Lecture 7 alt: The "other" form of field theory and S(k)

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We want $S(k) = \mathcal{F}_T\{\langle\hat\rho(r)\hat\rho(r')\rangle\} = \langle\rho_k\rho_{-k}\rangle$

Easiest method is the "other" form of FT

Don't use H-S Gaussian integrals, but use "Faddeev-Popov" transforms

Basically we use delta functionals to get rid of particle coords

Model

$$\beta U_0 = \frac{3}{2b^2}\sum_{j=1}^{n}\sum_{s=1}^{N-1}|r_{js}-r_{js+1}|^2$$

$$\beta U_1 = \frac{u_0}{2}\int dr[\hat\rho(r)]^2 - \frac{nNu_0}{2}$$

$$Z = \frac{z_0}{n!\lambda_T^{3nN}}\int dr^{nN}\left\{e^{-\beta U_0-\beta U_1}\int D\rho\ \delta[\rho(r)-\hat\rho(r)]\right\}$$

- $\rho(r)$ is a continuous, diff field
- write $\delta[\rho(r)-\hat\rho(r)] = \int Dw\ e^{i\rho\int dr\, w(r)[\rho(r)-\hat\rho(r)]}$

$$Z = \frac{z_0}{n!\lambda_T^{3n}}\int D\rho Dw\ e^{-\frac{u_0}{2}\int dr[\rho(r)]^2 + i\int dr\, w(r)\rho(r)}\underbrace{\int dr^{nN}\ e^{-\beta U_0 - i\int dr\, w(r)\hat\rho(r)}}_{[V\,Q[iw]]^n}$$

not $\hat\rho(r)$!

$$Z = \frac{z_1}{n!}V^n\int D\rho\int Dw\ e^{-\mathcal{H}[\rho,w]}$$

$$\mathcal{H} = \frac{u_0}{2}\int dr[\rho(r)]^2 - i\int dr\, w(r)\rho(r) - n\ln Q[iw]$$

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Why do this?

- no fn'l inverse needed, can have more cpx $u(r)$ or terms $\sim[\rho(r)]^3$

- Very easy to calculate $\langle \rho(r)\rho(r')\rangle = \langle \tilde\rho(r)\rho(r')\rangle$ in k-space in comb. w/ RPA approx for Q, $\tilde\rho$

Will get $S(k)$ for Model A, + Diblocks

- Use $\frac{\delta\mathcal{H}}{\delta w}=0$ to get a relation b/t $w(r)$, $\rho(r)$ at RPA level
- Eliminate $w(r)$ from $\mathcal{H}$
- Solve $\langle\rho(r)\rho(r')\rangle$ as 2^{nd} moment of a Gaussian

$$\frac{\delta\mathcal{H}}{\partial w} = i\rho(r) - n\frac{\delta\log Q[iw]}{\delta w} = 0 \qquad Q[iw] = e^{-w_0 N}\left[1 - \frac{N^2}{2V^2}\sum_k g_k w_k w_{-k}\right]$$

$$-i\rho(r) + i\tilde\rho(r;[iw]) = 0 = i\rho(r) + \rho_0 N g_k w_k$$

$$w_k = \frac{i\rho_k}{\rho_0 N g_k}$$

Plug into $\mathcal{H}$:

$$\mathcal{H} = \frac{u_0}{2V}\sum_k \rho_k\rho_{-k} + \frac{\cancel{i}}{V}\sum_k \frac{\cancel{i}\rho_k}{\rho_0 N g_k}\rho_{-k} + \underbrace{nNw_0}_{\text{ignore}} + \frac{\cancel{\rho_0 N}}{2V}\sum_k \frac{i}{\rho_0 N g_k}\rho_k \frac{i}{\cancel{\rho_0 N g_k}}\rho_{-k}\cancel{g_k}$$

$$= \frac{u_0}{2V}\sum_k \rho_k\rho_{-k} + \frac{1}{2V}\sum_k\frac{1}{\rho_0 N g_k}\rho_k\rho_{-k} = \frac{1}{2V}\sum_k \gamma_k\rho_k\rho_{-k}$$

$$\gamma_k = u_0 + \frac{1}{\rho_0 N g_k}$$

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$$Z = z_0 \int D\rho \; e^{-\frac{1}{2V}\sum_k \gamma_k \rho_k \rho_{-k}} \qquad \langle \rho_k \rho_{-k} \rangle = \frac{\int D\rho \; \rho_k \rho_{-k} \, e^{-\mathcal{H}}}{\int D\rho \; e^{-\mathcal{H}}} = \frac{1}{\gamma_k}$$, 2nd moment of a Gaussian

$$\boxed{S(k) = \frac{1}{u_0 + \frac{1}{\rho_0 N g_k}} = \frac{\rho_0 N g_k}{1 + u_0 \rho_0 N g_k}}$$

What about diblocks? Basically the same approach, just more equations

- Bonding potential
- Incompressibility $\delta[\hat{\rho}_T(r) - \rho_0]$
- Flory: $\beta U_1 = \frac{\chi}{\rho_0}\int dr \, \hat{\rho}_A(r) \hat{\rho}_B(r)$

Use 2 delta fn's in Z: $\int D\rho_A \int D\rho_B \, \delta[\rho_A(r) - \hat{\rho}_A(r)] \delta[\rho_B(r) - \hat{\rho}_B(r)]$

$$Z = z_0 \int D\{\rho, \omega\} \, e^{-\mathcal{H}} , \quad \mathcal{H} = \frac{\chi}{\rho_0}\int dr \, \rho_A(r) \rho_B(r) - i\int dr [\omega_A \rho_A + \omega_B \rho_B] - n \log Q[\mu_A, \mu_B]$$
$$- i \int dr \, \rho_0 \omega_+(r)$$

$\{\rho, \omega\} = \rho_A, \rho_B, \omega_A, \omega_B, \omega_+$

$\mu_A = i\omega_+ + i\omega_A$

$\mu_B = i\omega_+ + i\omega_B$

$i\omega_+$: enforces incompressibility : $\rho_A(r) = \rho_0 - \rho_B(r)$

Won't need to consider $i\omega_+$ beyond this fact

As before, we assume fields $\omega_A(r) = \omega_A^* + \alpha(r)$, $\omega_B(r) \approx \omega_B^* + \beta(r)$
w/ $\alpha(r), \beta(r)$ small

Now we use 2 MF eqns to relate $\alpha(r)$ to $\rho_A(r), \rho_B(r)$

At the level of RPA, partition function + density operators are:

$$Q = e^{-\omega_A^* N f} e^{-\omega_B N(1-f)} \left[1 - \frac{N^2}{2V} \sum_k \left(g_A \alpha_k \alpha_{-k} + 2 g_{AB} \alpha_k \beta_k + g_B \beta_k \beta_{-k} \right) \right]$$

$(i)^2$

$g_A = g_D(f,k) \qquad g_B = g_D(1-f,k) \qquad g_{AB} = g_{AB}(k)$

$$\tilde{\rho}_A = -n \frac{\delta \log Q}{\delta \omega_A}$$

$$\delta \tilde{\rho}_A(k) = \rho_0 N (g_A \alpha_k + g_{AB} \beta_k) = \tilde{\rho}_A(k) - f \rho_0 \delta(k)$$

$$\delta \tilde{\rho}_B(k) = \rho_0 N (g_B \beta_k + g_{AB} \alpha_k) = \tilde{\rho}_B(k) - (1-f) \rho_0 \delta(k)$$

From incompressibility, $\delta \rho_A(k) = -\delta \rho_B(k) = \rho_k$

Our mean-field equations:

$$\frac{\delta H}{\delta \omega_A} = i \rho_A - n \frac{\delta \log Q}{\delta \omega_A} = i \rho_k - \rho_0 N (g_A \alpha_k + g_{AB} \beta_k) = 0 \qquad (1)$$

$$\frac{\delta H}{\delta \omega_B} = i \rho_B - n \frac{\delta \log Q}{\delta \omega_B} = -i \rho_k - \rho_0 N (g_B \beta_k + g_{AB} \alpha_k) = 0 \qquad (2)$$

Solve for β_k, α_k to eliminate from the equations

From ②: $g_B\beta_k + g_{AB}\alpha_k = \frac{-i}{\rho_0 N}\rho_k$

$$\beta_k = \frac{-i}{\rho_0 N}\frac{\rho_k}{g_B} - \frac{g_{AB}}{g_B}\alpha_k = \frac{-i\rho_k - \rho_0 N g_{AB}\alpha_k}{\rho_0 N g_B} \quad ③$$

Plug into ①: $i\rho_k - \rho_0 N\left[g_A\alpha_k - g_{AB}\frac{i\rho_k + \rho_0 N g_{AB}\alpha_k}{\rho_0 N g_B}\right] = 0$

$$i\left(1+\frac{\cancel{\rho_0 N}\, g_{AB}}{\cancel{\rho_0 N}\, g_B}\right)\rho_k - \left[\rho_0 N g_A - \cancel{\rho_0 N}\,\frac{\rho_0 N g_{AB}^2}{\cancel{\rho_0 N}\, g_B}\right]\alpha_k = 0$$

$$i(g_B + g_{AB})\rho_k - \rho_0 N\underbrace{\left[g_A g_B - g_{AB}^2\right]}_{\equiv \mathbb{B}_k}\alpha_k = 0$$

$\equiv \mathbb{B}_k$: Note this is denominator of 5.34 in ETIP. prove w/ $g_D(f=1,k) = g_{AA} + 2g_{AB} + g_{BB}$

$$\alpha_k = i\,\frac{g_B+g_{AB}}{\mathbb{B}_k\,\rho_0 N}\,\rho_k \quad ④$$

Plug ④ into ③:

$$\beta_k = \frac{-i}{\rho_0 N}\frac{\rho_k}{g_B} - \frac{g_{AB}}{g_B}\, i\, \frac{g_B+g_{AB}}{B_k\,\rho_0 N}\,\rho_k$$

$$= \frac{-i}{\rho_0 N}\left(\frac{B_k + g_B g_{AB} + g_{AB}^2}{g_B B_k}\right)\rho_k = \frac{-i}{\rho_0 N}\left(\frac{g_A\cancel{g_B} + \cancel{g_B}\,g_{AB}}{\cancel{g_B}\,B_k}\right)\rho_k$$

$B_k = g_A g_B - g_{AB}^2$

$$\beta_k = \frac{-i}{\rho_0 N}\left(\frac{g_A+g_{AB}}{\mathbb{B}_k}\right)\rho_k$$

Now we go aaallllll the way back to H + plug in

$$w_A = \alpha_k = i\,\frac{g_B+g_{AB}}{B\rho_0 N}\,\rho_k \qquad w_B = \beta_k = \frac{-i}{\rho_0 N}\,\frac{g_A+g_{AB}}{\mathbb{B}_k}\,\rho_k$$

$\rho_A = \rho_k \qquad \rho_B = -\rho_k$

Only retaining the k-dependent terms

$(-)$ b/c $\rho_B = -\rho_k$

$$\mathcal{H} = \frac{-\chi}{\rho_0 V}\sum_k \rho_k \rho_k - \frac{i}{V}\sum_k \left\{ i\,\frac{g_B + g_{AB}}{B_k \rho_0 N}\rho_k \rho_{-k} + i\,\frac{g_A + g_{AB}}{\rho_0 N B_k}\rho_k \rho_{-k} \right\}$$

$$+ \frac{\rho_0 N}{2V}\sum_k \left\{ g_A i^2 \left(\frac{g_B + g_{AB}}{B_k \rho_0 N}\right)^2 - 2 g_{AB} i^2 \frac{(g_A + g_{AB})(g_B + g_{AB})}{(B_k \rho_0 N)^2} + g_B i^2 \left(\frac{g_A + g_{AB}}{B_k \rho_0 N}\right)^2 \right\} \rho_k \rho_{-k}$$

(2) (3) (4) (5) (6)

(2)+(3): $$\frac{g_B + 2g_{AB} + g_A}{B_k \rho_0 N} = \frac{g_D(f=1,k)}{B_k \rho_0 N} = \frac{G_k}{B_k \rho_0 N}$$

(4)+(5)+(6) $$\frac{1}{B_k^2 \rho_0 N}\Big[2g_{AB}\left(g_A g_B + g_B g_{AB} + g_A g_{AB} + g_{AB}^2\right) - g_A\left(g_B^2 + 2g_B g_{AB} + g_{AB}^2\right) - g_B\left(g_A^2 + 2 g_A g_{AB} + g_{AB}^2\right)\Big]$$

Multiply out term in brackets & collect powers of g_{AB}:

$$\frac{1}{B_k^2 \rho_0 N}\Big[2g_{AB}^3 + g_{AB}^2\left(\cancel{2}g_B + \cancel{2}g_A - \cancel{g_A} - \cancel{g_B}\right) + g_{AB}\left(2\cancel{g_A}g_B - 2g_A g_B - 2\cancel{g_A}g_B\right) - g_A g_B^2 - g_B g_A^2\Big]$$

$$= \frac{1}{B_k^2 \rho_0 N}\Big[2g_{AB}^3 + g_{AB}^2(g_B + g_A) - 2g_{AB}g_A g_B - g_A g_B^2 - g_B g_A^2\Big]$$

$$= \frac{1}{B_k^2 \rho_0 N}\Big[g_{AB}^2 \underbrace{\left[2g_{AB} + g_A + g_B\right]}_{G_k} - g_A g_B \underbrace{\left(g_A + g_B + 2g_{AB}\right)}_{G_k}\Big]$$

$$= \frac{G_k}{B_k^2 \rho_0 N}\left[g_{AB}^2 - g_A g_B\right] = -\frac{G_k}{B_k \rho_0 N}$$

$$= \frac{G_k}{B_k^2 \rho_0 N}\left[\underbrace{\rho_{AB}^2 - \rho_A\rho_B}_{-B_k}\right] = \frac{-G_k}{B_k \rho_0 N}$$

G_k $\qquad$ G_k

$$\mathcal{H} = \frac{-\chi}{\rho_0 V}\sum_k \rho_k \rho_{-k} + \frac{1}{V}\sum_k \frac{G_k}{B_k \rho_0 N}\rho_k\rho_{-k} - \frac{1}{2V}\sum_k \frac{G_k}{B_k \rho_0 N}\rho_k\rho_{-k}$$

$$\mathcal{H} = \frac{1}{2V}\sum_k\left(\frac{G_k}{B_k\rho_0 N} - \frac{2\chi N}{\rho_0 N}\right)\rho_k\rho_{-k} = \frac{1}{2V}\sum_k \gamma_k\,\rho_k\rho_{-k}$$

$$\gamma_k = \frac{G_k}{B_k \rho_0 N} - \frac{2\chi N}{\rho_0 N}$$

FINALLY, use the second moment formula to get

$$\langle \rho_k \rho_{-k}\rangle = \frac{1}{\gamma_k} = \frac{1}{\frac{G_k}{B_k\rho_0 N} - \frac{2\chi N}{\rho_0 N}}$$

$$\langle \rho_k \rho_{-k}\rangle = \frac{B_k \rho_0 N}{G_k - 2\chi N \rho_0 N B_k}$$

From ETIP:

$$\frac{\gamma_2}{V} = \frac{1}{V S(k)}\ ,\quad S(k) = \frac{1}{\gamma_2} \qquad 5.42$$

$$\gamma_2 = \Gamma_2(k) = \frac{1}{\rho_0 N}\left(\frac{G_k}{B_k} - 2\chi N\right) \qquad 5.33 + 5.34$$

GHF notation