Lecture 7: Calculating S(k)

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$$Z_c[J] = Z_1 \int D\omega \, e^{-\mathcal{H}[\omega, J]}$$

$$\mathcal{H} = \frac{1}{2u_0}\int dr [\omega(r)]^2 - n \log Q[\mu]$$

$$\mu(r) = i\omega(r) + J(r)$$

$$= i\left(\omega_* + \varepsilon(r)\right) + J(r)$$

At mean-field: $\frac{\delta \mathcal{H}}{\delta \omega} = 0 \Rightarrow \boxed{\frac{\omega(r)}{u_0} + i\tilde{\rho}(r)}$

If $J=0$: $\omega_* = \underline{-i u_0 \frac{nN}{V}}$

For $J(r) \neq 0$, use MF + WTE

$$\tilde{\rho}(r) \approx \frac{nN}{V}\left(1 - N\int dr' g_0(r-r')\underline{[i\varepsilon(r')} + J(r')]\right)$$

$\mathcal{F}$

$$\hat{\rho}(k) = \frac{nN}{V}\left(\delta(k) - N\hat{g}_D(k)\left(i\hat{\varepsilon}(k) + \hat{J}(k)\right)\right)$$

Mean-field equation:

$$\frac{\omega(r)}{u_0} + i\tilde{\rho}(r) = 0$$

$$\frac{\omega_* + \varepsilon(r)}{u_0} + i\frac{nN}{V}\left[1 - N\int dr' g_D(r-r')[i\varepsilon(r') + J(r')]\right] = 0$$

$$= \cancel{\frac{-iu_0\frac{nN}{V}}{u_0}} + \frac{\varepsilon(r)}{u_0} + \cancel{i\frac{nN}{V}} - i\frac{nN^2}{V}\int dr' g_D(r-r')[i\varepsilon(r') + J(r')]$$

$\mathcal{F}$

$$\frac{\hat{\varepsilon}(k)}{u_0} - i\frac{nN^2}{V}\hat{g}_D(k)\left(i\hat{\varepsilon}(k) + \hat{J}(k)\right) = 0$$

$\rho_0 = \frac{nN}{V}$

$$\hat{\varepsilon}(k) + \rho_0 u_0 N \hat{g}_0(k)\hat{\varepsilon}(k) - i\rho_0 u_0 N \hat{g}_0(k)\hat{J}(k) = 0$$

$$\hat{\varepsilon}(k) = \frac{i u_0 \rho_0 N \hat{g}_0(k)}{1 + u_0 \rho_0 N \hat{g}_0(k)} \hat{J}(k)$$

Plug into $\mathcal{H}$, Q to derive $A[J]$

$$\mathcal{H} = \frac{1}{2u_0}\int dr \, \underline{[-iu_0\rho_0 + \varepsilon(r)]}^2 - n \log Q$$

$$\frac{1}{2u_0}\int dr \left(-u_0^2\rho_0^2 - 2iu_0\rho_0\varepsilon(r) + \varepsilon^2(r)\right)$$

$$= -\frac{u_0^2\rho_0^2}{2u_0} V - 0 + \frac{1}{2u_0}\int dr [\varepsilon(r)]^2$$

$$= \frac{-u_0\rho_0^2 V}{2} + \frac{1}{2u_0 V}\underline{\sum_k \hat{\varepsilon}(k)\hat{\varepsilon}(-k)}$$

$$Q[\omega] = e^{-\omega_* N}\left[1 + \frac{N^2}{2V^2}\sum_k \hat{\varepsilon}(k)\hat{\varepsilon}(-k)\hat{g}_0(k)\right]$$

$$\omega(r) = \omega_* + \varepsilon(r)$$

Everywhere: $\omega_* \to i\omega_*$ $\quad \hat{\varepsilon}(k) \to i\hat{\varepsilon}(k) + \hat{J}(k)$

$$Q = e^{-i\omega_* N}\left[1 + \frac{N^2}{2V^2}\sum_k \left(i\hat{\varepsilon}(k) + \hat{J}(k)\right)\left(i\hat{\varepsilon}(-k) + \hat{J}(-k)\right)\hat{g}_0(k)\right]$$

$$-n\log Q = -n[-i\omega_* N] - n\log\left[1 + \frac{N^2}{2V^2}\sum_k \text{''} \quad \text{''} \quad \text{''}\right]$$

$\omega_* = -iu_0\rho_0$

$\log(1+x) \approx x$

$$-n\log Q \approx n N u_0 \rho_0 V - \frac{\rho_0 N}{2V}\sum_k \left(i\hat{\varepsilon}(k) + \hat{J}(k)\right)\left(i\hat{\varepsilon}(-k) + \hat{J}(-k)\right)\hat{g}_0(k)$$

$$-n\log Q \simeq n N u_0 \rho_0 V - \frac{\rho_0 N}{2V}\sum_k \left(i\hat{\varepsilon}(k)+\hat{J}(k)\right)\left(i\hat{\varepsilon}(-k)+\hat{J}(-k)\right)\hat{g}_0(k)$$

Plug back into $\mathcal{H}$:

$$\mathcal{H} = \underbrace{\frac{1}{2}\rho_0^2 u_0}_{\mathcal{H}_0} + \underbrace{\frac{1}{2u_0 V}\sum_k \hat{\varepsilon}(k)\,\hat{\varepsilon}(-k)}_{\text{Term 2}} - \underbrace{\frac{\rho_0 N}{2V}\sum_k \left(i\hat{\varepsilon}(k)+\hat{J}(k)\right)\left(i\hat{\varepsilon}(-k)+\hat{J}(-k)\right)\hat{g}_0(k)}_{\text{Term 3}}$$

Plug in $\hat{\varepsilon}(k) = \dfrac{i u_0 \rho_0 N \hat{g}_0(k)}{1+u_0\rho_0 N\hat{g}_0(k)}\cdot \hat{J}(k)$

Term 2: $$\frac{1}{2u_0 V}\sum_k \left(\frac{i u_0\rho_0 N\hat{g}_0(k)}{1+u_0\rho_0 N\hat{g}_0(k)}\right)^2 \hat{J}(k)\,\hat{J}(-k)$$

$$= \frac{1}{2u_0 V}\sum_k \frac{-u_0^2\rho_0^2 N^2 g_0^2(k)}{(1+u_0\rho_0 N\hat{g}_0(k))^2}\hat{J}(k)\,\hat{J}(-k)$$

Term 3:

$$-\frac{\rho_0 N}{2V}\sum_k \underset{\times\,\hat{g}_0(k)}{\hat{J}(k)}\,\hat{J}(-k)\left(\left[\cancel{i}\,\frac{-\cancel{i}\,u_0\rho_0 N\hat{g}_0(k)}{(1+u_0\rho_0 N\hat{g}_0(k))}+1\right]\left[\cancel{i}\,\frac{\cancel{-i}\,u_0\rho_0 N\hat{g}_0(k)}{1+u_0\rho_0 N\hat{g}_0(k)}+1\right]\right)$$

$$= -\frac{\rho_0 N}{2V}\sum_k \left\{\frac{u_0^2\rho_0^2 N^2\hat{g}_0^2}{(1+u_0\rho_0 N\hat{g}_0)^2} - \frac{2u_0\rho_0 N\hat{g}_0(k)}{1+u_0\rho_0 N\hat{g}_0(k)}+1\right\}\hat{g}_0\,\hat{J}(k)\,\hat{J}(-k)$$

Common denominator, cancel terms:

$$= -\frac{\rho_0 N}{2V u_0}\sum_k \frac{u_0\,\hat{g}_0(k)}{(1+u_0\rho_0 N\hat{g}_0(k))^2}\hat{J}(k)\,\hat{J}(-k)$$

$$= -\frac{1}{2u_0 V}\sum_k \frac{\rho_0 N u_0\,\hat{g}_0(k)}{(1+u_0\rho_0 N\hat{g}_0(k))^2}\hat{J}(k)\,\hat{J}(-k)$$

Term 2 + 3 ...

$$\ldots \sum_k (1+u_0\rho_0 N g_0(k))^2$$

Term 2+3:

$$\frac{-1}{2u_0V}\sum_k \frac{\rho_0 u_0 N\hat g_0(k)\,\cancel{(1+\rho_0u_0N\hat g_0(k))}}{(1+u_0\rho_0N\hat g_0(k))^{\cancel{2}}}\,\hat J(k)\,\hat J(-k)$$

Finally, we get for $\mathcal{H}$:

$$\mathcal{H} = \mathcal{H}_0 + \frac{-1}{2\cancel{u_0}V}\sum_k \frac{\cancel{u_0}\rho_0 N\hat g_0(k)}{1+u_0\rho_0N\hat g_0(k)}\,\hat J(k)\,\hat J(-k)$$ 5.24 in ETIP

$$= A[J]$$

$$\frac{\delta\mathcal{H}}{\delta J(r)} = \langle\hat\rho(r)\rangle \qquad \frac{\delta\mathcal{H}}{\delta\hat J(k)} = \hat\Delta\rho(k)$$

$$\frac{\delta\mathcal{H}}{\delta\hat J(k)} = \frac{-\rho_0N\hat g_0(k)}{1+u_0\rho_0N\hat g_0(k)}\,\hat J(k) = \hat\Delta\rho(k)$$

$$\hat J(k) = \frac{-(1+u_0\rho_0N\hat g_0(k))}{\rho_0N\hat g_0(k)}\,\hat\Delta\rho(k)$$

$$F[\hat\Delta\rho] = A[J] - \frac{1}{V}\sum_k \hat J(k)\,\hat\Delta\rho(-k)$$

$$= \mathcal{H}[\omega,J] - \frac{1}{V}\sum_k \hat J(k)\,\hat\Delta\rho(-k)$$

$$= \frac{-1}{2V}\sum_k \frac{\rho_0N\cancel{\hat g_0(k)}}{\cancel{(1+u_0\rho_0N\hat g_0(k))}}\left(\frac{1+u_0\rho_0N\hat g_0(k)}{\rho_0N\hat g_0(k)}\right)^{\cancel{2}}\hat\Delta\rho(k)\,\hat\Delta\rho(-k)$$

$$+\frac{1}{V}\sum_k \frac{+(1+u_0\rho_0N\hat g_0(k))}{\rho_0N\hat g_0(k)}\,\hat\Delta\rho(k)\cdot\hat\Delta\rho(-k) + \mathcal{H}_0$$

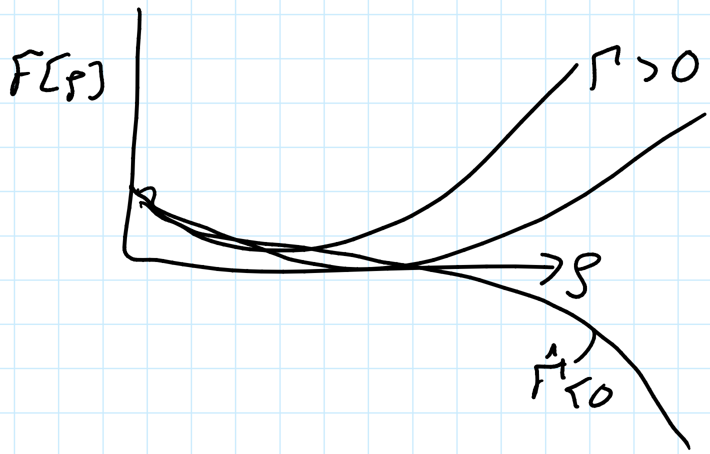
$$F[\hat\Delta\rho] = \mathcal{H}_0 + \frac{1}{2V}\sum_k \underbrace{\left(\frac{1}{\rho_0N\hat g_0(k)} + u_0\right)}_{=\hat\Gamma(k) = \frac{1}{\ldots}}\hat\Delta\rho(k)\,\hat\Delta\rho(-k)$$ ETIP 5.26

$$= \hat{\Gamma}(k) = \frac{1}{S(k)}$$

$$F[\hat{\Delta}_\rho] = \mathcal{F}_0 + \frac{1}{2V}\sum_k \hat{\Gamma}(k)\,\hat{\Delta}_\rho(k)\,\hat{\Delta}_\rho(-k)$$

Since $\hat{g}_D(k)$ is monotonically decreasing

System becomes unstable $\hat{\Gamma}(k=0) < 0$:



When $\Gamma = 0$, $\frac{1}{\rho_0 N g_D(0)} + u_0 = 0$ at the phase boundary

$\uparrow$ $=1$ at $k=0$

System is stable only when $u_0 > \frac{-1}{\rho_0 N}$

For a diblock, $\hat{\Gamma}(k)$ is non-monotonic in k

System goes unstable for $k^* > 0$

$\Rightarrow$ microphase separation on length scales

$$d \sim \frac{2\pi}{k^*}$$