SCFT for an Incompressible AB Diblock Melt in the Total/Exchange Formalism

Derivation Notes

1 Canonical model and microscopic densities

We consider a melt of n identical linear AB diblock copolymers in a periodic volume V at temperature T. Each chain is a space curve $\mathbf{R}_j(s)$ with contour variable $s \in [0, N]$. The A-block occupies $s \in [0, fN]$ and the B-block occupies $s \in [fN, N]$. Define the mean segment density

$$\rho_0 \equiv \frac{nN}{V} = \frac{1}{v_0}, \tag{1}$$

where v_0 is a reference segment volume.

Microscopic segment density operators.

$$\hat{\rho}_A(\mathbf{r}) \equiv \sum_{j=1}^{n} \int_0^{fN} \mathrm{d}s\, \delta\big(\mathbf{r} - \mathbf{R}_j(s)\big), \tag{2}$$

$$\hat{\rho}_B(\mathbf{r}) \equiv \sum_{j=1}^{n} \int_{fN}^{N} \mathrm{d}s\, \delta\big(\mathbf{r} - \mathbf{R}_j(s)\big). \tag{3}$$

Incompressibility constraint. The melt is strictly incompressible:

$$\hat{\rho}_A(\mathbf{r}) + \hat{\rho}_B(\mathbf{r}) = \rho_0 \quad \Longleftrightarrow \quad \delta\big[\hat{\rho}_A + \hat{\rho}_B - \rho_0\big]. \tag{4}$$

Gaussian chain model. The noninteracting (entropic) part of the Hamiltonian is

$$\beta U_0[\{\mathbf{R}_j\}] = \frac{3}{2b^2} \sum_{j=1}^{n} \int_0^N \mathrm{d}s \left| \frac{\mathrm{d}\mathbf{R}_j}{\mathrm{d}s} \right|^2, \tag{5}$$

with statistical segment length b and $\beta = (k_B T)^{-1}$.

Flory–Huggins contact interaction. Assume only A–B contact interactions:

$$\beta U_1[\{\mathbf{R}_j\}] = v_0 \chi_{AB} \int_V \mathrm{d}\mathbf{r}\, \hat{\rho}_A(\mathbf{r}) \hat{\rho}_B(\mathbf{r}). \tag{6}$$

Canonical partition function. Including the standard $n!$ and thermal wavelength λ_T prefactors,

$$Z_c(n, V, T) = \frac{1}{n!\, \left(\lambda_T^3\right)^{nN}} \prod_{j=1}^{n} \int \mathcal{D}\mathbf{R}_j\ \exp\Big[-\beta U_0 - \beta U_1\Big]\ \delta\big[\hat{\rho}_A + \hat{\rho}_B - \rho_0\big]. \tag{7}$$

2 Step 1: Introduce total and exchange density operators

Define the two linear combinations (your "two new variables"):

$$\hat{\rho}_+(\mathbf{r}) \equiv \hat{\rho}_A(\mathbf{r}) + \hat{\rho}_B(\mathbf{r}), \tag{8}$$

$$\hat{\rho}_-(\mathbf{r}) \equiv \hat{\rho}_A(\mathbf{r}) - \hat{\rho}_B(\mathbf{r}). \tag{9}$$

These imply the inverse relations

$$\hat{\rho}_A(\mathbf{r}) = \frac{1}{2}\big(\hat{\rho}_+(\mathbf{r}) + \hat{\rho}_-(\mathbf{r})\big), \tag{10}$$

$$\hat{\rho}_B(\mathbf{r}) = \frac{1}{2}\big(\hat{\rho}_+(\mathbf{r}) - \hat{\rho}_-(\mathbf{r})\big). \tag{11}$$

Incompressibility in the new variables. Equation (4) becomes simply

$$\delta\big[\hat{\rho}_A + \hat{\rho}_B - \rho_0\big] = \delta\big[\hat{\rho}_+ - \rho_0\big]. \tag{12}$$

Interaction in the new variables. Using (10)–(11),

$$\hat{\rho}_A(\mathbf{r})\hat{\rho}_B(\mathbf{r}) = \frac{1}{4}\Big(\hat{\rho}_+(\mathbf{r})^2 - \hat{\rho}_-(\mathbf{r})^2\Big), \tag{13}$$

so the Flory–Huggins interaction (6) becomes

$$\beta U_1 = \frac{v_0\chi_{AB}}{4}\int_V \mathrm{d}\mathbf{r}\,\Big(\hat{\rho}_+(\mathbf{r})^2 - \hat{\rho}_-(\mathbf{r})^2\Big). \tag{14}$$

3 Step 2: Use incompressibility to eliminate $\hat{\rho}_+$ from the interaction

Because $\delta[\hat{\rho}_+ - \rho_0]$ enforces $\hat{\rho}_+(\mathbf{r}) = \rho_0$ pointwise, we may replace $\hat{\rho}_+$ by ρ_0 *inside* any factor multiplying the delta-functional. In particular, (14) reduces to

$$\beta U_1 \;\to\; \frac{v_0\chi_{AB}}{4}\int_V \mathrm{d}\mathbf{r}\,\Big(\rho_0^2 - \hat{\rho}_-(\mathbf{r})^2\Big). \tag{15}$$

Therefore,

$$\exp\big[-\beta U_1\big] = \exp\left[-\frac{v_0\chi_{AB}}{4}\int_V \mathrm{d}\mathbf{r}\,\rho_0^2\right]\;\exp\left[+\frac{v_0\chi_{AB}}{4}\int_V \mathrm{d}\mathbf{r}\,\hat{\rho}_-(\mathbf{r})^2\right] \tag{16}$$

$$= \exp\left[-\frac{\chi_{AB}\rho_0 V}{4}\right]\;\exp\left[+\frac{v_0\chi_{AB}}{4}\int_V \mathrm{d}\mathbf{r}\,\hat{\rho}_-(\mathbf{r})^2\right], \tag{17}$$

where we used $\rho_0 = 1/v_0$ from (1).

4 Step 3: Introduce the pressure and exchange fields w_+ and w_-

4.1 3.1 Fourier representation of the incompressibility delta

Use the standard functional Fourier representation

$$\delta[F] = \int \mathcal{D}W\;\exp\!\left(-\mathrm{i}\int_V \mathrm{d}\mathbf{r}\,W(\mathbf{r})\,F(\mathbf{r})\right). \tag{18}$$

Applying (18) to (12) gives

$$\delta\big[\hat{\rho}_+ - \rho_0\big] = \int \mathcal{D}w_+\;\exp\left[-\mathrm{i}\int_V \mathrm{d}\mathbf{r}\,w_+(\mathbf{r})\big(\hat{\rho}_+(\mathbf{r}) - \rho_0\big)\right]. \tag{19}$$

4.2 3.2 Hubbard–Stratonovich decoupling of the $\hat{\rho}_-^2$ term

We use a Gaussian functional identity (Hubbard–Stratonovich type):

$$\exp\left(\frac{a}{2}\int_V \mathrm{d}\mathbf{r}\,\phi(\mathbf{r})^2\right) = \frac{\int \mathcal{D}W\ \exp\left[-\frac{1}{2a}\int_V \mathrm{d}\mathbf{r}\,W(\mathbf{r})^2 + \int_V \mathrm{d}\mathbf{r}\,W(\mathbf{r})\,\phi(\mathbf{r})\right]}{\int \mathcal{D}W\ \exp\left[-\frac{1}{2a}\int_V \mathrm{d}\mathbf{r}\,W(\mathbf{r})^2\right]}, \qquad a > 0. \tag{20}$$

Matching $\phi(\mathbf{r}) = \hat{\rho}_-(\mathbf{r})$ and choosing $a = v_0\chi_{AB}/2$ (so that $a/2 = v_0\chi_{AB}/4$), we obtain

$$\exp\left[+\frac{v_0\chi_{AB}}{4}\int_V \mathrm{d}\mathbf{r}\,\hat{\rho}_-(\mathbf{r})^2\right] = \frac{\int \mathcal{D}w_-\ \exp\left[-\frac{1}{v_0\chi_{AB}}\int_V \mathrm{d}\mathbf{r}\,w_-(\mathbf{r})^2 + \int_V \mathrm{d}\mathbf{r}\,w_-(\mathbf{r})\,\hat{\rho}_-(\mathbf{r})\right]}{\int \mathcal{D}w_-\ \exp\left[-\frac{1}{v_0\chi_{AB}}\int_V \mathrm{d}\mathbf{r}\,w_-(\mathbf{r})^2\right]}. \tag{21}$$

$$\frac{1}{v_0\chi_{AB}} = \frac{\rho_0}{\chi_{AB}}. \tag{22}$$

5 Step 4: Rewrite the partition function and isolate the single-chain problem

Insert Eqs. (17), (19), and (21) into Eq. (7). Keeping the HS normalization explicitly (the denominator in Eq. (21)), we obtain

$$\begin{aligned}
Z_c = {} & \frac{1}{n!\,\left(\lambda_T^3\right)^{nN}} \exp\left[-\frac{\chi_{AB}\rho_0 V}{4}\right] \int \mathcal{D}w_+ \int \mathcal{D}w_- \exp\left[\mathrm{i}\rho_0\int_V \mathrm{d}\mathbf{r}\,w_+(\mathbf{r}) - \frac{\rho_0}{\chi_{AB}}\int_V \mathrm{d}\mathbf{r}\,w_-(\mathbf{r})^2\right] \\
& \times \prod_{j=1}^{n} \int \mathcal{D}\mathbf{R}_j\ \exp\left[-\beta U_0[\mathbf{R}_j] - \mathrm{i}\int_V \mathrm{d}\mathbf{r}\,w_+(\mathbf{r})\hat{\rho}_+^{(j)}(\mathbf{r}) + \int_V \mathrm{d}\mathbf{r}\,w_-(\mathbf{r})\hat{\rho}_-^{(j)}(\mathbf{r})\right] \\
& \times \left[\int \mathcal{D}w_-\ \exp\left(-\frac{\rho_0}{\chi_{AB}}\int_V \mathrm{d}\mathbf{r}\,w_-(\mathbf{r})^2\right)\right]^{-1},
\end{aligned} \tag{23}$$

where $\hat{\rho}_\pm^{(j)}$ denotes the contribution from chain j alone.

5.1 4.1 Convert density couplings into contour integrals

For each chain j,

$$\int_V \mathrm{d}\mathbf{r}\,w_+(\mathbf{r})\hat{\rho}_+^{(j)}(\mathbf{r}) = \int_0^N \mathrm{d}s\,w_+\big(\mathbf{R}_j(s)\big), \tag{24}$$

$$\int_V \mathrm{d}\mathbf{r}\,w_-(\mathbf{r})\hat{\rho}_-^{(j)}(\mathbf{r}) = \int_0^{fN} \mathrm{d}s\,w_-\big(\mathbf{R}_j(s)\big) - \int_{fN}^N \mathrm{d}s\,w_-\big(\mathbf{R}_j(s)\big). \tag{25}$$

Therefore the chain-dependent exponential becomes

$$\begin{aligned}
& -\beta U_0[\mathbf{R}_j] - \mathrm{i}\int_0^N \mathrm{d}s\,w_+\big(\mathbf{R}_j(s)\big) + \int_0^{fN} \mathrm{d}s\,w_-\big(\mathbf{R}_j(s)\big) - \int_{fN}^N \mathrm{d}s\,w_-\big(\mathbf{R}_j(s)\big) \\
& \quad = -\beta U_0[\mathbf{R}_j] - \int_0^{fN} \mathrm{d}s\ \underbrace{\Big(\mathrm{i}w_+(\mathbf{R}_j(s)) - w_-(\mathbf{R}_j(s))\Big)}_{\equiv w_A(\mathbf{R}_j(s))} - \int_{fN}^N \mathrm{d}s\ \underbrace{\Big(\mathrm{i}w_+(\mathbf{R}_j(s)) + w_-(\mathbf{R}_j(s))\Big)}_{\equiv w_B(\mathbf{R}_j(s))}.
\end{aligned} \tag{26}$$

Definition of species fields from $w_\pm$. Motivated by (26), define

$$w_A(\mathbf{r}) \equiv \mathrm{i}w_+(\mathbf{r}) - w_-(\mathbf{r}), \tag{27}$$

$$w_B(\mathbf{r}) \equiv \mathrm{i}w_+(\mathbf{r}) + w_-(\mathbf{r}). \tag{28}$$

5.2 4.2 Single-chain partition function and normalized Q

Define the single-chain partition function in external fields w_A, w_B:

$$Z_{\text{chain}}[w_A, w_B] \equiv \int \mathcal{D}\mathbf{R}\ \exp\left[-\frac{3}{2b^2}\int_0^N \mathrm{d}s \left|\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}s}\right|^2 - \int_0^{fN} \mathrm{d}s\, w_A(\mathbf{R}(s)) - \int_{fN}^N \mathrm{d}s\, w_B(\mathbf{R}(s))\right]. \tag{29}$$

Also define the ideal-chain partition function (no external fields)

$$Z_0 \equiv \int \mathcal{D}\mathbf{R}\ \exp\left[-\frac{3}{2b^2}\int_0^N \mathrm{d}s \left|\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}s}\right|^2\right]. \tag{30}$$

The normalized single-chain partition function is

$$Q[w_A, w_B] \equiv \frac{Z_{\text{chain}}[w_A, w_B]}{Z_0}. \tag{31}$$

Because chains are independent given the fields,

$$\prod_{j=1}^n \int \mathcal{D}\mathbf{R}_j(\cdots) = \Big(Z_{\text{chain}}[w_A, w_B]\Big)^n = \big(Z_0\big)^n \exp\!\big(n \ln Q[w_A, w_B]\big). \tag{32}$$

6 Step 5: Final field theory and effective Hamiltonian

Insert Eq. (32) into Eq. (23). Absorb all field-independent prefactors—including the Hubbard–Stratonovich normalization (the Gaussian denominator in Eq. (21))—into an overall constant $\mathcal{N}$. Then the canonical partition function can be written in the standard field-theoretic form

$$Z_c = \mathcal{N} \int \mathcal{D}w_+ \int \mathcal{D}w_-\ \exp\!\Big(-\beta\mathcal{H}[w_+, w_-]\Big), \tag{33}$$

with effective Hamiltonian

$$\beta\mathcal{H}[w_+, w_-] = \frac{\rho_0}{\chi_{AB}} \int_V \mathrm{d}\mathbf{r}\, w_-(\mathbf{r})^2 - \mathrm{i}\rho_0 \int_V \mathrm{d}\mathbf{r}\, w_+(\mathbf{r}) - n \ln Q[w_A, w_B]. \tag{34}$$

Here w_A, w_B are the linear combinations of $w_\pm$,

$$w_A(\mathbf{r}) \equiv \mathrm{i}w_+(\mathbf{r}) - w_-(\mathbf{r}), \qquad w_B(\mathbf{r}) \equiv \mathrm{i}w_+(\mathbf{r}) + w_-(\mathbf{r}), \tag{35}$$

as defined previously in Eqs. (27)–(28).

Reality of saddle-point fields. At the mean-field (SCFT) saddle, one typically finds

$$w_-^\star(\mathbf{r}) \in \mathbb{R}, \qquad w_+^\star(\mathbf{r}) \in \mathrm{i}\,\mathbb{R}, \tag{36}$$

so it is convenient to introduce a real pressure-like field

$$\xi(\mathbf{r}) \equiv \mathrm{i}w_+(\mathbf{r}) \in \mathbb{R}. \tag{37}$$

Then the real saddle-point species fields become

$$w_A^\star(\mathbf{r}) = \xi^\star(\mathbf{r}) - w_-^\star(\mathbf{r}), \qquad w_B^\star(\mathbf{r}) = \xi^\star(\mathbf{r}) + w_-^\star(\mathbf{r}). \tag{38}$$

7 Step 6: Mean-field (SCFT) saddle-point equations

The SCFT approximation evaluates (33) by steepest descent:

$$\left.\frac{\delta\beta\mathcal{H}}{\delta w_+(\mathbf{r})}\right|_\star = 0, \qquad \left.\frac{\delta\beta\mathcal{H}}{\delta w_-(\mathbf{r})}\right|_\star = 0. \tag{39}$$

7.1 6.1 Functional derivatives of $\ln Q$ define densities

A key identity is that functional derivatives of $\ln Q$ generate single-chain densities. Define the mean segment densities (melt-averaged) by

$$\rho_A(\mathbf{r}) \equiv -n\,\frac{\delta \ln Q}{\delta w_A(\mathbf{r})}, \tag{40}$$

$$\rho_B(\mathbf{r}) \equiv -n\,\frac{\delta \ln Q}{\delta w_B(\mathbf{r})}. \tag{41}$$

(Equivalently, one may define volume fractions $\phi_K(\mathbf{r}) \equiv \rho_K(\mathbf{r})/\rho_0$.)

Using (27)–(28), the chain rule gives

$$\frac{\delta \ln Q}{\delta w_+(\mathbf{r})} = \frac{\delta \ln Q}{\delta w_A(\mathbf{r})}\frac{\delta w_A(\mathbf{r})}{\delta w_+(\mathbf{r})} + \frac{\delta \ln Q}{\delta w_B(\mathbf{r})}\frac{\delta w_B(\mathbf{r})}{\delta w_+(\mathbf{r})} = \mathrm{i}\left(\frac{\delta \ln Q}{\delta w_A(\mathbf{r})} + \frac{\delta \ln Q}{\delta w_B(\mathbf{r})}\right), \tag{42}$$

$$\frac{\delta \ln Q}{\delta w_-(\mathbf{r})} = \frac{\delta \ln Q}{\delta w_A(\mathbf{r})}\frac{\delta w_A(\mathbf{r})}{\delta w_-(\mathbf{r})} + \frac{\delta \ln Q}{\delta w_B(\mathbf{r})}\frac{\delta w_B(\mathbf{r})}{\delta w_-(\mathbf{r})} = -\frac{\delta \ln Q}{\delta w_A(\mathbf{r})} + \frac{\delta \ln Q}{\delta w_B(\mathbf{r})}. \tag{43}$$

7.2 6.2 Saddle equation for w_+: incompressibility

Differentiate (34) with respect to w_+:

$$\frac{\delta\beta\mathcal{H}}{\delta w_+(\mathbf{r})} = -\mathrm{i}\rho_0 - n\,\frac{\delta \ln Q}{\delta w_+(\mathbf{r})}. \tag{44}$$

Setting (44) to zero and using (42) gives

$$\begin{aligned} 0 &= -\mathrm{i}\rho_0 - n\,\mathrm{i}\left(\frac{\delta \ln Q}{\delta w_A(\mathbf{r})} + \frac{\delta \ln Q}{\delta w_B(\mathbf{r})}\right) \\ &= -\mathrm{i}\rho_0 + \mathrm{i}\Big(\rho_A(\mathbf{r}) + \rho_B(\mathbf{r})\Big), \end{aligned} \tag{45}$$

where we used (40)–(41). Therefore the saddle condition is

$$\rho_A^\star(\mathbf{r}) + \rho_B^\star(\mathbf{r}) = \rho_0. \tag{46}$$

In volume-fraction form,

$$\phi_A(\mathbf{r}) + \phi_B(\mathbf{r}) = 1. \tag{47}$$

7.3 6.3 Saddle equation for w_-: exchange self-consistency

Differentiate (34) with respect to w_-:

$$\frac{\delta\beta\mathcal{H}}{\delta w_-(\mathbf{r})} = \frac{2\rho_0}{\chi_{AB}} w_-(\mathbf{r}) - n\,\frac{\delta \ln Q}{\delta w_-(\mathbf{r})}. \tag{48}$$

Setting (48) to zero and using (43) yields

$$\begin{aligned} 0 &= \frac{2\rho_0}{\chi_{AB}} w_-(\mathbf{r}) - n\left(-\frac{\delta \ln Q}{\delta w_A(\mathbf{r})} + \frac{\delta \ln Q}{\delta w_B(\mathbf{r})}\right) \\ &= \frac{2\rho_0}{\chi_{AB}} w_-(\mathbf{r}) + \rho_A(\mathbf{r}) - \rho_B(\mathbf{r}). \end{aligned} \tag{49}$$

Thus the exchange field satisfies

$$w_-^\star(\mathbf{r}) = \frac{\chi_{AB}}{2\rho_0}\Big(\rho_B^\star(\mathbf{r}) - \rho_A^\star(\mathbf{r})\Big) = \frac{\chi_{AB}}{2}\Big(\phi_B(\mathbf{r}) - \phi_A(\mathbf{r})\Big). \tag{50}$$

8 Step 7: Standard propagator representation of ϕ_A, ϕ_B

To make ϕ_A, ϕ_B explicit, introduce the forward and backward propagators $q(\mathbf{r}, s)$ and $q^\dagger(\mathbf{r}, s)$, defined by the modified diffusion equations (MDEs).

8.1 7.1 Modified diffusion equations

Define the contour-dependent potential

$$W(\mathbf{r}, s) = \begin{cases} w_A(\mathbf{r}), & 0 \le s \le fN, \\ w_B(\mathbf{r}), & fN \le s \le N. \end{cases} \tag{51}$$

Then the forward propagator satisfies

$$\frac{\partial q(\mathbf{r}, s)}{\partial s} = \frac{b^2}{6} \nabla^2 q(\mathbf{r}, s) - W(\mathbf{r}, s)\, q(\mathbf{r}, s), \qquad q(\mathbf{r}, 0) = 1, \tag{52}$$

and the backward propagator satisfies

$$\frac{\partial q^\dagger(\mathbf{r}, s)}{\partial s} = \frac{b^2}{6} \nabla^2 q^\dagger(\mathbf{r}, s) - W(\mathbf{r}, N - s)\, q^\dagger(\mathbf{r}, s), \qquad q^\dagger(\mathbf{r}, 0) = 1. \tag{53}$$

8.2 7.2 Single-chain partition function from propagators

The normalized single-chain partition function can be computed as

$$Q[w_A, w_B] = \frac{1}{V} \int_V \mathrm{d}\mathbf{r}\, q(\mathbf{r}, N). \tag{54}$$

8.3 7.3 Volume fractions

The standard SCFT expressions for the volume fractions are

$$\phi_A(\mathbf{r}) = \frac{1}{Q} \frac{1}{N} \int_0^{fN} \mathrm{d}s\; q(\mathbf{r}, s)\, q^\dagger(\mathbf{r}, N - s), \tag{55}$$

$$\phi_B(\mathbf{r}) = \frac{1}{Q} \frac{1}{N} \int_{fN}^{N} \mathrm{d}s\; q(\mathbf{r}, s)\, q^\dagger(\mathbf{r}, N - s). \tag{56}$$

9 Summary: SCFT equations in the total/exchange formalism

The SCFT (mean-field) solution is the saddle point $\{w_+^\star, w_-^\star\}$ (equivalently $\{\xi^\star, w_-^\star\}$) that minimizes the mean-field free energy (per chain) while being self-consistent with the single-chain statistics in the corresponding external fields.

(0) Mean-field free energy (evaluated at the saddle). With the effective Hamiltonian $\beta\mathcal{H}[w_+, w_-]$ in Eq. (34), the mean-field free energy follows from the saddle-point approximation $Z_c \approx \mathcal{N} \exp\bigl(-\beta\mathcal{H}[w_+^\star, w_-^\star]\bigr)$:

$$A = -k_B T \ln Z_c \approx \mathcal{H}[w_+^\star, w_-^\star] + (\text{field-independent constants}). \tag{57}$$

It is often convenient to quote the dimensionless free energy per chain (dropping constants that do not affect the saddle):

$$\frac{\beta A}{n} = -\ln Q[w_A^\star, w_B^\star] + \frac{\rho_0}{n\chi_{AB}} \int_V \mathrm{d}\mathbf{r}\, \bigl(w_-^\star(\mathbf{r})\bigr)^2 - \mathrm{i}\, \frac{\rho_0}{n} \int_V \mathrm{d}\mathbf{r}\, w_+^\star(\mathbf{r}) \quad (+\,\text{constants}). \tag{58}$$

Equivalently, using the real pressure field $\xi(\mathbf{r}) \equiv \mathrm{i}w_+(\mathbf{r}) \in \mathbb{R}$ at the saddle,

$$\frac{\beta A}{n} = -\ln Q[w_A^\star, w_B^\star] + \frac{\rho_0}{n\chi_{AB}} \int_V \mathrm{d}\mathbf{r}\, \big(w_-^\star(\mathbf{r})\big)^2 - \frac{\rho_0}{n} \int_V \mathrm{d}\mathbf{r}\, \xi^\star(\mathbf{r}) \quad (+\,\text{constants}). \tag{59}$$

The last term enforces incompressibility and acts as a Lagrange-multiplier contribution if we further defined

$$\mu_+(\mathbf{r}) = N\xi^*(\mathbf{r}), \tag{60}$$

$$\mu_-(\mathbf{r}) = Nw_-^*(\mathbf{r}). \tag{61}$$

Using $\rho_0 = nN/V$, Eq. (59) can be rewritten compactly in terms of $\mu_\pm$ as

$$\frac{\beta A}{n} = -\ln Q[w_A^\star, w_B^\star] + \frac{1}{V} \int_V \mathrm{d}\mathbf{r} \left[\frac{\big(\mu_-(\mathbf{r})\big)^2}{\chi_{AB} N} - \mu_+(\mathbf{r}) \right] \quad (+\,\text{constants}). \tag{62}$$

The μ_+ term plays the role of a Lagrange multiplier enforcing incompressibility; its spatial average may be fixed by a gauge choice (e.g. $\int_V \mathrm{d}\mathbf{r}\, \mu_+ = 0$).

(i) Species fields in the $\mu_\pm$ representation. At the saddle, define the dimensionless species fields

$$\mu_A(\mathbf{r}) \equiv Nw_A^\star(\mathbf{r}), \qquad \mu_B(\mathbf{r}) \equiv Nw_B^\star(\mathbf{r}), \tag{63}$$

which are related to $\mu_\pm^\star$ by

$$\mu_A(\mathbf{r}) = \mu_+(\mathbf{r}) - \mu_-(\mathbf{r}), \tag{64}$$

$$\mu_B(\mathbf{r}) = \mu_+(\mathbf{r}) + \mu_-(\mathbf{r}). \tag{65}$$

Equivalently,

$$w_A^\star(\mathbf{r}) = \frac{1}{N}\mu_A(\mathbf{r}), \qquad w_B^\star(\mathbf{r}) = \frac{1}{N}\mu_B(\mathbf{r}). \tag{66}$$

(ii) Modified diffusion equations (propagators) in a unit contour variable. Introduce the normalized contour variable $t \equiv s/N \in [0,1]$ and the radius of gyration $R_g^2 \equiv Nb^2/6$. Define the piecewise contour potential

$$\mu(\mathbf{r}, t) = \begin{cases} \mu_A(\mathbf{r}), & 0 \le t \le f, \\ \mu_B(\mathbf{r}), & f \le t \le 1. \end{cases} \tag{67}$$

Then the forward and backward propagators satisfy

$$\frac{\partial q(\mathbf{r}, t)}{\partial t} = R_g^2 \nabla^2 q(\mathbf{r}, t) - \mu(\mathbf{r}, t)\, q(\mathbf{r}, t), \qquad q(\mathbf{r}, 0) = 1, \tag{68}$$

$$\frac{\partial q^\dagger(\mathbf{r}, t)}{\partial t} = R_g^2 \nabla^2 q^\dagger(\mathbf{r}, t) - \mu(\mathbf{r}, 1-t)\, q^\dagger(\mathbf{r}, t), \qquad q^\dagger(\mathbf{r}, 0) = 1. \tag{69}$$

(iii) Single-chain partition function.

$$Q[w_A^\star, w_B^\star] = \frac{1}{V} \int_V \mathrm{d}\mathbf{r}\, q(\mathbf{r}, 1). \tag{70}$$

(iv) Volume fractions generated by the propagators.

$$\phi_A(\mathbf{r}) = \frac{1}{Q} \int_0^f \mathrm{d}t\; q(\mathbf{r}, t)\, q^\dagger(\mathbf{r}, 1-t), \tag{71}$$

$$\phi_B(\mathbf{r}) = \frac{1}{Q} \int_f^1 \mathrm{d}t\; q(\mathbf{r}, t)\, q^\dagger(\mathbf{r}, 1-t). \tag{72}$$

(v) Saddle-point (self-consistency) conditions. The SCFT solution is obtained when the fields and densities are mutually consistent:

$$\phi_A(\mathbf{r}) + \phi_B(\mathbf{r}) = 1, \tag{73}$$

$$\frac{2\mu_-(\mathbf{r})}{N\chi_{AB}} + \phi_A(\mathbf{r}) - \phi_B(\mathbf{r}) = 0. \tag{74}$$

Equations (64)–(65) and (68)–(72), together with (73)–(74), close the SCFT loop.