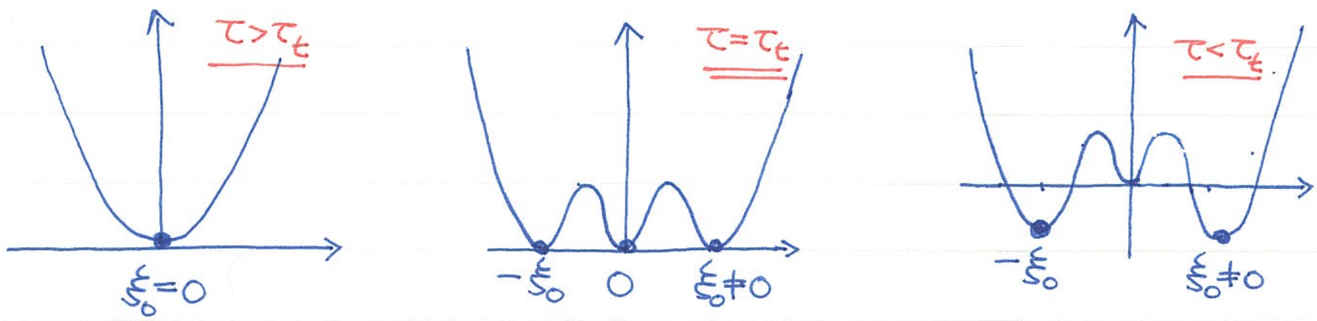
Thus, the specific heat has a jump crossing $\tau = \tau_c$. Because $\frac{\partial^2 F}{\partial \tau^2}$ is singular, it is called the 2^{nd} order phase transition.

② 1^{st} order phase transition:

When $b < 0$, one must include ξ^6 term to ensure stability.

$$\boxed{F_L(\xi, \tau) = F_0 + \frac{1}{2}a(\tau - \tau_0)\xi^2 - \frac{1}{4}|b|\xi^4 + \frac{1}{6}c\,\xi^6}$$

The evolution of $F_L(\xi, \tau)$ profiles is different:



One can follow the same logic to compute ξ_0:

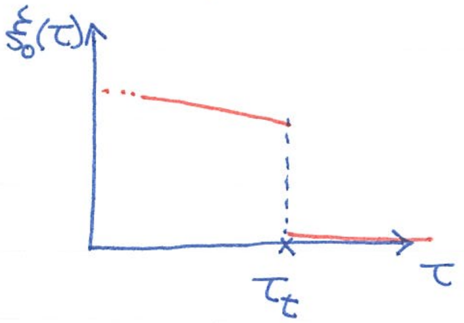
$$\frac{\partial F_L}{\partial \xi} = 0 \longrightarrow a(\tau - \tau_0)\xi_0 - |b|\xi_0^3 + c\,\xi_0^5 = 0$$

for $\tau \le \tau_t$ case.

$$\boxed{\xi_0^2 = \frac{1}{2c}\left[|b| + \sqrt{b^2 - 4ac(\tau - \tau_0)}\right]}$$

The other root corresponds to the local max.

If one plots the order parameter ξ, it is clear to see a jump.



The transition temperature τ_t can be computed,

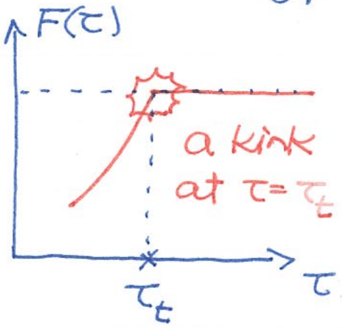
$$\boxed{F_L(\xi_0=0, \tau_t) = F_L(\xi_0\neq 0, \tau_t)}$$

After some algebra,

transition temp

$$\tau_t = \tau_0 + \frac{3b^2}{16ac}$$

The free energy can be computed as well and is plotted below.



$$\sigma(\tau_t^+) - \sigma(\tau_t^-) = \Delta\sigma = -\left[\frac{\partial F}{\partial \tau_+} - \frac{\partial F}{\partial \tau_-}\right] > 0$$

Thus, the latent heat is not zero.

$$\boxed{L = \tau_t \Delta\sigma > 0}$$

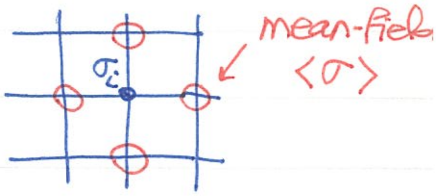
Since $\partial F/\partial\tau$ is already singular, it's called the 1st order phase transition

⊘ Revisit Ising model.

It is helpful to revisit the Ising model discussed before.

The energy of a spin at site i is

$$E_i = {\sum_j}' \langle\sigma_j\rangle\sigma_i \cdot (-\varepsilon) = -\varepsilon z \langle\sigma\rangle \sigma_i$$



The average energy of the whole system is

$$\boxed{U = \langle E\rangle = \frac{1}{2}\sum_i \langle E_i\rangle = -\frac{N}{2}\varepsilon z m^2}$$

$m = \langle\sigma\rangle$ to avoid confusion with entropy σ.

For given spin polarization $m = \langle\sigma\rangle$, the probability distribation is quite simple:

$\uparrow$ $\quad$ $\downarrow$

$P_\uparrow = \frac{1+m}{2}$ $\quad$ $P_\downarrow = \frac{1-m}{2}$

The corresponding entropy for one spin is

$$\boxed{\begin{aligned}\sigma_1 &= -\sum_s P_s \log P_s \\ &= -\left(\frac{1+m}{2}\right)\log\left(\frac{1+m}{2}\right) - \left(\frac{1-m}{2}\right)\log\left(\frac{1-m}{2}\right)\end{aligned}}$$

Treating m as order parameter, the Landau free energy function is

$$F(m,\tau) = U(m,\tau) - \tau\sigma(m,\tau)$$

$\tau_c = \varepsilon z$ critical temperature

$$= -\frac{N}{2}\tau_c m^2 + \underbrace{N\tau\left(\frac{1+m}{2}\right)\log\left(\frac{1+m}{2}\right) + N\tau\left(\frac{1-m}{2}\right)\log\left(\frac{1-m}{2}\right)}_{\text{just add up all spins} \to N \text{ times } \sigma_1}$$

Expand $F(m,\tau)$ near $m=0$, one gets the following series,

$$\boxed{F(m,\tau) = \frac{N}{2}(\tau-\tau_c)m^2 + \frac{N}{12}\tau m^4 + O(m^6)}$$

Landau is smart to get the form right with doing actual calculations ☺

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