Landau-Ginzburg approach

Order parameter may vary slowly in space to represent a fluctuation from a perfectly ordered system.

free energy functional — general d-dimensional space

$$F[m(\vec{r})] = \int d^d r \left\{ a m^2 + b m^4 + c|\vec{\nabla} m|^2 \right\}$$

where $a = a_0(T - T_c)$ vanishes at T_c as before

$b =$ constant

$c =$ constant — measures stiffness to spatial variations in $m(\vec{r})$.

Consider small fluctuations away from the mean field solution m_0. $m_0 = 0$ for $T > T_c$, $m_0 = \sqrt{\frac{a_0(T_c - T)}{2b}}$ for $T < T_c$

$m(\vec{r}) = m_0 + \delta m(\vec{r})$ expand F to $O(\delta m^2)$

$$F[m(\vec{r})] = \int d^d r \{ a m_0^2 + 2 a m_0 \delta m + a\,\delta m^2 + b m_0^4 + 4 b m_0^3 \delta m + 6 b m_0^2 \delta m^2 + c|\vec{\nabla}\delta m|^2 \}$$

the constant terms $a m_0^2 + b m_0^4$ give the mean field free energy.

the linear terms $(2 a m_0 + 4 b m_0^3)\delta m$ vanish because m_0 minimizes F.

The remaining quadratic terms are

$$\delta F = \int d^d r \left\{ \left[a + 6 b m_0^2 \right] \delta m^2 + c \, |\vec{\nabla} \delta m|^2 \right\}$$

$\uparrow$ integral is over vol L^d $\qquad$ let $a' \equiv a + 6 b m_0^2$

Fourier transforms

$$\delta m(\vec{r}) = \frac{1}{L^{d/2}} \sum_{q} e^{i \vec{q} \cdot \vec{r}} \, \delta m_q$$

sum over all q s.t. $q_\mu = \frac{2\pi n_\mu}{L}$, n_μ integer

$$\delta m_q = \frac{1}{L^{d/2}} \int d^d r \, e^{-i \vec{q} \cdot \vec{r}} \, \delta m(\vec{r})$$

Then

$$\delta F = \frac{1}{L^{d/2}} \frac{1}{L^{d/2}} \sum_{q} \sum_{q'} \left[a' - c \, \vec{q} \cdot \vec{q}\,' \right] \delta m_q \, \delta m_{q'} \times \underbrace{\int d^d r \, e^{i (\vec{q} + \vec{q}\,') \cdot \vec{r}}}_{L^d \delta(\vec{q} + \vec{q}\,')}$$

$$\boxed{\delta F = \sum_{q} \left[a' + c q^2 \right] \delta m_q \, \delta m_{-q}}$$

Correlation function

To average over fluctuations we should compute the partition function averaged over $\delta m(\vec{r})$

$$Z = \prod_{r} \int_{-\infty}^{\infty} d\delta m(\vec{r})\; e^{-\beta \delta F[\delta m(\vec{r})]}$$

integrate over all values of $\delta m(\vec{r})$

$$= \prod_{q} \int d\delta m_q\; e^{-\beta \delta F[\delta m_q]}$$

transform integration from $\delta m(\vec{r})$ to δm_q

Note; δm_q is complex $\Rightarrow \delta m_q = \underbrace{\delta m_{q1}}_{\text{real part}} + \underbrace{i\delta m_{q2}}_{\text{complex part}}$

Since $\delta m(\vec{r})$ is real, $\delta m_q^* = \delta m_{-q}$, so δm_q and δm_q^* are not independent. When we integrate over δm_q we should integrate over real values δm_{q1} and δm_{q2} but restrict q to $q_z > 0$ so as not to double count δm_q and δm_{-q}.

$$Z = \prod_{\substack{q \\ \text{st } q_z > 0}} \int_{-\infty}^{\infty} d\delta m_{q1} \int_{-\infty}^{\infty} d\delta m_{q2}\; e^{-\beta \delta F[\delta m_{q1} + i\delta m_{q2}]}$$

Now ~~Note~~: $\langle \delta m_q \delta m_{-q} \rangle = \langle \delta m_{q1}^2 + \delta m_{q2}^2 \rangle$

$$= \frac{\int d\delta m_{q1} \int d\delta m_{q2}\; e^{-\beta[a' + cq^2](\delta m_{q1}^2 + \delta m_{q2}^2)} (\delta m_{q1}^2 + \delta m_{q2}^2)}{\int d\delta m_{q1} \int d\delta m_{q2}\; e^{-\beta[a' + cq^2](\delta m_{q1}^2 + \delta m_{q2}^2)}}$$

$$= \frac{k_B T}{a' + cq^2}$$ doing the Gaussian integrals

Real space correlation function is then

$$\langle \delta m(\vec{r})\, \delta m(0) \rangle = \frac{1}{L^{d/2}} \frac{1}{L^{d/2}} \sum_{q} \sum_{q'} e^{i\vec{q}\cdot\vec{r}} \langle \delta m_q\, \delta m_{q'} \rangle$$

$$= \frac{1}{L^d} \sum_{q} e^{i\vec{q}\cdot\vec{r}} \langle \delta m_q\, \delta m_{-q} \rangle$$

$$= \frac{1}{L^d} \sum_{q} e^{i\vec{q}\cdot\vec{r}} \frac{k_B T}{a' + cq^2}$$

$$= \int \frac{d^d q}{(2\pi)^d} e^{i\vec{q}\cdot\vec{r}} \frac{k_B T}{a' + cq^2}$$

$$\sim \frac{e^{-r/\xi}}{r^{d-2}} \quad \text{Ornstein - Zernike form}$$

where $\xi = \sqrt{\frac{c}{a'}}$ is the "correlation length"

gives length scale over which fluctuations $\delta m(\vec{r})$ decay

Result comes from the integrand having its poles at $\pm i \sqrt{a'/c} = q$

For $T > T_c$, $a' = a$ since $m_0 = 0$

$$= a_0 (T - T_c)$$

$$\xi \sim \frac{1}{\sqrt{a'}} \sim \frac{1}{\sqrt{T - T_c}} \sim \frac{1}{|t|^{\nu}} \quad \text{with } \nu = 1/2$$

ν is correlation length exponent

For $T<T_c$, $a' = a + 6bm_0^2$

$$= a_0(T-T_c) + 6b\left(\frac{a_0(T_c-T)}{2b}\right)$$

$$= 2a_0(T_c-T)$$

$$\xi \sim \frac{1}{\sqrt{a'}} \sim \frac{1}{\sqrt{T_c-T}} \sim \frac{1}{|t|^{\nu}} \quad \text{with } \nu = 1/2$$

As $T \to T_c$ the correlation length diverges

Since fluctuations propagate out a distance ξ

$\Rightarrow$ fluctuations can be important at critical point!

<u>Contribution of fluctuations</u> to the total free energy

$$\delta F = \sum_q \left[a' + cq^2\right] \delta m_q \delta m_{-q}$$

$$Z = \prod_{\substack{q \\ \text{st } q_3>0}} \int_{-\infty}^{\infty} d\delta m_{q_1} \int_{-\infty}^{\infty} d\delta m_{q_2}\, e^{-\beta[a'+cq^2](\delta m_{q_1}^2 + \delta m_{q_2}^2)}$$

$$= \prod_{\substack{q \\ \text{st. } q_3>0}} \left[\frac{2\pi k_B T}{2(a'+cq^2)}\right]$$

$$\delta G = -k_B T \ln Z = -k_B T \sum_{\substack{q \\ \text{st } q_3>0}} \ln\left(\frac{\pi k_B T}{a'+cq^2}\right)$$

$$= \frac{-k_B T}{2} \sum_q \ln\left(\frac{\pi k_B T}{a'+cq^2}\right) = \frac{-k_B T L^d}{2} \int \frac{d^d q}{(2\pi)^d} \ln\left(\frac{\pi k_B T}{a'+cq^2}\right)$$

all q – add in $q_3<0$ and compensate with prefactor of $1/2$

Contribution to specific heat per volume δC

$$\delta C = -\frac{T}{L^d}\frac{\partial^2 \delta G}{\partial T^2}$$

Consider $T > T_c$ so $a' = a_0(T - T_c)$

$$\frac{1}{L^d}\frac{\partial \delta G}{\partial T} = -\frac{k_B}{2}\int \frac{d^dq}{(2\pi)^d} \ln\left(\frac{\pi k_B T}{a' + cq^2}\right)$$

$$- \frac{k_B T}{2}\int \frac{d^dq}{(2\pi)^d}\left\{\frac{1}{T} - \frac{a_0}{a' + cq^2}\right\}$$

τ comes from T dependence of $a' = a_0(T - T_c)$

$$\frac{1}{L^d}\frac{\partial^2 \delta G}{\partial T^2} = -\frac{k_B}{2}\int \frac{d^dq}{(2\pi)^d}\left\{\frac{1}{T} - \frac{a_0}{a' + cq^2}\right\}$$

$$+ \frac{k_B}{2}\int \frac{d^dq}{(2\pi)^d}\left\{\frac{a_0}{a' + cq^2}\right\}$$

$$- \frac{k_B T}{2}\int \frac{d^dq}{(2\pi)^d}\left\{\frac{a_0^2}{(a' + cq^2)^2}\right\}$$

$$\delta C = \frac{k_B}{2}\int \frac{d^dq}{(2\pi)^d}\left\{1 - \frac{2T a_0}{a' + cq^2} + \frac{T^2 a_0^2}{(a' + cq^2)^2}\right\}$$

this gives classical $\frac{1}{2}k_B$ per degree freedom

corrections due to T-dependence of $a(T)$ in δF

To see how the integrals behave as $T \to T_c$

$I_1 = \int d^d q \, \frac{a_0}{a_0 t + c q^2}$ where $t = T - T_c$

let $q^2 = t q'^2$

$I_1 = t^{d/2} \int d^d q' \, \frac{a_0}{a_0 t + c t q'^2} = t^{\frac{d}{2}-1} \underbrace{\int d^d q' \, \frac{a_0}{a_0 + c q'^2}}_{\text{just some number}}$

$I_1 \sim t^{\frac{d}{2}-1} = t^{\frac{d-2}{2}} \propto \xi^{2-d}$

(since $\xi \sim t^{-1/2}$)

Similarly

$I_2 = \int d^d q \, \frac{a_0^2}{(a_0 t + c q^2)^2} \propto t^{\frac{d}{2}-2} = t^{\frac{d-4}{2}} \propto \xi^{4-d}$

The second integral is the more singular one

For mean field theory to be valid as $T \to T_c$, we want the correction δC to be small compared to C_{MF} the mean field value.

In mean field theory, $C_{MF} \sim$ finite at T_c

$$\delta C \sim t^{\frac{d-4}{2}}$$

δC will diverge whenever $d < 4$

$\to$ $d > 4 \Rightarrow$ fluctuations negligible
mean field theory gives correct critical exponents

$d < 4 \to$ fluctuations give singular corrections
mean field theory breaks down
$\Rightarrow$ Renormalization Group approach.

$d_c = 4$ is called the <u>upper critical dimension</u>
the value of d_c can vary with the symmetry of $F[m(r)]$.
$d_c = 4$ for spherically symmetric n component spin models
mean field theory is OK only when $d > d_c$

Also a <u>lower critical dimension</u> – depends on n
For $d <$ lower critical dimension, there is no phase transition at finite temperature