Lecture 5: Weak Inhomogeneity Expansion

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Recall 2 FT properties:

$$\int dr' f(r-r')g(r') = \mathcal{F}^{-1}[\hat{f}(k)\hat{g}(k)]$$

$$\int dr\, f(r)g(r) = \frac{1}{V}\sum_k \hat{f}(k)\hat{g}(-k)$$

Begin w/ homopoly Q:

$$Q = \frac{1}{V}\int d\underline{r}^N e^{-\omega(r_N)}\phi(r_N - r_{N-1})e^{-\omega(r_{N-1})}\cdots\phi(r_2-r_1)e^{-\omega(r_1)}$$

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

$\omega_* =$ M.F. solution

$\varepsilon(r)$: small, spatially varying perturbations

$$\int dr\, \varepsilon(r) = 0$$

$$Q = \frac{e^{-N\omega_*}}{V}\int dr^N e^{-\varepsilon_N}\phi_{N,N-1}e^{-\varepsilon_{N-1}}\cdots\phi_{2,1}e^{-\varepsilon_1}, \qquad \varepsilon_N = \varepsilon(r_N)$$

Taylor expand $e^{-\varepsilon_N} \approx \left(1 - \varepsilon_N + \frac{1}{2}\varepsilon_N^2 + \dots\right)$

$$Q = \frac{e^{-N\omega_*}}{V}\int dr^N\left(1-\underline{\varepsilon_N}+\frac{1}{2}\varepsilon_N^2\right)\phi_{N,N-1}\left(1-\underline{\varepsilon_{N-1}}+\frac{1}{2}\varepsilon_{N-1}^2\right)\cdots$$

After multiplying out, all linear terms in $\varepsilon(r)$ can be ignored $\int dr\, \varepsilon(r) = 0$

$$Q = \frac{e^{-N\omega_*}}{V}\int dr^N\, \Phi(r^N)\left[1 + \frac{1}{2}\varepsilon_N^2 + \varepsilon_N\cdot\varepsilon_{N-1}\dots + \varepsilon_N\varepsilon_1 + \frac{1}{2}\varepsilon_{N-1}^2\right.$$

$$Q = \frac{e}{V} \int dr^N \, \Phi(r^N) \Big[1 + \tfrac{1}{2}\varepsilon_N^2 + \varepsilon_N \cdot \varepsilon_{N-1} \ldots + \varepsilon_N \varepsilon_1 + \tfrac{1}{2}\varepsilon_{N-1}^2$$

$\phi_{N,N-1} \cdot \phi_{N-1,N-2} \ldots$

$$+ \ldots \varepsilon_2 \varepsilon_1 + \tfrac{1}{2}\varepsilon_1^2 \Big]$$

Rewrite the sum:

$$Q = \frac{e^{-\omega_s N}}{V} \int dr^N \, \Phi(r^N) \Big[1 + \frac{1}{2} \sum_{n=1}^{N} \sum_{j=1}^{N} \varepsilon_n \varepsilon_j \Big]$$

$$= \frac{e^{-\omega_s N}}{V} \Big[V + \underline{\frac{1}{2} \sum_{n} \sum_{j} \int dr^N \Phi(r^N) \, \varepsilon_n} \, \varepsilon_j \Big]$$

To see how to evaluate this: examine specific case of $N=5$

$$\frac{1}{2} \sum_{n=1}^{5} \sum_{j=1}^{5} \int dr_5 \, dr_4 \, dr_3 \, dr_2 \, dr_1 \; \phi_{5,4} \, \phi_{4,3} \, \phi_{3,2} \, \phi_{2,1} \; \varepsilon_n \varepsilon_j$$

Pick one term: $n=4$, $j=2$

$$\int dr_5 \ldots dr_1 \; \phi_{5,4} \, \varepsilon_4 \, \phi_{4,3} \, \phi_{3,2} \, \varepsilon_2 \, \phi_{2,1}$$

$$= \int dr_5 \ldots dr_2 \; \phi_{5,4} \, \varepsilon_4 \, \phi_{4,3} \, \phi_{3,2} \, \varepsilon_2 \underbrace{\int dr_1 \, \phi(r_2 - r_1)}_{=1}$$

For a fixed r_2, integrating over r_1

$r_{12} = r_1 - r_2 \qquad dr_{12} = dr_1$

$$\int dr_{12} \, \phi(r_{12}) = 1 \quad \Big(\text{similarly} \int dr_{54} \, \phi_{54} = 1 \Big)$$

$$= \int dr_4 \, dr_3 \, dr_2 \; \varepsilon_4 \, \phi_{4,3} \, \phi_{3,2} \, \varepsilon_2$$

$$= \int dr_4\, \varepsilon_4 \int dr_3\, \phi_{4,3} \underline{\int dr_2\, \phi(r_3 - r_2)\, \varepsilon(r_2)}$$

$$f_1(r_3) = \int dr_2\, \phi(r_3 - r_2)\, \varepsilon(r_2)$$

$$= \mathcal{F}^{-1}\left[\hat{\phi}(k)\hat{\varepsilon}(k)\right]$$

$$= \int dr_4\, \varepsilon_4 \int dr_3\, \phi(r_4 - r_3)\, f_1(r_3)$$

$$f_2(r_4) = \mathcal{F}^{-1}\left[\hat{\phi} \hat{f}_1\right]$$

$$= \mathcal{F}^{-1}\left[\hat{\phi}\hat{\phi}\hat{\varepsilon}\right]$$

$$= \int dr_4\, \varepsilon_4\, f_2(r_4)$$

Use the other FT rule:

$$= \frac{1}{V} \sum_k \hat{\varepsilon}(k)\, \hat{f}_2(-k)$$

$$= \frac{1}{V} \sum_k \hat{\phi}(-k)\, \hat{\phi}(-k)\, \hat{\varepsilon}(k)\, \hat{\varepsilon}(-k)$$

$$\hat{\phi}(k) = e^{-k^2 b^2/6}$$

$$= \frac{1}{V} \sum_k \hat{\phi}(k)^2\, \hat{\varepsilon}(k)\, \hat{\varepsilon}(-k)$$

$$\phi^2(k) = e^{-\frac{k^2 b^2}{6} \cdot 2}$$

4-2: the # of bonds separating m + j on the chain

Each term has the form:

$$\frac{1}{V} \sum_k \hat{\varepsilon}(k)\, \hat{\varepsilon}(-k)\, e^{-\frac{k^2 b^2}{6} |m-j|}$$

$$\frac{1}{V}\sum_k \varepsilon(k)\,\varepsilon(-k)\,e^{\cdots}$$

Plug into Q above:

this was wrong in the live lecture I believe

$$Q=\frac{e^{-w_k N}}{V}\left[V+\frac{1}{2V}\sum_n\sum_j\sum_k \hat{\varepsilon}(k)\,\hat{\varepsilon}(-k)\,e^{-\frac{k^2b^2}{6}|n-k|}\right]$$

$|n-j|$

Now we take continuum limit:

$$\sum_n\sum_j \Rightarrow \int_0^N dn\int_0^N dj$$

$$\int_0^N dn\int_0^N dj\; e^{-\frac{k^2b^2}{6}|n-j|}=\int_0^N dn\int_0^n dj\; e^{-\frac{k^2b^2}{6}(n-j)}+\int_0^N dj\int_0^j dn\; e^{-\frac{k^2b^2}{6}(j-n)}$$

Sum of 2 identical terms:

$$=2\int_0^N dn\int_0^n dj\; e^{-\frac{k^2b^2}{6}(n-j)}$$

$$=2\int_0^N dn\; e^{-k^2b^2/6\cdot n}\cdot\int_0^n dj\; e^{+\frac{k^2b^2}{6}j}$$

$$=2\int_0^N dn\; e^{-\frac{k^2b^2}{6}\cdot n}\,\frac{6}{k^2b^2}\left(e^{\frac{k^2b^2}{6}j}\Big|_{j=0}^{j=n}\right.$$

$$=2\,\frac{6}{k^2b^2}\int_0^N dn\; e^{-\frac{k^2b^2}{6}n}\cdot\left(e^{\frac{k^2b^2}{6}n}-1\right)$$

$$=2\,\frac{6}{k^2b^2}\int_0^N dn\left(1-e^{-\frac{k^2b^2}{6}n}\right)$$

$$=2\,\frac{6}{k^2b^2}\left[N-0+\frac{6}{k^2b^2}\left(e^{-\frac{k^2b^2n}{6}}\Big|_{n=0}^{n=N}\right]$$

$$=\frac{N^2}{\cdots}\,2\left(\frac{6}{k^2b^2}\right)^2\left[N\frac{k^2b^2}{6}+e^{-\frac{k^2b^2N}{6}}-1\right]$$

$$= \frac{N^2}{N^2}\, 2 \left(\frac{6}{k^2 b^2}\right)^2 \left[N \frac{k^2 b^2}{6} + e^{-\frac{k^2 b^2 N}{6}} - 1 \right]$$

$$R_g^2 = N b^2 / 6$$

$$= N^2 \underbrace{\frac{2}{k^4 R_g^4}\left(k^2 R_g^2 + e^{-k^2 R_g^2} - 1\right)}_{\text{Debye function}}$$

$$= N^2 \hat{g}_D(k)$$

Full version of Q

$$Q = e^{-w_A N}\left[1 + \frac{N^2}{2V^2} \sum_k \hat{\varepsilon}(k)\, \hat{\varepsilon}(-k)\, \hat{g}_D(k)\right]$$

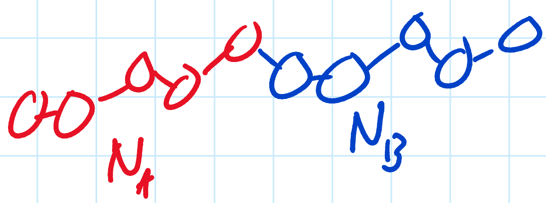
OR in r-space:

$$Q = e^{-w_A N}\left[1 + \frac{N^2}{2V} \underline{\int dr \int dr'}\, \varepsilon(r)\, g_D(r-r')\, \varepsilon(r')\right]$$

Density operator: $\tilde{\rho} = \frac{-n}{Q} \frac{\delta Q}{\delta w(r)}$

$$\tilde{\rho}(r) = \frac{nN}{V} - \frac{nN^2}{V} \int dr'\, \varepsilon(r')\, g_D(r-r')$$

Diblocks



$$f = \frac{N_A}{N}$$

The key difference: A & B experience dif't fields!

$$\omega_A(r) = \omega_A^* + \varepsilon_A^*(r)$$

$$\omega_B(r) = \omega_B^* + \varepsilon_B^*(r)$$

The quadratic term changes:

$$\sum_{m=0}^{N}\sum_{j=0}^{N} \hat{\varepsilon}_m(k)\,\hat{\varepsilon}_j(-k)\, e^{-\frac{k^2b^2}{6}|n-j|}$$

There are three contributions:

$$= 2\sum_{n=1}^{N_A}\sum_{j=1}^{\cancel{N_A}\,m} \hat{\varepsilon}_A(k)\,\hat{\varepsilon}_A(-k)\, e^{-\frac{k^2b^2}{6}(n-j)}$$

$$+ 2\sum_{n=N_A}^{N}\sum_{j=N_A}^{\cancel{N}\,m} \hat{\varepsilon}_B(k)\,\hat{\varepsilon}_B(-k)\, e^{-\frac{k^2b^2}{6}(n-j)}$$

$$+ 2\sum_{m=N_A}^{N}\sum_{j=N_A}^{N} \hat{\varepsilon}_A(k)\,\hat{\varepsilon}_B(-k)\, e^{-\frac{k^2b^2}{6}(j-m)}$$

Integrate & collect terms:

$$Q = e^{-\omega_A^* \cdot N \cdot f}\, e^{-\omega_B^* N(1-f)}$$

$$\cdot \Big[1 - \frac{N^2}{2V}\sum_k \Big(\hat{\varepsilon}_A(k)\,\hat{\varepsilon}_A(-k)\,\hat{g}_D(f,k)$$

$$+ 2\hat{g}_{AB}(f,k)\,\hat{\varepsilon}_A(k)\,\hat{\varepsilon}_B(-k)$$

$$+ \hat{g}_D(1-f,k)\,\hat{\varepsilon}_B(k)\,\hat{\varepsilon}_B(-k)\Big)\Big]$$

$$\hat{g}_D(f,k) = \frac{1}{k^4R_g^4}\left[f k^2 R_g^2 + e^{-k^2R_g^2 f} - 1\right]$$

$$\hat{g}_{hg}(f,k) = \frac{1}{k^4 R_g^4}\left(1 - e^{-k^2 R_g^2 f}\right)\left(1 - e^{-k^2 R_g^2 (1-f)}\right)$$