SCFT and Numerical Methods for Polymeric Systems

Kai Jiang*
School of Mathematics and Computational Science,
Xiangtan University, Xiangtan 411105, P.R. China and
Hunan Key Laboratory for Computation and Simulation in Science and Engineering,
Xiangtan University, Xiangtan 411105, P.R. China
(Dated: December 7, 2017)

* kaijiang@xtu.edu.cn

CONTENTS

I. LINEAR COIL-COIL DIBLOCK COPOLYMER MELT

A. Self-consistent field theory

Within mean-field approximation to statistical mechanics of the Edwards model of polymers, the free energy functional for AB diblock copolymer melt is

$$\begin{aligned} H =& \frac{1}{V}\int d\mathbf{r}\{\chi N\phi_A(\mathbf{r})\phi_B(\mathbf{r}) - w_A(\mathbf{r})\phi_A(\mathbf{r}) \\ & - w_B(\mathbf{r})\phi_B(\mathbf{r}) - \xi(\mathbf{r})[1-\phi_A(\mathbf{r})-\phi_B(\mathbf{r})]\} - \log Q[w_A, w_B], \end{aligned} \tag{1}$$

where χ is the Flory-Huggins parameter to describe the interaction between segments A and B. $\phi_A(\mathbf{r})$ and $\phi_B(\mathbf{r})$ are the monomer density fields. $w_A(\mathbf{r})$ and $w_B(\mathbf{r})$ are the mean external fields acting on blocks A and B, produced by the surrounding chains. $\xi(\mathbf{r})$ is a pressure field that ensures the local incompressibility. Q is the single chain partition functional subjected to mean fields $w_A(\mathbf{r})$ and $w_B(\mathbf{r})$. Minimizing the free energy with respect to the density fields and the external fields leads to the following self-consistent field (SCF) equations,

$$w_A(\mathbf{r}) = \chi N\phi_B(\mathbf{r}) + \xi(\mathbf{r}), \tag{2}$$
$$w_B(\mathbf{r}) = \chi N\phi_A(\mathbf{r}) + \xi(\mathbf{r}), \tag{3}$$
$$\phi_A(\mathbf{r}) + \phi_B(\mathbf{r}) = 1, \tag{4}$$
$$Q = \frac{1}{V}\int d\mathbf{r}\, q(\mathbf{r}, s)q^\dagger(\mathbf{r}, s), \quad \forall s \in [0, 1], \tag{5}$$
$$\phi_A(\mathbf{r}) = \frac{1}{Q}\int_0^f ds\, q(\mathbf{r}, s)q^\dagger(\mathbf{r}, s), \tag{6}$$
$$\phi_B(\mathbf{r}) = \frac{1}{Q}\int_f^1 ds\, q(\mathbf{r}, s)q^\dagger(\mathbf{r}, s). \tag{7}$$

The forward propagator $q(\mathbf{r}, s)$ represents the probability weight that the chain of contour length s has its end at position $\mathbf{r}$, where the variable s is used to parameterize each copolymer chain. $s = 0$ represents the tail of the A block and $s = f$ is the junction between the A and B blocks.

From the flexible Gaussian chain model [3], we know that it satisfies the modified diffusion equation

$$\frac{\partial q}{\partial s} = \begin{cases} \nabla^2 q - \omega_A(\mathbf{r})q, & 0 \le s \le f, \\ \nabla^2 q - \omega_B(\mathbf{r})q, & f < s \le 1, \end{cases} \tag{8}$$

with the initial condition $q(\mathbf{r}, 0) = 1$, R_g is the radius of gyration. The reverse propagator $q^\dagger(\mathbf{r}, s)$, which represents the probability weight from $s = 1$ to $s = 0$, satisfies Eqn. (193) only with the right-hand side multiplied by -1, and the initial condition, $q^\dagger(\mathbf{r}, 1) = 1$.

B. Numerical methods

Self-consistent iterative procedure

Step 1: Given initial estimations of fields w_A and w_B, and freeze computational box;

Step 2: Compute forward (back) propagator operators q and $q^\dagger$ (see Sec. I B 1);

Step 3: Obtain Q, ϕ_C and ϕ_B by integral equations (see Sec. I B 2), and calculate the value of effective Hamiltonian H;

Step 4: Update fields w_A and w_B using some iterative methods (see Sec. I B 3);

Step 5: Goto **Step 2** until the Hamiltonian does not change or SCF equations are satisfied.

---

1. Numerical schemes for solving PDEs of coil chain

2. Solving integral equations

A fourth-order integral formula can be used to approximate s-direction integral equations

$$\int_0^{n_s} ds\, f(s) = \Delta s \left\{ -\frac{5}{8}(f_0 + f_{n_s}) + \frac{1}{6}(f_1 + f_{n_s-1}) - \frac{1}{24}(f_2 + f_{n_s-2}) + \sum_{j=0}^{n_s} f_j \right\}. \tag{9}$$

3. Nonlinear iterative methods

II. LINEAR COIL-COIL DIBLOCK COPOLYMER MELT ON A GENERAL CURVED SURFACE

A. Self-consistent field theory (SCFT) on a general curved surface

Consider n AB diblock copolymers with the polymerization of N confined on a curved surface with a total area S. The volume fraction of A block is f and the two blocks disfavor with each other characterized by the Flory-Huggins parameter χ. Within mean-field approximation, the free energy density of this system in the unit of k_BT can be written as

$$\begin{aligned}\frac{F}{nk_BT} =& \frac{1}{S}\int d\mathbf{s}\{\chi N\phi_A(\mathbf{u})\phi_B(\mathbf{u}) - w_A(\mathbf{u})\phi_A(\mathbf{u}) \\ & - w_B(\mathbf{u})\phi_B(\mathbf{u}) - \xi(\mathbf{u})[1-\phi_A(\mathbf{u})-\phi_B(\mathbf{u})]\} - \log Q[w_A, w_B]\end{aligned} \tag{10}$$

In the above equation, χ is the Flory-Huggins parameter to describe the interaction between segments A and B. $w_A(\mathbf{u})$ and $w_B(\mathbf{u})$ are the mean external fields acting on blocks A and B, produced by the surrounding chains. $\xi(\mathbf{r})$ is a pressure field that ensures the local incompressibility. Q is the single chain partition functional subjected to mean fields w_A and w_B. $\phi_A(\mathbf{u})$ and $\phi_B(\mathbf{u})$ are A and B monomer densities. $d\mathbf{s}$ is the element of the surface. First-order variations of the free energy functional with respect to the density fields and the external fields lead to the following self-consistent field (SCF) equations,

$$w_A(\mathbf{u}) = \chi N\phi_B(\mathbf{u}) + \xi(\mathbf{u}), \tag{11}$$

$$w_B(\mathbf{u}) = \chi N\phi_A(\mathbf{u}) + \xi(\mathbf{u}), \tag{12}$$

$$\phi_A(\mathbf{u}) + \phi_B(\mathbf{u}) = 1, \tag{13}$$

$$Q = \frac{1}{S}\int d\mathbf{u}\, q(\mathbf{u}, s)q^\dagger(\mathbf{u}, 1-s), \quad \forall s \in [0,1], \tag{14}$$

$$\phi_A(\mathbf{u}) = \frac{1}{Q}\int_0^f ds\, q(\mathbf{u}, s)q^\dagger(\mathbf{u}, 1-s), \tag{15}$$

$$\phi_B(\mathbf{u}) = \frac{1}{Q}\int_f^1 ds\, q(\mathbf{u}, s)q^\dagger(\mathbf{u}, 1-s). \tag{16}$$

The forward propagator $q(\mathbf{u}, s)$ represents the probability weight that the chain of contour length s has its end at surface position $\mathbf{u}$, where the variable s is used to parameterize each copolymer chain. $s = 0$ represents the tail of the A block and $s = f$ is the junction between the A and B blocks. From the flexible Gaussian chain model [3], the forward propagator $q(\mathbf{u}, s)$ satisfies the modified diffusion equation

$$\begin{aligned}\frac{\partial}{\partial s}q(\mathbf{u}, s) &= [\nabla^2_{LB} - w(\mathbf{u}, s)]q(\mathbf{u}, s) \\ q(\mathbf{u}, 0) &= 1\end{aligned} \tag{17}$$

where ∇^2_{LB} is the Laplace-Beltrami operator which is actually the divergence operator for the curved surface. $w(\mathbf{u}, s) = w_A(\mathbf{u})$, $0 \le s \le f$, and $w(\mathbf{u}, s) = w_B(\mathbf{u})$, $f \le s \le 1$. The backward propagator $q^\dagger(\mathbf{u}, s)$, which represents the probability weight from $s = 1$ to $s = 0$, satisfies

$$\begin{aligned}\frac{\partial}{\partial s}q^\dagger(\mathbf{u}, s) &= [\nabla^2_{LB} - w^\dagger(\mathbf{u}, s)]q^\dagger(\mathbf{u}, s) \\ q^\dagger(\mathbf{u}, 0) &= 1\end{aligned} \tag{18}$$

where $w^\dagger(\mathbf{u}, s) = w_B(\mathbf{u})$, $0 \le s \le 1-f$, and $w^\dagger(\mathbf{u}, s) = w_A(\mathbf{u})$, $1-f \le s \le 1$.

B. Numerical methods

Self-consistent iterative procedure

Step 1: Given initial estimations of fields w_A and w_B;

Step 2: Compute forward (back) propagator operators q and $q^\dagger$ on a general curved surface (see Sec.);

Step 3: Obtain Q, ϕ_A and ϕ_B by integral equations (see Sec.), and calculate the free energy density F/nk_BT;

Step 4: Update fields w_A and w_B using some iterative methods (see Sec.);

Step 5: Goto **Step 2** until the Hamiltonian does not change or SCF equations are satisfied.

---

1. Basic numerical methods

• Integral formula along s-direction

A fourth-order integral formula can be used to approximate s-direction integral equations

$$\int_0^{n_s} ds\, f(s) = \Delta s \left\{ -\frac{5}{8}(f_0 + f_{n_s}) + \frac{1}{6}(f_1 + f_{n_s-1}) - \frac{1}{24}(f_2 + f_{n_s-2}) + \sum_{j=0}^{n_s} f_j \right\}. \tag{19}$$

• Second-order operator-splitting method

The propagator of coil subchain satisfies the following PDEs

$$\frac{\partial}{\partial s} q(\mathbf{u}, s) = \nabla^2_{LB} q(\mathbf{u}, s) - w_C(\mathbf{u}) q(\mathbf{u}, s) := \mathcal{L}_1 q + \mathcal{L}_2 q \tag{20}$$

From s to $s + h$, the second-order operator-splitting is specified by

$$q(\mathbf{u}, s + h) = e^{\frac{h}{2}\mathcal{L}_2} e^{h\mathcal{L}_1} e^{\frac{h}{2}\mathcal{L}_2} q(\mathbf{u}, s) \tag{21}$$

• Simple mixing method

The k iteration in the simple mixing method begins with the evaluation of new fields from the SCF equations

$$\xi^{(k)}(\mathbf{u}) = \frac{w_A(\mathbf{u}) + w_B(\mathbf{u}) - \chi N}{2} \tag{22}$$

$$\bar{w}_A^{(k)}(\mathbf{u}) = \chi N \phi_B^{(k)}(\mathbf{u}) + \xi(\mathbf{u}), \tag{23}$$

$$\bar{w}_B^{(k)}(\mathbf{u}) = \chi N \phi_A^{(k)}(\mathbf{u}) + \xi(\mathbf{u}), \tag{24}$$

In the above expressions, $w_\alpha^{(k)}$, $\alpha = A, B$, are the old fields. The simple mixing method is

$$w_\alpha^{(k+1)}(\mathbf{u}) = (1 - \lambda) w_\alpha^{(k)}(\mathbf{u}) + \lambda \bar{w}_\alpha^{(k)}(\mathbf{u}) \tag{25}$$

• Anderson mixing method

The k iteration in the Anderson mixing method begins with the evaluation of new fields from the SCF equations

$$\xi^{(k)}(\mathbf{u}) = \frac{w_A(\mathbf{u}) + w_B(\mathbf{u}) - \chi N}{2} \tag{26}$$

$$\bar{w}_A^{(k)}(\mathbf{u}) = \chi N \phi_B^{(k)}(\mathbf{u}) + \xi(\mathbf{u}), \tag{27}$$

$$\bar{w}_B^{(k)}(\mathbf{u}) = \chi N \phi_A^{(k)}(\mathbf{u}) + \xi(\mathbf{u}), \tag{28}$$

In the above expressions, $w_\alpha^{(k)}$, $\alpha = A, B$, are the old fields. Next we evaluate the deviation,

$$d^{(k)} = \bar{w}^{(k)}(\mathbf{u}) - w^{(k)}(\mathbf{u}), \tag{29}$$

where $d^{(k)} = [d_A^{(k)}(\mathbf{u}), d_B^{(k)}(\mathbf{u})]^T$, $\bar{w}^{(k)}(\mathbf{u}) = [\bar{w}_A^{(k)}(\mathbf{u}), \bar{w}_B^{(k)}(\mathbf{u})]^T$, $w^{(k)}(\mathbf{u}) = [w_A^{(k)}(\mathbf{u}), w_B^{(k)}(\mathbf{u})]^T$. From the deviation, we can specify an error tolerance through the inner product

$$(g(\mathbf{u}), f(\mathbf{u})) = \frac{1}{S} \int d\mathbf{u}\, g(\mathbf{u}) f(\mathbf{u}), \tag{30}$$

where $g(\mathbf{u})$ and $f(\mathbf{u})$ are arbitrary functions. The error tolerance is defined by

$$\varepsilon_1 = \left[\frac{\sum_{\alpha=A,B}(d_\alpha^{(k)}(\mathbf{u}), d_\alpha^{(k)}(\mathbf{u}))}{\sum_{\alpha=A,B}(w_\alpha^{(k)}(\mathbf{u}), w_\alpha^{(k)}(\mathbf{u}))} \right]^{1/2} \tag{31}$$

as a measure of the numerical inaccuracy in the field Eqns. (11)-(12).

The simple mixing method is performed until a certain tolerance is reached where a morphology has begun to develop. From our experience, $\varepsilon_1 < 10^{-2}$, is sufficient in most cases. We then switch to the Anderson mixing procedure by the previous n steps to update fields. We assemble the symmetric matrix in this way

$$U_{ij}^{(k)} = (d^{(k)} - d^{(k-i)},\ d^{(k)} - d^{(k-j)}), \tag{32}$$

for $i, j = 1, 2, \ldots, n$, and vector

$$V_i^{(k)} = (d^{(k)} - d^{(k-i)},\ d^{(k)}) = (d^{(k)},\ d^{(k)}) - (d^{(k-i)},\ d^{(k)}). \tag{33}$$

From these, we calculate the coefficients

$$C_i = \sum_j^n (U^{-1})_{ij} V_j, \tag{34}$$

and combine the previous histories as

$$T_\alpha^{(k)} = w_\alpha^{(k)} + \sum_{i=1}^n C_i (w_\alpha^{(k-i)} - w_\alpha^{(k)}), \tag{35}$$

$$D_\alpha^{(k)} = d_\alpha^{(k)} + \sum_{i=1}^n C_i (d_\alpha^{(k-i)} - d_\alpha^{(k)}). \tag{36}$$

Finally, the new fields are obtained from

$$w_{\alpha,j}^{(k+1)} = T_{\alpha,j}^{(k)} + \lambda D_{\alpha,j}^{(k)}, \tag{37}$$

where $0 < \lambda = 1.0 - 0.9^k < 1$.

In our implementation, the used previous steps are usually much less than the number of basis functions or grid points. Therefore assembling the n-order linear system spends more computation time than solving this system. To save computational amount, we decompose Eqn. (32) into

$$U_{ij}^{(k)} = (d^{(k)},\ d^{(k)}) - (d^{(k-i)},\ d^{(k)}) - (d^{(k)},\ d^{(k-j)}) + (d^{(k-i)},\ d^{(k-j)}). \tag{38}$$

In k iteration, only the terms related to $d^{(k)}$ in the right term of Eqn. (38) are required to calculate, but the last terms $(d^{(k-i)},\ d^{(k-j)})$, $i, j = 1, \ldots, n$, should be not computed repeatedly which will save the main computational cost in assembling matrix U. In practical calculations, we store the following inner product matrix

$$M = \begin{pmatrix} (d^{(k)}, d^{(k)}) & (d^{(k)}, d^{(k-1)}) & \cdots & (d^{(k)}, d^{(k-n)}) \\ (d^{(k-1)}, d^{(k)}) & (d^{(k-1)}, d^{(k-1)}) & \cdots & (d^{(k-1)}, d^{(k-n)}) \\ \vdots & \vdots & \ddots & \vdots \\ (d^{(k-n)}, d^{(k)}) & (d^{(k-n)}, d^{(k-1)}) & \cdots & (d^{(k-n)}, d^{(k-n)}) \end{pmatrix}. \tag{39}$$

Then we can assemble the matrix U and vector V according to the expressions of Eqns. (38) and (33) using the elements of matrix M. Note that the inner product matrix is symmetric, therefore only a row (or a column, equivalently) of M is required to update in each iteration.

2. *Finite element discretization on general surface (TBA)*

3. *Surface integral (TBA)*

III. SCFT OF AB_2 STAR COPOLYMER MELT

Within mean-field approximation to statistical mechanics of the Edwards model of polymers, the free energy functional for AB_2 diblock copolymer melt is

$$\begin{aligned} H =& \frac{1}{V}\int d\mathbf{r}\{\chi N\phi_A(\mathbf{r})\phi_B(\mathbf{r}) - w_A(\mathbf{r})\phi_A(\mathbf{r}) \\ & - w_B(\mathbf{r})\phi_B(\mathbf{r}) - \xi(\mathbf{r})[1-\phi_A(\mathbf{r})-\phi_B(\mathbf{r})]\} - \log Q[w_A, w_B]. \end{aligned} \tag{40}$$

Minimizing the mean-field Hamiltonian leads to self-consistent field equations

$$w_A(\mathbf{r}) = \chi N\phi_B(\mathbf{r}) + \xi(\mathbf{r}), \tag{41}$$

$$w_B(\mathbf{r}) = \chi N\phi_A(\mathbf{r}) + \xi(\mathbf{r}), \tag{42}$$

$$\phi_A(\mathbf{r}) + \phi_B(\mathbf{r}) = 1, \tag{43}$$

$$Q = \frac{1}{V}\int d\mathbf{r}\, q(\mathbf{r}, s)q^\dagger(\mathbf{r}, s), \quad \forall s \in [0, 1], \tag{44}$$

$$\phi_A(\mathbf{r}) = \frac{1}{Q}\int_0^{f_A} ds\, q(\mathbf{r}, s)q^\dagger(\mathbf{r}, s), \tag{45}$$

$$\phi_B(\mathbf{r}) = \frac{1}{Q}\left\{\int_0^{f_{B_1}} ds\, q(\mathbf{r}, s)q^\dagger(\mathbf{r}, s) + \int_0^{f_{B_2}} ds\, q(\mathbf{r}, s)q^\dagger(\mathbf{r}, s)\right\}, \tag{46}$$

where $f_{B_1} + f_{B_2} = f_B$, and $f_A + f_B = 1$. The propagators of the star triblock copolymer satisfy the modified diffusion equations,

$$\frac{\partial}{\partial s}q_\alpha(\mathbf{r}, s) = \nabla^2_{\mathbf{r}}q_\alpha(\mathbf{r}, s) - w_\alpha q_\alpha(\mathbf{r}, s), \quad q_\alpha(\mathbf{r}, 0) = 1, \quad s \in [0, f_\alpha], \tag{47}$$

$$\frac{\partial}{\partial s}q^\dagger_\alpha(\mathbf{r}, s) = \nabla^2_{\mathbf{r}}q^\dagger_\alpha(\mathbf{r}, s) - w_\alpha q^\dagger_\alpha(\mathbf{r}, s), \quad q^\dagger_\alpha(\mathbf{r}, 0) = q_\beta(\mathbf{r}, f_\beta)q_\gamma(\mathbf{r}, f_\gamma), \tag{48}$$

where $(\alpha\beta\gamma) \in \{(AB_1B_2), (B_1B_2A), (B_2AB_1)\}$, and $w_{B_1} = w_{B_2} = w_B$.

The field-based effective Hamiltonian by Gaussian functional integral technology is

$$H = \frac{1}{V}\int d\mathbf{r}\,\{-\mu_+(\mathbf{r}) + \frac{\mu^2_-(\mathbf{r})}{\chi N}\} - \log \mathcal{Q}[w_A, w_B], \tag{49}$$

where $w_A = \mu_+ - \mu_-$, $w_B = \mu_+ + \mu_-$. The corresponding SCFT equations are

$$\phi_A(\mathbf{r}) + \phi_B(\mathbf{r}) = 1, \tag{50}$$

$$\phi_A(\mathbf{r}) - \phi_B(\mathbf{r}) = \frac{2\mu_-(\mathbf{r})}{\chi N}. \tag{51}$$

IV. AB DIBLOCK COPOLYMER BLENDS

A. SCFT in the canonical (nVT) ensemble

Within mean-field approximation, the free energy functional in the canonical ensemble

$$\frac{F}{k_BT(n_l+\kappa n_s)} = \frac{1}{V}\int d\mathbf{r}\Big\{\chi N_l\phi_A(\mathbf{r})\phi_B(\mathbf{r}) - w_A(\mathbf{r})\phi_A(\mathbf{r}) - w_B(\mathbf{r})\phi_B(\mathbf{r}) + \xi(\mathbf{r})[\phi_A(\mathbf{r})+\phi_B(\mathbf{r})-1]\Big\} - \frac{n_l}{n_l+\kappa n_s}\log Q_l - \frac{n_s}{n_l+\kappa n_s}\log Q_s \tag{52}$$

First variations lead to SCF equations

$$w_A(\mathbf{r}) = \chi N_l\phi_B(\mathbf{r}) + \xi(\mathbf{r}) \tag{53}$$
$$w_B(\mathbf{r}) = \chi N_l\phi_A(\mathbf{r}) + \xi(\mathbf{r}) \tag{54}$$
$$1 = \phi_A(\mathbf{r}) + \phi_B(\mathbf{r}) \tag{55}$$
$$Q_l = \frac{1}{V}\int d\mathbf{r}\, q_{l,A}(\mathbf{r},1) \tag{56}$$
$$Q_s = \frac{1}{V}\int d\mathbf{r}\, q_{s,A}(\mathbf{r},\kappa) \tag{57}$$
$$\phi_A(\mathbf{r}) = \frac{n_l}{n_l+\kappa n_s}\frac{1}{Q_l}\int_0^{f_{l,A}} ds\, q_{l,A}(\mathbf{r},s)q^\dagger_{l,A}(\mathbf{r},f_{l,A}-s) + \frac{n_s}{n_l+\kappa n_s}\frac{1}{Q_s}\int_0^{\kappa f_{s,A}} ds\, q_{s,A}(\mathbf{r},s)q^\dagger_{s,A}(\mathbf{r},\kappa f_{s,A}-s) \tag{58}$$
$$\phi_B(\mathbf{r}) = \frac{n_l}{n_l+\kappa n_s}\frac{1}{Q_l}\int_0^{f_{l,B}} ds\, q_{l,B}(\mathbf{r},s)q^\dagger_{l,B}(\mathbf{r},f_{l,B}-s) + \frac{n_s}{n_l+\kappa n_s}\frac{1}{Q_s}\int_0^{\kappa f_{s,B}} ds\, q_{s,B}(\mathbf{r},s)q^\dagger_{s,B}(\mathbf{r},\kappa f_{s,B}-s) \tag{59}$$

The propagators of long and short AB diblock copolymers satisfy

$$\frac{\partial}{\partial s}q_\alpha(\mathbf{r},s) = \varepsilon^2[\nabla^2_{\mathbf{r}} - w(\mathbf{r},s)]q_\alpha(\mathbf{r},s) \qquad s\in[0,\kappa_\alpha] \tag{60}$$
$$q_\alpha(\mathbf{r},0) = 1, \tag{61}$$

In the above expression, $\varepsilon = b_A/b_B$ represents the ratio of the A and B statistical segment lengths. $\alpha = l, s$, $\kappa_l = 1$, and $\kappa_s = \kappa$. When $\alpha = l$, $w(\mathbf{r},s) = w_A(\mathbf{r})$ $(0\le s\le f_{l,A})$, $w(\mathbf{r},s) = w_B(\mathbf{r})$ $(f_{l,A}\le s\le 1)$. When $\alpha = s$, $w(\mathbf{r},s) = w_A(\mathbf{r})$ $(0\le s\le \kappa f_{s,A})$, $w(\mathbf{r},s) = w_B(\mathbf{r})$ $(\kappa f_{l,A}\le s\le \kappa)$.

$$\frac{\partial}{\partial s}q^\dagger_\alpha(\mathbf{r},s) = \varepsilon^2[\nabla^2_{\mathbf{r}} - w^\dagger(\mathbf{r},s)]q^\dagger_\alpha(\mathbf{r},s) \qquad s\in[0,\kappa_\alpha] \tag{62}$$
$$q^\dagger_\alpha(\mathbf{r},0) = 1, \tag{63}$$

In the above expression, $\alpha = l, s$, $\kappa_l = 1$, and $\kappa_s = \kappa$. When $\alpha = l$, $w^\dagger(\mathbf{r},s) = w_B(\mathbf{r})$ $(0\le s\le 1-f_{l,A})$, $w^\dagger(\mathbf{r},s) = w_A(\mathbf{r})$ $(1-f_{l,A}\le s\le 1)$. When $\alpha = s$, $w^\dagger(\mathbf{r},s) = w_B(\mathbf{r})$ $(0\le s\le \kappa f_{s,A})$, $w^\dagger(\mathbf{r},s) = w_A(\mathbf{r})$ $[\kappa(1-f_{s,A})\le s\le\kappa]$.

B. From SCFT to Landau's theory

We apply the asymptotic expansion tool to solve the MDE

$$\frac{\partial}{\partial s}q_l(\mathbf{r},s) = [\nabla^2_{\mathbf{r}} - w(\mathbf{r},s)]q_l(\mathbf{r},s) \qquad s\in[0,1] \tag{64}$$
$$q_l(\mathbf{r},0) = 1 \tag{65}$$
$$w(\mathbf{r},s) = \begin{cases} w_A(\mathbf{r}), & 0\le s\le f_{l,A} \\ w_B(\mathbf{r}), & f_{l,A}\le s\le 1 \end{cases} \tag{66}$$

$$w_A(\mathbf{r}) = w_{0,A} + \epsilon w_{1,A}(\mathbf{r}) \tag{67}$$
$$w_B(\mathbf{r}) = w_{0,B} + \epsilon w_{1,B}(\mathbf{r}) \tag{68}$$

where

$$w_{0,A} = \frac{1}{V}\int d\mathbf{r}\, w_A(\mathbf{r}), \qquad w_{0,B} = \frac{1}{V}\int d\mathbf{r}\, w_B(\mathbf{r}) \tag{69}$$

And

$$\delta w_A = w_A(\mathbf{r}) - w_{0,A}, \qquad \delta w_B = w_B(\mathbf{r}) - w_{0,B} \tag{70}$$

$$q(\mathbf{r},s) = e^{-\int_0^s d\tau\, w_0(\tau)}[1 + \epsilon p_1(\mathbf{r},s) + \epsilon^2 p_2(\mathbf{r},s) + O(\epsilon^3)] \tag{71}$$

$w_0(s) = w_{0,A}$ when $0 \le s \le f_A$, and $w_0(s) = w_{0,B}$ when $f_A \le s \le 1$.

- $O(\epsilon^0)$:

$$\begin{cases} \frac{\partial}{\partial s} p_0(\mathbf{r},s) &= \nabla^2 p_0(\mathbf{r},s) \\ p_0(\mathbf{r},0) &= 1 \end{cases} \tag{72}$$

Solving the equation will lead to

$$p_0(\mathbf{r},s) = 1, \qquad 0 \le s \le 1 \tag{73}$$

- $O(\epsilon^1)$:

$$\begin{cases} \frac{\partial}{\partial s} p_1(\mathbf{r},s) &= \nabla^2 p_1(\mathbf{r},s) - w_1(\mathbf{r},s) p_0(\mathbf{r},s) \\ p_1(\mathbf{r},0) &= 0 \end{cases} \tag{74}$$

Solving the equation will lead to

$$0 \le s \le f_A: \quad \hat{p}_1(\mathbf{k},s) = \frac{\hat{w}_{1,A}(\mathbf{k})}{|\mathbf{k}|^2}(e^{-|\mathbf{k}|^2 s} - 1) \tag{75}$$

$$f_A \le s \le 1: \quad \hat{p}_1(\mathbf{k},s) = \frac{\hat{w}_{1,A}(\mathbf{k})}{|\mathbf{k}|^2}(1 - e^{|\mathbf{k}|^2 f_A})e^{-|\mathbf{k}|^2 s} + \frac{\hat{w}_{1,B}(\mathbf{k})}{|\mathbf{k}|^2}(e^{-|\mathbf{k}|^2(s-f_A)} - 1) \tag{76}$$

- $O(\epsilon^2)$:

$$\begin{cases} \frac{\partial}{\partial s} p_2(\mathbf{r},s) &= \nabla^2 p_2(\mathbf{r},s) - w_1(\mathbf{r},s) p_1(\mathbf{r},s) \\ p_2(\mathbf{r},0) &= 0 \end{cases} \tag{77}$$

$$0 \le s \le f_A: \quad \hat{p}_2(\mathbf{k},s) = \sum_{\mathbf{k}'} \frac{\hat{w}_{1,A}(\mathbf{k}')\hat{w}_{1,A}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}|^2|\mathbf{k}-\mathbf{k}'|^2}\left[\frac{|\mathbf{k}|^2}{|\mathbf{k}|^2 - |\mathbf{k}-\mathbf{k}'|^2}\left(e^{-|\mathbf{k}|^2 s} - e^{-|\mathbf{k}-\mathbf{k}'|^2 s}\right) + 1 - e^{-|\mathbf{k}|^2 s}\right] \tag{78}$$

$f_A \le s \le 1$:

$$\begin{aligned} \frac{\partial}{\partial s}\hat{p}_2(\mathbf{k},s) = -\mathbf{k}^2\hat{p}_2(\mathbf{k},s) &- \sum_{\mathbf{k}'} \frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,A}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}(1 - e^{|\mathbf{k}-\mathbf{k}'|^2 f_A})e^{-|\mathbf{k}-\mathbf{k}'|^2 s} \\ &- \sum_{\mathbf{k}'} \frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,B}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}(e^{-|\mathbf{k}-\mathbf{k}'|^2(s-f_A)} - 1) \end{aligned} \tag{79}$$

$$\hat{p}_2(\mathbf{k},f_A) = -\sum_{\mathbf{k}'} \frac{\hat{w}_{1,A}(\mathbf{k}')\hat{w}_{1,A}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}\left(\frac{e^{-|\mathbf{k}-\mathbf{k}'|^2 f_A}}{\mathbf{k}^2 - |\mathbf{k}-\mathbf{k}'|^2} - \frac{1}{\mathbf{k}^2} + \frac{e^{-\mathbf{k}^2 s}}{\mathbf{k}^2} - \frac{e^{-\mathbf{k}^2 s}}{\mathbf{k}^2 - |\mathbf{k}-\mathbf{k}'|^2}\right)$$

Solving the homogeneous equation will lead to

$$\frac{\partial}{\partial s}\hat{p}_2(\mathbf{k},s) = -\mathbf{k}^2\hat{p}_2(\mathbf{k},s) \Longrightarrow \hat{p}_2(\mathbf{k},s) = C(s)e^{-\mathbf{k}^2 s} \tag{80}$$

By the constant variation method,

$$\begin{aligned} C'(s)e^{-\mathbf{k}^2 s} - \mathbf{k}^2 C(s)e^{-\mathbf{k}^2 s} = -\mathbf{k}^2 C(s)e^{-\mathbf{k}^2 s} &- \sum_{\mathbf{k}'} \frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,A}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}(1-e^{|\mathbf{k}-\mathbf{k}'|^2 f_A})e^{-|\mathbf{k}-\mathbf{k}'|^2 s} \\ &- \sum_{\mathbf{k}'} \frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,B}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}(e^{-|\mathbf{k}-\mathbf{k}'|^2(s-f_A)}-1) \end{aligned} \tag{81}$$

$$\begin{aligned} C'(s) = &- \sum_{\mathbf{k}'} \frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,A}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}(1-e^{|\mathbf{k}-\mathbf{k}'|^2 f_A})e^{(\mathbf{k}^2-|\mathbf{k}-\mathbf{k}'|^2)s} \\ &- \sum_{\mathbf{k}'} \frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,B}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}(e^{-|\mathbf{k}-\mathbf{k}'|^2(s-f_A)}-1)e^{\mathbf{k}^2 s} \end{aligned} \tag{82}$$

$$\begin{aligned} C(s) = -\sum_{\mathbf{k}'} \Big[&\frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,A}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}(1-e^{|\mathbf{k}-\mathbf{k}'|^2 f_A})\frac{e^{(\mathbf{k}^2-|\mathbf{k}-\mathbf{k}'|^2)s}}{\mathbf{k}^2-|\mathbf{k}-\mathbf{k}'|^2} \\ &- \frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,B}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}\Big(e^{|\mathbf{k}-\mathbf{k}'|^2 f_A}\frac{e^{(\mathbf{k}^2-|\mathbf{k}-\mathbf{k}'|^2)s}}{\mathbf{k}^2-|\mathbf{k}-\mathbf{k}'|^2} - \frac{e^{\mathbf{k}^2 s}}{\mathbf{k}^2}\Big) + \tilde{C}\Big] \end{aligned} \tag{83}$$

$$\begin{aligned} \hat{p}_2(\mathbf{k},s) =& C(s)e^{-\mathbf{k}^2 s} \\ = &-\sum_{\mathbf{k}'} \Big[\frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,A}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}(1-e^{|\mathbf{k}-\mathbf{k}'|^2 f_A})\frac{e^{-|\mathbf{k}-\mathbf{k}'|^2 s}}{\mathbf{k}^2-|\mathbf{k}-\mathbf{k}'|^2} \\ &- \frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,B}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}\Big(e^{|\mathbf{k}-\mathbf{k}'|^2 f_A}\frac{e^{-|\mathbf{k}-\mathbf{k}'|^2 s}}{\mathbf{k}^2-|\mathbf{k}-\mathbf{k}'|^2} - \frac{1}{\mathbf{k}^2}\Big) + \tilde{C}e^{-\mathbf{k}^2 s}\Big] \end{aligned} \tag{84}$$

We use the initial value to determine the constant $\tilde{C}$

$$\begin{aligned} \hat{p}_2(\mathbf{k},f_A) = -\sum_{\mathbf{k}'} \Big[&\frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,A}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}\frac{1}{\mathbf{k}^2-|\mathbf{k}-\mathbf{k}'|^2}(e^{-|\mathbf{k}-\mathbf{k}'|^2 f_A}-1) \\ &- \frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,B}(\mathbf{k}-\mathbf{k}')}{|\mathbf{k}-\mathbf{k}'|^2}\Big(\frac{1}{\mathbf{k}^2-|\mathbf{k}-\mathbf{k}'|^2} - \frac{1}{\mathbf{k}^2}\Big) + \tilde{C}e^{-\mathbf{k}^2 f_A}\Big] \end{aligned} \tag{85}$$

Definition: Debye's function $g(\mathbf{k},s) = \frac{2}{\mathbf{k}^2}(e^{-s\mathbf{k}} + s\mathbf{k} - 1)$

Now let us only consider the case of $\mathbf{k} = \mathbf{0}$. The initial value becomes

$$\hat{p}_2(\mathbf{0},f_A) = \frac{1}{2}\sum_{\mathbf{k}'} \hat{w}_{1,A}(\mathbf{k}')\hat{w}_{1,A}(-\mathbf{k}')g(|\mathbf{k}'|^2,f_A) \tag{86}$$

The solution of $\hat{p}_2$ at $\mathbf{k} = \mathbf{0}$ is

$$\begin{aligned} \hat{p}_2(\mathbf{0},s) = &\sum_{\mathbf{k}'} \frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,A}(-\mathbf{k}')}{|\mathbf{k}'|^4}(1-e^{|\mathbf{k}'|^2 f_A})e^{-|\mathbf{k}'|^2 s} \\ &+ \frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,B}(-\mathbf{k}')}{|\mathbf{k}'|^4}\Big(e^{-|\mathbf{k}'|^2(s-f_A)} - s|\mathbf{k}'|^2\Big) + \tilde{C} \end{aligned} \tag{87}$$

$$\begin{aligned}\tilde{C} =& \frac{1}{2}\sum_{\mathbf{k}'}\hat{w}_{1,A}(\mathbf{k}')\hat{w}_{1,A}(-\mathbf{k}')g(|\mathbf{k}'|^2,f_A)\\ &-\sum_{\mathbf{k}'}\frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,A}(-\mathbf{k}')}{|\mathbf{k}'|^4}(e^{-|\mathbf{k}'|^2 f_A}-1)\\ &-\frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,B}(-\mathbf{k}')}{|\mathbf{k}'|^4}(1-f_A|\mathbf{k}'|^2)\end{aligned} \tag{88}$$

$$\begin{aligned}\hat{p}_2(\mathbf{0},s)=\sum_{\mathbf{k}'}\Big[&\frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,A}(-\mathbf{k}')}{|\mathbf{k}'|^4}(1-e^{|\mathbf{k}'|^2 f_A})(e^{-|\mathbf{k}'|^2 s}-e^{-|\mathbf{k}'|^2 f_A})+\\ &\frac{1}{2}\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,B}(-\mathbf{k}')g(|\mathbf{k}'|^2,s-f_A)+\frac{1}{2}\hat{w}_{1,A}(\mathbf{k}')\hat{w}_{1,A}(-\mathbf{k}')g(|\mathbf{k}'|^2,f_A)\Big]\end{aligned} \tag{89}$$

$$0\le s\le f_A:\quad \hat{p}_2(\mathbf{0},s)=\frac{1}{2}\sum_{\mathbf{k}'}\hat{w}_{1,A}(\mathbf{k}')\hat{w}_{1,A}(-\mathbf{k}')g(|\mathbf{k}'|^2,s) \tag{90}$$

$$f_A\le s\le 1:\quad \hat{p}_2(\mathbf{0},s)=\frac{1}{2}\sum_{\mathbf{k}'}\Big[\frac{\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,A}(-\mathbf{k}')}{|\mathbf{k}'|^4}\left[g(|\mathbf{k}'|^2,s)-g(|\mathbf{k}'|^2,s-f_A)-g(|\mathbf{k}'|^2,f_A)\right]+ \tag{91}$$

$$\hat{w}_{1,B}(\mathbf{k}')\hat{w}_{1,B}(-\mathbf{k}')g(|\mathbf{k}'|^2,s-f_A)+\hat{w}_{1,A}(\mathbf{k}')\hat{w}_{1,A}(-\mathbf{k}')g(|\mathbf{k}'|^2,f_A)\Big] \tag{92}$$

Now we consider the conformationally asymmetric case

$$\frac{\partial}{\partial s}q(\mathbf{r},s)=[\varepsilon^2\nabla_{\mathbf{r}}^2-w(\mathbf{r},s)]q(\mathbf{r},s)\qquad s\in[0,1] \tag{93}$$

$$q(\mathbf{r},0)=1 \tag{94}$$

$$w(\mathbf{r},s)=\begin{cases}w_A(\mathbf{r}), & 0\le s\le f_A\\ w_B(\mathbf{r}), & f_A\le s\le 1\end{cases} \tag{95}$$

- $O(\epsilon^0)$:

$$\begin{cases}\frac{\partial}{\partial s}p_0(\mathbf{r},s) &= \varepsilon^2\nabla^2 p_0(\mathbf{r},s)\\ p_0(\mathbf{r},0) &= 1\end{cases} \tag{96}$$

Solving the equation will lead to

$$p_0(\mathbf{r},s)=1,\qquad 0\le s\le 1 \tag{97}$$

- $O(\epsilon^1)$:

$$\begin{cases}\frac{\partial}{\partial s}p_1(\mathbf{r},s) &= \nabla^2 p_1(\mathbf{r},s)-w_1(\mathbf{r},s)p_0(\mathbf{r},s)\\ p_1(\mathbf{r},0) &= 0\end{cases} \tag{98}$$

Solving the equation will lead to

$$0\le s\le f_A:\quad \hat{p}_1(\mathbf{k},s)=\frac{\hat{w}_{1,A}(\mathbf{k})}{\varepsilon^2|\mathbf{k}|^2}(e^{-\varepsilon^2|\mathbf{k}|^2 s}-1) \tag{99}$$

$$f_A\le s\le 1:\quad \hat{p}_1(\mathbf{k},s)=\frac{\hat{w}_{1,A}(\mathbf{k})}{\varepsilon^2|\mathbf{k}|^2}(1-e^{\varepsilon^2|\mathbf{k}|^2 f_A})e^{-\varepsilon^2|\mathbf{k}|^2 s}+\frac{\hat{w}_{1,B}(\mathbf{k})}{\varepsilon^2|\mathbf{k}|^2}(e^{-\varepsilon^2|\mathbf{k}|^2(s-f_A)}-1) \tag{100}$$

$$0\le s\le f_A:\quad \hat{p}_1(\mathbf{0},s)=-\hat{w}_{1,A}(\mathbf{0})s \tag{101}$$

$$f_A\le s\le 1:\quad \hat{p}_1(\mathbf{0},s)=-\hat{w}_{1,A}(\mathbf{0})f_A-\hat{w}_{1,B}(\mathbf{0})(s-f_A) \tag{102}$$

- $O(\epsilon^2)$:

$$\begin{cases} \frac{\partial}{\partial s} p_2(\mathbf{r}, s) &= \varepsilon^2 \nabla^2 p_2(\mathbf{r}, s) - w_1(\mathbf{r}, s) p_1(\mathbf{r}, s) \\ p_2(\mathbf{r}, 0) &= 0 \end{cases} \tag{103}$$

$$0 \le s \le f_A: \quad \hat{p}_2(\mathbf{0}, s) = \frac{1}{2} \sum_{\mathbf{k}'} \hat{w}_{1,A}(\mathbf{k}') \hat{w}_{1,A}(-\mathbf{k}') g(\varepsilon |\mathbf{k}'|^2, s) \tag{104}$$

$$f_A \le s \le 1: \quad \hat{p}_2(\mathbf{0}, s) = \frac{1}{2} \sum_{\mathbf{k}'} \Big[\hat{w}_{1,B}(\mathbf{k}') \hat{w}_{1,A}(-\mathbf{k}') \left[g(\varepsilon |\mathbf{k}'|^2, s) - g(\varepsilon |\mathbf{k}'|^2, s - f_A) - g(\varepsilon |\mathbf{k}'|^2, f_A) \right] + \tag{105}$$

$$\hat{w}_{1,B}(\mathbf{k}') \hat{w}_{1,B}(-\mathbf{k}') g(\varepsilon |\mathbf{k}'|^2, s - f_A) + \hat{w}_{1,A}(\mathbf{k}') \hat{w}_{1,A}(-\mathbf{k}') g(\varepsilon |\mathbf{k}'|^2, f_A) \Big] \tag{106}$$

The single chain partition functional of long diblock copolymer can be approximated by

$$\begin{aligned} Q_l[w_A, w_B] &= \frac{1}{V} \int d\mathbf{r}\, q_l(\mathbf{r}, 1) = \hat{q}_l(\mathbf{0}, 1) \\ &\approx \underbrace{e^{-\int_0^1 ds\, w_0(s)}}_{Constant} [1 + \epsilon \hat{p}_{l,1}(\mathbf{0}, 1) + \epsilon^2 \hat{p}_{l,2}(\mathbf{0}, 1)] \\ &= e^{-\int_0^1 ds\, w_0(s)} \Bigg\{ 1 - f_{l,A} \epsilon \hat{w}_{1,A}(\mathbf{0}) - (1 - f_{l,A}) \epsilon \hat{w}_{1,B}(\mathbf{0}) \\ &\quad + \frac{\epsilon^2}{2} \sum_{\mathbf{k}'} \Big[\hat{w}_{1,B}(\mathbf{k}') \hat{w}_{1,A}(-\mathbf{k}') \left[g(\varepsilon |\mathbf{k}'|^2, 1) - g(\varepsilon |\mathbf{k}'|^2, 1 - f_{l,A}) - g(\varepsilon |\mathbf{k}'|^2, f_{l,A}) \right] \\ &\quad + \hat{w}_{1,B}(\mathbf{k}') \hat{w}_{1,B}(-\mathbf{k}') g(\varepsilon |\mathbf{k}'|^2, 1 - f_{l,A}) + \hat{w}_{1,A}(\mathbf{k}') \hat{w}_{1,A}(-\mathbf{k}') g(\varepsilon |\mathbf{k}'|^2, f_{l,A}) \Big] \Bigg\} \end{aligned} \tag{107}$$

$$\begin{aligned} Q_s[w_A, w_B] &= \frac{1}{V} \int d\mathbf{r}\, q_s(\mathbf{r}, \kappa) = \hat{q}_s(\mathbf{0}, \kappa) \\ &\approx \underbrace{e^{-\int_0^1 ds\, w_0(s)}}_{Constant} [1 + \epsilon \hat{p}_{s,1}(\mathbf{0}, 1) + \epsilon^2 \hat{p}_{s,2}(\mathbf{0}, 1)] \\ &= e^{-\int_0^1 ds\, w_0(s)} \Bigg\{ 1 - \kappa f_{s,A} \epsilon \hat{w}_{1,A}(\mathbf{0}) - \kappa (1 - f_{s,A}) \epsilon \hat{w}_{1,B}(\mathbf{0}) \\ &\quad + \frac{\epsilon^2}{2} \sum_{\mathbf{k}'} \Big[\hat{w}_{1,B}(\mathbf{k}') \hat{w}_{1,A}(-\mathbf{k}') \left[g(\varepsilon |\mathbf{k}'|^2, \kappa) - g(\varepsilon |\mathbf{k}'|^2, \kappa(1 - f_{s,A})) - g(\varepsilon |\mathbf{k}'|^2, \kappa f_{s,A}) \right] \\ &\quad + \hat{w}_{1,B}(\mathbf{k}') \hat{w}_{1,B}(-\mathbf{k}') g(\varepsilon |\mathbf{k}'|^2, \kappa(1 - f_{s,A})) + \hat{w}_{1,A}(\mathbf{k}') \hat{w}_{1,A}(-\mathbf{k}') g(\varepsilon |\mathbf{k}'|^2, \kappa f_{s,A}) \Big] \Bigg\} \end{aligned} \tag{108}$$

Some notations:

$$\begin{aligned} P_l(\mathbf{k}) &= g(\varepsilon^2 |\mathbf{k}|^2, 1) \\ P_{l,A}(\mathbf{k}) &= g(\varepsilon^2 |\mathbf{k}|^2, f_{l,A}) \\ P_{l,B}(\mathbf{k}) &= g(\varepsilon^2 |\mathbf{k}|^2, 1 - f_{l,A}) \\ P_s(\mathbf{k}) &= g(\varepsilon^2 |\mathbf{k}|^2, \kappa) \\ P_{s,A}(\mathbf{k}) &= g(\varepsilon^2 |\mathbf{k}|^2, \kappa f_{s,A}) \\ P_{s,B}(\mathbf{k}) &= g(\varepsilon^2 |\mathbf{k}|^2, \kappa(1 - f_{s,A})) \end{aligned} \tag{109}$$

An important fact:

$$\frac{\partial F}{\partial \hat{w}(-\mathbf{k})} = \int \frac{\delta F}{\delta w(\mathbf{r})} \frac{\delta w(\mathbf{r})}{\delta \hat{w}(-\mathbf{k})}\, d\mathbf{r} = \int \frac{\delta F}{\delta w(\mathbf{r})} e^{i\mathbf{k}\mathbf{r}}\, d\mathbf{r} = V\widehat{\left(\frac{\delta F}{\delta w(\mathbf{r})}\right)}(\mathbf{k})$$

where the Fourier transform and its inverse transform are defined as following

$$f(\mathbf{r}) = \int \hat{f}(\mathbf{k}) e^{i\mathbf{k}\mathbf{r}}\, d\mathbf{k}$$
$$\hat{f}(\mathbf{k}) = \frac{1}{V}\int f(\mathbf{r}) e^{-i\mathbf{k}\mathbf{r}}\, d\mathbf{r}$$

$$\begin{aligned}
\hat{\phi}_A(\mathbf{k}; w_A, w_B) &= -\frac{n_l}{n_l+\kappa n_s} V\widehat{\left(\frac{\delta \log Q_l}{\delta(\epsilon w_{1,A}(\mathbf{r}))}\right)}(\mathbf{k}) - \frac{n_s}{n_l+\kappa n_s} V\widehat{\left(\frac{\delta \log Q_s}{\delta(\epsilon w_{1,A}(\mathbf{r}))}\right)}(\mathbf{k}) \\
&= -\frac{n_l}{n_l+\kappa n_s}\frac{\partial \log Q_l}{\partial(\epsilon \hat{w}_A(-\mathbf{k}))} - \frac{n_s}{n_l+\kappa n_s}\frac{\partial \log Q_s}{\partial(\epsilon \hat{w}_A(-\mathbf{k}))} \\
&\approx \frac{n_l}{n_l+\kappa n_s}\left\{ f_{l,A}\delta_{\mathbf{k},\mathbf{0}} - P_{l,A}(\mathbf{k})\epsilon\hat{w}_{1,A} - \frac{1}{2}\left[P_l(\mathbf{k}) - P_{l,B}(\mathbf{k}) - P_{l.A}(\mathbf{k})\right]\epsilon\hat{w}_{1,B}\right\} \\
&\quad + \frac{n_s}{n_l+\kappa n_s}\left\{ \kappa f_{s,A}\delta_{\mathbf{k},\mathbf{0}} - P_{s,A}(\mathbf{k})\epsilon\hat{w}_{1,A} - \frac{1}{2}\left[P_s(\mathbf{k}) - P_{s,B}(\mathbf{k}) - P_{s,A}(\mathbf{k})\right]\epsilon\hat{w}_{1,B}\right\}
\end{aligned} \tag{110}$$

$$\begin{aligned}
\hat{\phi}_B(\mathbf{k}; w_A, w_B) &= -\frac{n_l}{n_l+\kappa n_s} V\widehat{\left(\frac{\delta \log Q_l}{\delta(\epsilon w_{1,B}(\mathbf{r}))}\right)}(\mathbf{k}) - \frac{n_s}{n_l+\kappa n_s} V\widehat{\left(\frac{\delta \log Q_s}{\delta(\epsilon w_{1,B}(\mathbf{r}))}\right)}(\mathbf{k}) \\
&= -\frac{n_l}{n_l+\kappa n_s}\frac{\partial \log Q_l}{\partial(\epsilon \hat{w}_B(-\mathbf{k}))} - \frac{n_s}{n_l+\kappa n_s}\frac{\partial \log Q_s}{\partial(\epsilon \hat{w}_B(-\mathbf{k}))} \\
&\approx \frac{n_l}{n_l+\kappa n_s}\left\{ (1-f_{l,A})\delta_{\mathbf{k},\mathbf{0}} - P_{l,B}(\mathbf{k})\epsilon\hat{w}_{1,B} - \frac{1}{2}\left[P_l(\mathbf{k}) - P_{l,B}(\mathbf{k}) - P_{l.A}(\mathbf{k})\right]\epsilon\hat{w}_{1,A}\right\} \\
&\quad + \frac{n_s}{n_l+\kappa n_s}\left\{ \kappa(1-f_{s,A})\delta_{\mathbf{k},\mathbf{0}} - P_{s,B}(\mathbf{k})\epsilon\hat{w}_{1,B} - \frac{1}{2}\left[P_s(\mathbf{k}) - P_{s,B}(\mathbf{k}) - P_{s,A}(\mathbf{k})\right]\epsilon\hat{w}_{1,A}\right\}
\end{aligned} \tag{111}$$

The above expressions are the first order weak inhomogeneity expansion of $\phi_A(\mathbf{r}; w_A, w_B)$ and $\phi_B(\mathbf{r}; w_A, w_B)$. Now we denote that

$$\begin{aligned}
\delta w_A(\mathbf{r}; J_A) &= \epsilon w_{1,A}(\mathbf{r}; J_A) = w_A(\mathbf{r}; J_A) - w_{0,A} \\
\delta w_B(\mathbf{r}; J_B) &= \epsilon w_{1,B}(\mathbf{r}; J_B) = w_B(\mathbf{r}; J_B) - w_{0,B} \\
\delta\phi_A(\mathbf{r}; J_A) &= \epsilon\phi_{1,A}(\mathbf{r}; J_A) = \phi_A(\mathbf{r}; J_A) - \phi_{0,A} \\
\delta\phi_B(\mathbf{r}; J_B) &= \epsilon\phi_{1,B}(\mathbf{r}; J_B) = \phi_B(\mathbf{r}; J_B) - \phi_{0,B} \\
\delta\xi(\mathbf{r}; J_B) &= \frac{\delta w_A(\mathbf{r}; J_A) + \delta w_B(\mathbf{r}; J_B)}{2}
\end{aligned} \tag{112}$$

Using the mean-field equations, we can obtain that

$$\delta w_A(\mathbf{r}; J_A) = \chi N_l \delta\phi_B(\mathbf{r}; J_A) + \delta\xi(\mathbf{r}; J_A) \tag{113}$$
$$\delta w_B(\mathbf{r}; J_A) = \chi N_l \delta\phi_A(\mathbf{r}; J_A) + \delta\xi(\mathbf{r}; J_A) \tag{114}$$

Actually, the above expressions are SCF equations of the first order expansion with respect to ϵ. The incompressible condition is

$$\delta\phi_A(\mathbf{r}) + \delta\phi_B(\mathbf{r}) = 0 \tag{115}$$

In Fourier space, the above equation becomes

$$\delta\hat{\phi}_A(\mathbf{k}) + \delta\hat{\phi}_B(\mathbf{k}) = 0 \tag{116}$$

$$\begin{aligned}\delta\hat{\phi}_A(\mathbf{k}) \approx \frac{n_l}{n_l+\kappa n_s}\left\{-P_{l,A}(\mathbf{k})[N_l\hat{J}_A(\mathbf{k}) + \chi N_l\delta\hat{\phi}_B(\mathbf{k}) + \delta\hat{\xi}(\mathbf{k})] - \frac{1}{2}\left[P_l(\mathbf{k}) - P_{l,B}(\mathbf{k}) - P_{l.A}(\mathbf{k})\right][\chi N_l\delta\hat{\phi}_A(\mathbf{k}) + \delta\hat{\xi}(\mathbf{k})]\right\} \\ + \frac{n_s}{n_l+\kappa n_s}\left\{-P_{s,A}(\mathbf{k})[N_l\hat{J}_A(\mathbf{k}) + \chi N_l\delta\hat{\phi}_B(\mathbf{k}) + \delta\hat{\xi}(\mathbf{k})] - \frac{1}{2}\left[P_s(\mathbf{k}) - P_{s,f_B}(\mathbf{k}) - P_{s,A}(\mathbf{k})\right][\chi N_l\delta\hat{\phi}_A(\mathbf{k}) + \delta\hat{\xi}(\mathbf{k})]\right\}\end{aligned} \tag{117}$$

$$\begin{aligned}\delta\hat{\phi}_B(\mathbf{k}) \approx \frac{n_l}{n_l+\kappa n_s}\left\{-P_{l,B}(\mathbf{k})[\chi N_l\delta\hat{\phi}_A(\mathbf{k}) + \hat{\xi}(\mathbf{k})] - \frac{1}{2}\left[P_l(\mathbf{k}) - P_{l,B}(\mathbf{k}) - P_{l.A}(\mathbf{k})\right][N_l\hat{J}_A(\mathbf{k}) + \chi N_l\delta\hat{\phi}_B(\mathbf{k}) + \delta\hat{\xi}(\mathbf{k})]\right\} \\ + \frac{n_s}{n_l+\kappa n_s}\left\{-P_{s,B}(\mathbf{k})[\chi N_l\delta\hat{\phi}_A(\mathbf{k}) + \hat{\xi}(\mathbf{k})] - \frac{1}{2}\left[P_s(\mathbf{k}) - P_{s,B}(\mathbf{k}) - P_{s,A}(\mathbf{k})\right][N_l\hat{J}_A(\mathbf{k}) + \chi N_l\delta\hat{\phi}_B(\mathbf{k}) + \delta\hat{\xi}(\mathbf{k})]\right\}\end{aligned} \tag{118}$$

From above three equations, we can obtain

$$\delta\hat{\phi}_A(\mathbf{k}) \approx -s(\mathbf{k})\hat{J}(\mathbf{k}) \tag{119}$$

In the above expression,

$$s(\mathbf{k}) = N_l\left[\frac{1}{c_A}(\tilde{n}_l\tilde{Q}_l + \tilde{n}_s\tilde{Q}_s) - \frac{1}{c_B}(\tilde{n}_lP_{l,A} + \tilde{n}_sP_{s,A})\right]\left(\frac{c_Ac_B}{c_Bd_A - c_Ad_B}\right) \tag{120}$$

where

$$\begin{aligned}\tilde{n}_l &= \frac{n_l}{n_l+\kappa n_s}, \quad \tilde{n}_s = \frac{n_s}{n_l+\kappa n_s}, \\ \tilde{Q}_l(\mathbf{k}) &= P_l(\mathbf{k}) - P_{l,B}(\mathbf{k}) - P_{l,A}(\mathbf{k}), \\ \tilde{Q}_s(\mathbf{k}) &= P_s(\mathbf{k}) - P_{s,B}(\mathbf{k}) - P_{s,A}(\mathbf{k}), \\ c_A(\mathbf{k}) &= \tilde{n}_lP_{l.A} + \tilde{n}_sP_{s.A} + \frac{1}{2}(\tilde{n}_s\tilde{Q}_s + \tilde{n}_l\tilde{Q}_l) \\ c_B(\mathbf{k}) &= \tilde{n}_lP_{l.B} + \tilde{n}_sP_{s.B} + \frac{1}{2}(\tilde{n}_s\tilde{Q}_s + \tilde{n}_l\tilde{Q}_l) \\ d_A(\mathbf{k}) &= -1 + \chi N_l(\tilde{n}_lP_{l,A} + \tilde{n}_sP_{s,A}) - \frac{1}{2}\chi N_l(\tilde{n}_s\tilde{Q}_s + \tilde{n}_l\tilde{Q}_l) \\ d_B(\mathbf{k}) &= 1 - \chi N_l(\tilde{n}_lP_{l,B} + \tilde{n}_sP_{s,B}) + \frac{1}{2}\chi N_l(\tilde{n}_s\tilde{Q}_s + \tilde{n}_l\tilde{Q}_l)\end{aligned} \tag{121}$$

Therefore,

$$\hat{J}_A(\mathbf{k}) \approx -s^{-1}(\mathbf{k})\delta\hat{\phi}_A(\mathbf{k}) \tag{122}$$

$$\widehat{\left(\frac{\delta F}{\delta\phi_A}\right)}(\mathbf{k}) = -\rho_0\hat{J}_A(\mathbf{k}) \tag{123}$$

$$\widehat{\left(\frac{\delta F}{\delta\phi_A}\right)}(\mathbf{k}) = \frac{1}{V}\frac{\delta F}{\delta\hat{\phi}_A(-\mathbf{k})} \tag{124}$$

Therefore,

$$\frac{\delta F}{\delta\hat{\phi}_A(-\mathbf{k})} \approx (n_l+\kappa n_s)N_ls^{-1}(\mathbf{k})\delta\hat{\phi}_A(\mathbf{k}) \tag{125}$$

Integraling the above equation, we can obtain the free energy density

$$\frac{F}{n_l+\kappa n_s}=\frac{F_0}{n_l+\kappa n_s}+\frac{1}{2}\sum_{\mathbf{k}}N_l s^{-1}(\mathbf{k})\delta\hat{\phi}_A(\mathbf{k})\delta\hat{\phi}_A(-\mathbf{k}) \tag{126}$$

F_0 is the energy value of the homogeneous phase. For the homogeneous phase, the propagators $q_\alpha(\mathbf{r},s)=q_\alpha^\dagger(\mathbf{r},s)=1$, and the fields $w_A(\mathbf{r})=w_B(\mathbf{r})=0$. The density functions are

$$\begin{aligned}\phi_{A,h}&=\frac{n_l}{n_l+\kappa n_s}f_{l,A}+\frac{n_s}{n_l+\kappa n_s}f_{s,A}\\ \phi_{B,h}&=\frac{n_l}{n_l+\kappa n_s}f_{l,B}+\frac{n_s}{n_l+\kappa n_s}f_{s,B}\end{aligned} \tag{127}$$

Therefore

$$\frac{F_0}{n_l+\kappa n_s}=\chi N_l\phi_A\phi_B=\frac{\chi N_l}{(n_l+\kappa n_s)^2}\Big\{(n_l f_{l,A}+\kappa n_s f_{s,A})[n_l(1-f_{l,A})+\kappa n_s(1-f_{s,A})]\Big\} \tag{128}$$

Defining $S^{-1}(\mathbf{k})=N_l s^{-1}(\mathbf{k})$, and assume that $\phi(\mathbf{r})\equiv\delta\phi_A(\mathbf{r})=\phi_A(\mathbf{r})-\phi_{A,h}$. Then the free energy density becomes

$$\frac{F}{n_l+\kappa n_s}=\frac{F_0}{n_l+\kappa n_s}+\frac{1}{2}\sum_{\mathbf{k}}S^{-1}(\mathbf{k})\delta\hat{\phi}_A(\mathbf{k})\delta\hat{\phi}_A(-\mathbf{k}) \tag{129}$$

In the following, we will analyse the properties of correlation function $S^{-1}(\mathbf{k})$, i.e.,

$$S^{-1}(\mathbf{k})=\frac{c_B(\mathbf{k})d_A(\mathbf{k})-c_A(\mathbf{k})d_B(\mathbf{k})}{c_B(\mathbf{k})\big[\tilde{n}_l\tilde{Q}(\mathbf{k})+\tilde{n}_s\tilde{Q}_s(\mathbf{k})\big]-c_A(\mathbf{k})\big[\tilde{n}_l P_{l,A}(\mathbf{k})+\tilde{n}_s P_{s,A}(\mathbf{k})\big]} \tag{130}$$

V. SCFT OF ABC STAR COPOLYMER MELT

The field-based effective Hamiltonian by δ-functional technology is

$$H = \frac{n}{V}\int d\mathbf{r}\,[\chi_{AB}N\rho_A\rho_B + \chi_{BC}N\rho_B\rho_C + \rho_{AC}N\rho_A\rho_C - w_A\rho_A - w_B\rho_B - w_B\rho_B - \xi(1-\rho_A-\rho_B-\rho_C)] - n\log Q[w_A, w_B, w_C]. \tag{131}$$

Minimizing the mean-field Hamiltonian leads to self-consistent field equations

$$w_A(\mathbf{r}) = \chi_{AB}N_C\rho_B(\mathbf{r}) + \chi_{AC}N_C\rho_C(\mathbf{r}) + w_+(\mathbf{r}), \tag{132}$$
$$w_B(\mathbf{r}) = \chi_{AB}N_C\rho_A(\mathbf{r}) + \chi_{BC}N_C\rho_C(\mathbf{r}) + w_+(\mathbf{r}), \tag{133}$$
$$w_C(\mathbf{r}) = \chi_{AC}N_C\rho_A(\mathbf{r}) + \chi_{BC}N_C\rho_B(\mathbf{r}) + w_+(\mathbf{r}), \tag{134}$$
$$\rho_A + \rho_B + \rho_C = 1, \tag{135}$$
$$\rho_A = \frac{1}{Q}\int_0^{f_A} ds\, q_A(\mathbf{r}, s)q_A^\dagger(\mathbf{r}, f_A - s), \tag{136}$$
$$\rho_B = \frac{1}{Q}\int_0^{f_B} ds\, q_B(\mathbf{r}, s)q_B^\dagger(\mathbf{r}, f_B - s), \tag{137}$$
$$\rho_C = \frac{1}{Q}\int_0^{f_C} ds\, q_C(\mathbf{r}, s)q_C^\dagger(\mathbf{r}, f_C - s), \tag{138}$$
$$Q = \frac{1}{V}\int d\mathbf{r}\, q_\alpha(\mathbf{r}, s)q_\alpha^\dagger(\mathbf{r}, f_\alpha - s), \qquad \forall s, \alpha. \tag{139}$$

The propagators of the star triblock copolymer satisfy the modified diffusion equations,

$$\frac{\partial}{\partial s}q_\alpha(\mathbf{r}, s) = \nabla_{\mathbf{r}}^2 q_\alpha(\mathbf{r}, s) - w_\alpha q_\alpha(\mathbf{r}, s), \quad q_\alpha(\mathbf{r}, 0) = 1, \quad s \in [0, f_\alpha], \tag{140}$$
$$\frac{\partial}{\partial s}q_\alpha^\dagger(\mathbf{r}, s) = \nabla_{\mathbf{r}}^2 q_\alpha^\dagger(\mathbf{r}, s) - w_\alpha q_\alpha^\dagger(\mathbf{r}, s), \quad q_\alpha^\dagger(\mathbf{r}, 0) = q_\beta(\mathbf{r}, f_\beta)q_\gamma(\mathbf{r}, f_\gamma), \tag{141}$$

where $(\alpha\beta\gamma) \in \{(ABC), (BCA), (CAB)\}$.

The field-based effective Hamiltonian by Gaussian functional integral technology is

$$H = \frac{n}{V}\int d\mathbf{r}\left(\frac{1}{4N\zeta_1}\mu_1^2 + \frac{1}{4N\zeta_2}\mu_2^2 - \mu_+\right) - n\log Q[\omega_A, \omega_B, \omega_C], \tag{142}$$
$$\omega_\alpha = \mu_+ - \sigma_{1\alpha}\mu_1 - \sigma_{2\alpha}\mu_2, \quad \alpha \in \{A, B, C\}. \tag{143}$$

In this expression,

$$\zeta_1 = \frac{-\Delta}{4\chi_{AC}}, \qquad \zeta_2 = \chi_{AC}, \tag{144}$$
$$\Delta = \chi_{AB}^2 + \chi_{AC}^2 + \chi_{BC}^2 - 2\chi_{AB}\chi_{AC} - 2\chi_{AB}\chi_{BC} - 2\chi_{AC}\chi_{BC}. \tag{145}$$

The coefficients $\sigma_{k\alpha}$ are

$$\begin{aligned} &\sigma_{1A} = \frac{1}{3}, \qquad \sigma_{1B} = -\frac{2}{3}, \qquad \sigma_{1C} = \frac{1}{3}, \\ &\sigma_{2A} = \frac{1+\alpha}{3}, \quad \sigma_{2B} = \frac{1-2\alpha}{3}, \quad \sigma_{2C} = \frac{\alpha-2}{3}, \quad \alpha = \frac{\chi_{AC}+\chi_{AB}-\chi_{BC}}{2\chi_{AC}}. \end{aligned} \tag{146}$$

The corresponding SCFT equations are

$$\rho_A + \rho_B + \rho_C - 1 = 0, \tag{147}$$
$$\frac{1}{2N\zeta_1}\mu_1 - \sigma_{1A}\rho_A - \sigma_{1B}\rho_B - \sigma_{1C}\rho_C = 0, \tag{148}$$
$$\frac{1}{2N\zeta_2}\mu_2 - \sigma_{2A}\rho_A - \sigma_{2B}\rho_B - \sigma_{2C}\rho_C = 0. \tag{149}$$

VI. SCFT OF ABC STAR COPOLYMER AND B HOMOPOLYMER BLENDS

A detailed derivation process of the SCFT of ABC star triblock copolymer and B homopolymer blends is given in this section.

	Notations
Kuhn length	$b_A = b_B = b_C = b$
Volume of the system	V
Degree of polymerization of ABC star triblock copolymer	N_C
Degree of polymerization of α block	N_α, $\alpha = A, B, C$
α-segment fraction	$f_\alpha = N_\alpha/N_C$
Degree of polymerization of B homopolymer	N_H
Ratio of polymerization of two polymers	$\kappa = N_H/N_C$
Number of ABC star triblock copolymer	n_C
Number of B homopolymer	n_H
Average Number density of segments	$\rho_0 = (n_C N_C + n_H N_H)/V$
Molecular configuration of ABC star triblock copolymer	Γ_i, $i = 1, \cdots, n$
Molecular configuration of B homopolymer	$\tilde{\Gamma}_j$, $j = 1, \cdots, n_H$

Microscopic segment density operators

$$\hat{\rho}_A(\mathbf{r}) = \frac{N_C}{\rho_0} \sum_{i=1}^{n_C} \int_0^{f_A} ds\, \delta(\mathbf{r} - \Gamma_i(s)), \tag{150}$$

$$\hat{\rho}_B(\mathbf{r}) = \frac{N_C}{\rho_0} \sum_{i=1}^{n_C} \int_0^{f_B} ds\, \delta(\mathbf{r} - \Gamma_i(s)) + \frac{N_H}{\rho_0} \sum_{j=1}^{n_H} \int_0^1 ds\, \delta(\mathbf{r} - \tilde{\Gamma}_j(s)), \tag{151}$$

$$\hat{\rho}_C(\mathbf{r}) = \frac{N_C}{\rho_0} \sum_{i=1}^{n_C} \int_0^{f_C} ds\, \delta(\mathbf{r} - \Gamma_i(s)). \tag{152}$$

In the following, we denote $\hat{\rho}_+ = \sum_\alpha \hat{\rho}_\alpha$.

Elastic potential energy based on continuous Gaussian chain model

$$\beta U_0 = \sum_{i=1}^{n_C} \int_0^1 ds\, \frac{3}{2N_C b^2} \Big| \frac{d\Gamma_i(s)}{ds} \Big|^2 + \sum_{j=1}^{n_H} \int_0^1 ds\, \frac{3}{2N_H b^2} \Big| \frac{d\tilde{\Gamma}_j(s)}{ds} \Big|^2. \tag{153}$$

Segment-segment interaction potential energy

$$\beta U_1 = \rho_0 \chi_{AB} \int d\mathbf{r}\, \hat{\rho}_A \hat{\rho}_B + \rho_0 \chi_{AC} \int d\mathbf{r}\, \hat{\rho}_A \hat{\rho}_C + \rho_0 \chi_{BC} \int d\mathbf{r}\, \hat{\rho}_B \hat{\rho}_C. \tag{154}$$

The partition function for the incompressible star triblock copolymer-homoploymer blends is

$$Z[\Gamma, \tilde{\Gamma}] = \prod_{i=1}^{n_C} \int D\Gamma_i \prod_{j=1}^{n_H} \int D\tilde{\Gamma}_j \, \exp\Big\{ - \beta U_0 - \beta U_1 \Big\} \delta(1 - \hat{\rho}_+) \tag{155}$$

In order to obtain the field based partition function, we use the particle-to-field transformation through introducing δ functional

$$\int D\rho_\alpha \, \delta[\rho_\alpha(\mathbf{r}) - \hat{\rho}_\alpha(\mathbf{r})] = 1, \tag{156}$$

and corresponding Fourier transformations.

$$\delta[\rho_\alpha - \hat{\rho}_\alpha] = \int DW_\alpha \exp\Big\{ \int d\mathbf{r}\, iW_\alpha(\rho_\alpha - \hat{\rho}_\alpha) \Big\}. \tag{157}$$

The partition function becomes

$$
\begin{aligned}
Z[\Gamma,\tilde{\Gamma}] = &\prod_{\alpha}\int DW_{\alpha}\prod_{\alpha}\int D\rho_{\alpha}\int DW_{+}\,\exp\Big\{-\int d\mathbf{r}\sum_{\alpha\neq\beta}\rho_0\chi_{\alpha\beta}\rho_{\alpha}\rho_{\beta}+\int d\mathbf{r}\sum_{\alpha}iW_{\alpha}\rho_{\alpha}-\int d\mathbf{r}\,iW_{+}(\rho_{+}-1)\Big\}\\
&\times\prod_{i=1}^{n_C}\int D\Gamma_i\prod_{j=1}^{n_H}\int D\tilde{\Gamma}_j\,\exp\Big\{-\int d\mathbf{r}\sum_{\alpha}iW_{\alpha}\hat{\rho}_{\alpha}-\sum_{i=1}^{n_C}\int_0^1 ds\,\frac{3}{2N_Cb^2}\Big|\frac{d\Gamma_i(s)}{ds}\Big|^2-\sum_{i=1}^{n_H}\int_0^1 ds\,\frac{3}{2N_Hb^2}\Big|\frac{d\tilde{\Gamma}_j(s)}{ds}\Big|^2\Big\}\\
=&\prod_{\alpha}\int DW_{\alpha}\prod_{\alpha}\int D\rho_{\alpha}\int DW_{+}\,\exp\Big\{-\int d\mathbf{r}\sum_{\alpha\neq\beta}\rho_0\chi_{\alpha\beta}\rho_{\alpha}\rho_{\beta}+\int d\mathbf{r}\sum_{\alpha}iW_{\alpha}\rho_{\alpha}-\int d\mathbf{r}\,iW_{+}(\rho_{+}-1)\Big\}\\
&\times\prod_{i=1}^{n_C}\int D\Gamma_i\exp\Big\{-\frac{N_C}{\rho_0}\sum_{i=1}^{n_C}\Big[\sum_{\alpha}\int_0^{f_{\alpha}}ds\,iW_{\alpha}(\Gamma_i(s))\Big]-\sum_{i=1}^{n_C}\int_0^1 ds\,\frac{3}{2N_Cb^2}\Big|\frac{d\Gamma_i(s)}{ds}\Big|^2\Big\}\\
&\times\prod_{j=1}^{n_H}\int D\tilde{\Gamma}_j\,\exp\Big\{-\frac{N_H}{\rho_0}\sum_{j=1}^{n_H}\int_0^1 ds\,iW_B(\tilde{\Gamma}_j(s))-\sum_{i=1}^{n_H}\int_0^1 ds\,\frac{3}{2N_Hb^2}\Big|\frac{d\tilde{\Gamma}_j(s)}{ds}\Big|^2\Big\},
\end{aligned}
\tag{158}
$$

where $\alpha,\beta\in\{A,B,C\}$. In order to simplify the above expression, letting $w_{\alpha}=\frac{N_C}{\rho_0}iW_{\alpha}$, $w_{+}=\frac{N_C}{\rho_0}iW_{+}$, and introducing the single-chain partition function for the ABC star triblock copolymer

$$
Q_C=\int D\Gamma\exp\Big\{-\sum_{\alpha}\int_0^{f_{\alpha}}ds\,w_{\alpha}(\Gamma_i(s))-\frac{3}{2N_Cb^2}\int_0^1 ds\,\Big|\frac{d\Gamma_i(s)}{ds}\Big|^2\Big\},
\tag{159}
$$

and the B-homopolymer

$$
Q_H=\int D\tilde{\Gamma}\,\exp\Big\{-\int_0^{\kappa}ds\,w_B(\tilde{\Gamma}_j(s))-\frac{3}{2N_Cb^2}\int_0^{\kappa}ds\,\Big|\frac{d\tilde{\Gamma}_j(s)}{ds}\Big|^2\Big\},
\tag{160}
$$

one can obtain

$$
\begin{aligned}
Z[\Gamma,\tilde{\Gamma}]=\prod_{\alpha}\int Dw_{\alpha}\prod_{\alpha}\int D\rho_{\alpha}\int Dw_{+}\,\exp\Big\{\frac{\rho_0}{N_C}\Big[&-\int d\mathbf{r}\sum_{\alpha\neq\beta}N_C\chi_{\alpha\beta}\rho_{\alpha}\rho_{\beta}+\int d\mathbf{r}\sum_{\alpha}w_{\alpha}\rho_{\alpha}\\
&-\int d\mathbf{r}\,w_{+}(\rho_{+}-1)\Big]+n_C\ln Q_C[w_A,w_B,w_C]+n_H\ln Q_H[w_B]\Big\}.
\end{aligned}
\tag{161}
$$

Note ρ_0 is the number density of segments, the partition function can be rewritten as

$$
Z[w_{\alpha},w_{+},\rho_{\alpha}]=\prod_{\alpha}\int Dw_{\alpha}\prod_{\alpha}\int D\rho_{\alpha}\int Dw_{+}\,\exp\Big\{-(n_C+\kappa n_H)H[w_{\alpha},w_{+},\rho_{\alpha}]\Big\},
\tag{162}
$$

the field-based Hamiltonian is

$$
\begin{aligned}
H[w_{\alpha},w_{+},\rho_{\alpha}]=&\frac{1}{V}\int d\mathbf{r}\sum_{\alpha\neq\beta}N_C\chi_{\alpha\beta}\rho_{\alpha}\rho_{\beta}-\frac{1}{V}\int d\mathbf{r}\sum_{\alpha}w_{\alpha}\rho_{\alpha}+\frac{1}{V}\int d\mathbf{r}\,w_{+}(\rho_{+}-1)\\
&-\frac{n_C}{n_C+\kappa n_H}\ln Q_C[w_A,w_B,w_C]-\frac{n_H}{n_C+\kappa n_H}\ln Q_H[w_B].
\end{aligned}
\tag{163}
$$

Within mean-field (saddle-point) approximation, at equilibrium configuration $[w_{\alpha}^{*},w_{+}^{*},\rho_{\alpha}^{*}]$,

$$
Z[w_{\alpha},w_{+},\rho_{\alpha}]\Big|_{[w_{\alpha}^{*},w_{+}^{*},\rho_{\alpha}^{*}]}\approx H[w_{\alpha}^{*},w_{+}^{*},\rho_{\alpha}^{*}].
\tag{164}
$$

For brevity, we will omit the * in the following. Minimizing the mean-field Hamiltonian leads to self-consistent field

equations

$$w_A(\mathbf{r}) = \chi_{AB}N_C\rho_B(\mathbf{r}) + \chi_{AC}N_C\rho_C(\mathbf{r}) + w_+(\mathbf{r}), \tag{165}$$
$$w_B(\mathbf{r}) = \chi_{AB}N_C\rho_A(\mathbf{r}) + \chi_{BC}N_C\rho_C(\mathbf{r}) + w_+(\mathbf{r}), \tag{166}$$
$$w_C(\mathbf{r}) = \chi_{AC}N_C\rho_A(\mathbf{r}) + \chi_{BC}N_C\rho_B(\mathbf{r}) + w_+(\mathbf{r}), \tag{167}$$
$$\rho_A + \rho_B + \rho_C = 1, \tag{168}$$
$$\rho_A = \frac{n_C}{n_C + \kappa n_H}\frac{1}{Q_C}\int_0^{f_A} ds\, q_A(\mathbf{r}, s)q_A^\dagger(\mathbf{r}, 1-s), \tag{169}$$
$$\rho_B = \frac{n_C}{n_C + \kappa n_H}\frac{1}{Q_C}\int_0^{f_B} ds\, q_B(\mathbf{r}, s)q_B^\dagger(\mathbf{r}, 1-s) + \frac{n_H}{n_C + \kappa n_H}\frac{1}{Q_H}\int_0^{\kappa} ds\, q_H(\mathbf{r}, s)q_H^\dagger(\mathbf{r}, 1-s), \tag{170}$$
$$\rho_C = \frac{n_C}{n_C + \kappa n_H}\frac{1}{Q_C}\int_0^{f_C} ds\, q_C(\mathbf{r}, s)q_C^\dagger(\mathbf{r}, 1-s), \tag{171}$$
$$Q_C = \frac{1}{V}\int d\mathbf{r}\, q_\alpha(\mathbf{r}, s)q_\alpha^\dagger(\mathbf{r}, 1-s) \quad \forall s, \alpha, \tag{172}$$
$$Q_H = \frac{1}{V}\int d\mathbf{r}\, q_H(\mathbf{r}, \kappa). \tag{173}$$

In the above expression, the functions $q_\alpha(\mathbf{r}, s)$, $q_\alpha^\dagger(\mathbf{r}, s)$, ($\alpha \in A, B, C$) and $q_H(\mathbf{r}, s)$, $q_H^\dagger(\mathbf{r}, s)$ are the end-integrated segment distribution functions, or propagators, representing the probability of finding the s-th segment at a particular position $\mathbf{r}$. The propagators of the star triblock copolymer satisfy the modified diffusion equations,

$$\frac{\partial}{\partial s}q_\alpha(\mathbf{r}, s) = \nabla_{\mathbf{r}}^2 q_\alpha(\mathbf{r}, s) - w_\alpha q_\alpha(\mathbf{r}, s), \quad q_\alpha(\mathbf{r}, 0) = 1, \quad s \in [0, f_\alpha], \tag{174}$$
$$\frac{\partial}{\partial s}q_\alpha^\dagger(\mathbf{r}, s) = \nabla_{\mathbf{r}}^2 q_\alpha^\dagger(\mathbf{r}, s) - w_\alpha q_\alpha^\dagger(\mathbf{r}, s), \quad q_\alpha^\dagger(\mathbf{r}, 0) = q_\beta(\mathbf{r}, f_\beta)q_\gamma(\mathbf{r}, f_\gamma), \tag{175}$$

where $(\alpha\beta\gamma) \in \{(ABC), (BCA), (CAB)\}$. The propagators of the B-homopolymer satisfy the modified diffusion equations,

$$\frac{\partial}{\partial s}q_H(\mathbf{r}, s) = \nabla_{\mathbf{r}}^2 q_H(\mathbf{r}, s) - w_B q_H(\mathbf{r}, s), \quad q_H(\mathbf{r}, 0) = 1, \quad s \in [0, \kappa], \tag{176}$$
$$\frac{\partial}{\partial s}q_H^\dagger(\mathbf{r}, s) = \nabla_{\mathbf{r}}^2 q_H^\dagger(\mathbf{r}, s) - w_B q_H^\dagger(\mathbf{r}, s), \quad q_H^\dagger(\mathbf{r}, 0) = 1, \quad s \in [0, \kappa]. \tag{177}$$

Then we can solve the integrated SCFT system of Eqns. (165)-(177).

The field-based effective Hamiltonian by Gaussian functional integral technology is

$$H = \frac{1}{V}\int d\mathbf{r}\left(\frac{1}{4N\zeta_1}\mu_1^2 + \frac{1}{4N\zeta_2}\mu_2^2 - \mu_+\right) - \frac{n_C}{n_C + \kappa n_H}\ln Q_C[w_A, w_B, w_C] - \frac{n_H}{n_C + \kappa n_H}\ln Q_H[w_B]. \tag{178}$$
$$\omega_\alpha = \mu_+ - \sigma_{1\alpha}\mu_1 - \sigma_{2\alpha}\mu_2, \quad \alpha \in \{A, B, C\}. \tag{179}$$

The coefficients $\sigma_{k\alpha}$ are

$$\begin{aligned} &\sigma_{1A} = \frac{1}{3}, \qquad \sigma_{1B} = -\frac{2}{3}, \qquad \sigma_{1C} = \frac{1}{3}, \\ &\sigma_{2A} = \frac{1+\alpha}{3}, \quad \sigma_{2B} = \frac{1-2\alpha}{3}, \quad \sigma_{2C} = \frac{\alpha-2}{3}, \quad \alpha = \frac{\chi_{AC} + \chi_{AB} - \chi_{BC}}{2\chi_{AC}}. \end{aligned} \tag{180}$$

The corresponding SCFT equations are

$$\rho_A + \rho_B + \rho_C - 1 = 0, \tag{181}$$
$$\frac{1}{2N\zeta_1}\mu_1 - \sigma_{1A}\rho_A - \sigma_{1B}\rho_B - \sigma_{1C}\rho_C = 0, \tag{182}$$
$$\frac{1}{2N\zeta_2}\mu_2 - \sigma_{2A}\rho_A - \sigma_{2B}\rho_B - \sigma_{2C}\rho_C = 0. \tag{183}$$

VII. SCFT OF ABA'C LINEAR TETRABLOCK COPOLYMERS

The effective mean-field Hamiltonian of ABA'C linear tetrablock terpolymer system is

$$\frac{H}{nk_BT} = -\ln Q[w_A, w_B, w_C] + \frac{1}{V}\int d\mathbf{r}\,[\chi_{AB}N\rho_A\rho_B + \chi_{BC}N\rho_B\rho_C + \rho_{AC}N\rho_A\rho_C - w_A\rho_A - w_B\rho_B - w_B\rho_B - w_+(1-\rho_A-\rho_B-\rho_C)]. \tag{184}$$

Minimizing the above Hamiltonian leads to the SCF equations

$$w_A(\mathbf{r}) = \chi_{AB}N\rho_B(\mathbf{r}) + \chi_{AC}N\rho_C(\mathbf{r}) + w_+(\mathbf{r}), \tag{185}$$
$$w_B(\mathbf{r}) = \chi_{AB}N\rho_A(\mathbf{r}) + \chi_{BC}N\rho_C(\mathbf{r}) + w_+(\mathbf{r}), \tag{186}$$
$$w_C(\mathbf{r}) = \chi_{AC}N\rho_A(\mathbf{r}) + \chi_{BC}N\rho_B(\mathbf{r}) + w_+(\mathbf{r}), \tag{187}$$
$$\rho_A + \rho_B + \rho_C = 1, \tag{188}$$

where

$$Q = \frac{1}{V}\int d\mathbf{r}\, q(\mathbf{r},s)q^\dagger(\mathbf{r},1-s), \quad \forall s\in[0,1], \tag{189}$$
$$\rho_A(\mathbf{r}) = \frac{1}{Q}\left[\int_0^{f_{A_1}} + \int_{f_{A_1}+f_B}^{f_{A_1}+f_B+f_{A_2}}\right] ds\, q(\mathbf{r},s)q^\dagger(\mathbf{r},1-s), \tag{190}$$
$$\rho_B(\mathbf{r}) = \frac{1}{Q}\int_{f_{A_1}}^{f_{A_1}+f_B} ds\, q(\mathbf{r},s)q^\dagger(\mathbf{r},1-s), \tag{191}$$
$$\rho_C(\mathbf{r}) = \frac{1}{Q}\int_{f_{A_1}+f_B+f_{A_2}}^{1} ds\, q(\mathbf{r},s)q^\dagger(\mathbf{r},1-s). \tag{192}$$

The forward propagator operator satisfies the following modified diffusion equation

$$\frac{\partial}{\partial s}q(\mathbf{r},s) = \nabla^2 q(\mathbf{r},s) - w(\mathbf{r},s)q(\mathbf{r},s), \quad q(\mathbf{r},0)=1, \tag{193}$$

where

$$w(\mathbf{r},s) = \begin{cases} w_A(\mathbf{r}), & 0\leqslant s\leqslant f_{A_1}, \text{ or } f_{A_1}+f_B+f_C\leqslant s\leqslant 1,\\ w_B(\mathbf{r}), & f_{A_1}\leqslant s\leqslant f_{A_1}+f_B,\\ w_C(\mathbf{r}), & f_{A_1}+f_B\leqslant s\leqslant f_{A_1}+f_B+f_C. \end{cases} \tag{194}$$

The back propagator operator satisfies

$$\frac{\partial}{\partial s}q^\dagger(\mathbf{r},s) = \nabla^2 q^\dagger(\mathbf{r},s) - w^\dagger(\mathbf{r},s)q^\dagger(\mathbf{r},s), \quad q^\dagger(\mathbf{r},0)=1, \tag{195}$$

where

$$w^\dagger(\mathbf{r},s) = \begin{cases} w_A(\mathbf{r}), & 0\leqslant s\leqslant f_{A_2}, \text{ or } f_{A_2}+f_C+f_B\leqslant s\leqslant 1,\\ w_B(\mathbf{r}), & f_{A_2}+f_C\leqslant s\leqslant f_{A_2}+f_C+f_B,\\ w_C(\mathbf{r}), & f_{A_2}\leqslant s\leqslant f_{A_2}+f_C. \end{cases} \tag{196}$$

VIII. SCFT OF AB SEMIFLEXIBLE-FLEXIBLE DIBLOCK COPOLYMER MELT

	Notations
Volume of the system	V
Size Asymmetry ratio measuring different block	$\nu = (a/b)(6N)^{1/2}$
Maier-Saupe interaction parameter	η
Stiff parameter of semiflexible chain	λ

The mean-field Hamiltonian functional is

$$H[\mu_+,\mu_-,\mathbf{M}] = \frac{n}{\chi NV}\int d\mathbf{r}\,\mu_-^2(\mathbf{r}) - \frac{n}{V}\int d\mathbf{r}\,\mu_+(\mathbf{r}) + \frac{n}{2\eta NV}\int d\mathbf{r}\,\mathbf{M}(\mathbf{r}):\mathbf{M}(\mathbf{r}) - n\log Q. \tag{197}$$

The SCF equations system is composed of

$$\rho_A + \rho_B - 1 = 0, \tag{198}$$

$$\frac{2}{\chi N}\mu_- - (\rho_A - \rho_B) = 0, \tag{199}$$

$$\frac{1}{\eta N}\mathbf{M} - \mathbf{S} = 0. \tag{200}$$

The expressions of singe partition functional and order parameters are

$$Q = \frac{1}{V}\int d\mathbf{r}\int d\mathbf{u}\,q_B^\dagger(\mathbf{r},\mathbf{u},1-f)q_A(\mathbf{r},f), \tag{201}$$

$$\rho_A(\mathbf{r}) = \frac{1}{Q}\int_0^f ds\,q_A(\mathbf{r},s)q_A^\dagger(\mathbf{r},1-s), \tag{202}$$

$$\rho_B(\mathbf{r}) = \frac{4\pi}{Q}\int_f^1 ds\int d\mathbf{u}\,q_B(\mathbf{r},\mathbf{u},s)q_B^\dagger(\mathbf{r},\mathbf{u},1-s), \tag{203}$$

$$\mathbf{S}(\mathbf{r}) = \frac{4\pi}{Q}\int_f^1 ds\int d\mathbf{u}\,q_B(\mathbf{r},\mathbf{u},s)\left(\mathbf{uu}-\frac{1}{3}\mathbf{I}\right)q_B^\dagger(\mathbf{r},\mathbf{u},1-s). \tag{204}$$

The propagators satisfy the following PDEs

$$\frac{\partial}{\partial s}q_A(\mathbf{r},s) = \nabla_{\mathbf{r}}^2 q_A(\mathbf{r},s) - w_A(\mathbf{r})q_A(\mathbf{r},s), \quad 0\leqslant s\leqslant f, \tag{205}$$

$$\frac{\partial}{\partial s}q_B(\mathbf{r},\mathbf{u},s) = -\nu\mathbf{u}\cdot\nabla_{\mathbf{r}}q_B(\mathbf{r},\mathbf{u},s) - \left[w_B(\mathbf{r}) - \mathbf{M}(\mathbf{r}):\left(\mathbf{uu}-\frac{1}{3}\mathbf{I}\right)\right]q_B(\mathbf{r},\mathbf{u},s) + \frac{1}{2\lambda}\nabla_{\mathbf{u}}^2 q_B(\mathbf{r},\mathbf{u},s), \quad f\leqslant s\leqslant 1, \tag{206}$$

and the corresponding initial values are

$$q_A(\mathbf{r},0) = 1, \quad q_B(\mathbf{r},\mathbf{u},f) = \frac{q_A(\mathbf{r},f)}{4\pi}. \tag{207}$$

Similarly, the inverse propagators satisfy the MDEs

$$\frac{\partial}{\partial s}q_A^\dagger(\mathbf{r},s) = \nabla_{\mathbf{r}}^2 q_A^\dagger(\mathbf{r},s) - w_A(\mathbf{r})q_A^\dagger(\mathbf{r},s), \quad 1-f\leqslant s\leqslant 1, \tag{208}$$

$$\frac{\partial}{\partial s}q_B^\dagger(\mathbf{r},\mathbf{u},s) = \nu\mathbf{u}\cdot\nabla_{\mathbf{r}}q_B^\dagger(\mathbf{r},\mathbf{u},s) - \left[w_B(\mathbf{r}) - \mathbf{M}(\mathbf{r}):\left(\mathbf{uu}-\frac{1}{3}\mathbf{I}\right)\right]q_B^\dagger(\mathbf{r},\mathbf{u},s) + \frac{1}{2\lambda}\nabla_{\mathbf{u}}^2 q_B^\dagger(\mathbf{r},\mathbf{u},s), \quad 0\leqslant s\leqslant 1-f, \tag{209}$$

the initial values are

$$q_A(\mathbf{r},1-f) = \int d\mathbf{u}\,q_B^\dagger(\mathbf{r},\mathbf{u},1-f), \quad q_B^\dagger(\mathbf{r},\mathbf{u},0) = \frac{1}{4\pi}. \tag{210}$$

The fields of (w_A, w_B) and (μ_+,μ_-) have the following relationship

$$w_A(\mathbf{r}) = \mu_+(\mathbf{r}) - \mu_-(\mathbf{r}), \quad w_B(\mathbf{r}) = \mu_+(\mathbf{r}) + \mu_-(\mathbf{r}). \tag{211}$$

IX. AB ROD-COIL DIBLOCK COPOLYMER MELT

A. Self-consistent field theory

	Notations
Volume of the system	V
Number of the polymers	n
Degree of polymerization	N
Flory-Huggins interaction parameter	χ
Size Asymmetry ratio measuring different block	$\nu = (a/b)(6N)^{1/2}$
Maier-Saupe interaction parameter	η

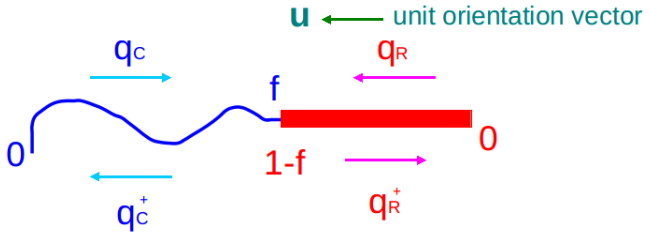

FIG. 1: Schematic diagram of coil-rod liquid-crystal diblock copolymer.

To develop a statistical mechanical description of the self-assembly behavior, we consider an incompressible melt of n monodisperse rod-coil block polymers in a volume V. The flexible (coil) part of the polymer is modeled as a Gaussian chain where the conformation of the polymers is represented by continuous space curves $\mathbf{R}_\alpha(s)$, where $\alpha = 1, \ldots, n$ indexes the different polymers and s is an arc length variable running from 0 to N_C the number of coil segments along each chain contour. The stiffer block of the rod-coil polymer is modeled as a wormlike chain of finite thickness with a unit orientation vector $\mathbf{u}_\alpha$ characterizing its conformation. The monomeric units of the flexible coil are characterized by a statistical segment length b, while the diameter of the rod's monomers are denoted as d. For simplicity, we define the statistical segment length of the rod, a, by assuming equal monomeric volumes ρ_0 for the coil and rods, i.e., $b^3 = ad^2 = \rho_0^{-1}$. In this notation the block copolymer is assumed to be characterized by N_f coil segments and $N(1-f)$ rod segments.

Within saddle-point approximation, the mean-field Hamiltonian functional is

$$H[\mu_+, \mu_-, \mathbf{M}] = \frac{n}{\chi N V}\int d\mathbf{r}\, \mu_-^2(\mathbf{r}) - \frac{n}{V}\int d\mathbf{r}\, \mu_+(\mathbf{r}) + \frac{n}{2\eta N V}\int d\mathbf{r}\, \mathbf{M}(\mathbf{r}) : \mathbf{M}(\mathbf{r}) - n\log Q. \tag{212}$$

The SCF equations system is composed of

$$\rho_C + \rho_R - 1 = 0, \tag{213}$$

$$\frac{2}{\chi N}\mu_- - (\rho_C - \rho_R) = 0, \tag{214}$$

$$\frac{1}{\eta N}\mathbf{M} - \mathbf{S} = 0, \tag{215}$$

where $\mathbf{M}, \mathbf{S} \in \mathbb{R}^{3\times 3}$.

Before going ahead, let us introduce some notations:

$$w_C = \mu_+ - \mu_-, \quad w_R = \mu_+ + \mu_-, \quad \Gamma(\mathbf{r}, \mathbf{u}) = w_R(\mathbf{r}) - \mathbf{M}(\mathbf{r}) : \left(\mathbf{uu} - \frac{1}{3}\mathbf{I}\right) \tag{216}$$

The expressions of singe partition functional and order parameters are

$$Q = \frac{1}{V}\int d\mathbf{r}\int d\mathbf{u}\, q_R^\dagger(\mathbf{r},\mathbf{u},1-f)q_C(\mathbf{r},f), \tag{217}$$

$$\rho_C(\mathbf{r}) = \frac{1}{Q}\int_0^f ds\, q_C(\mathbf{r},s)q_C^\dagger(\mathbf{r},f-s), \tag{218}$$

$$\rho_R(\mathbf{r}) = \frac{4\pi}{Q}\int_f^1 ds\int d\mathbf{u}\, q_R(\mathbf{r},\mathbf{u},s)q_R^\dagger(\mathbf{r},\mathbf{u},1-f-s), \tag{219}$$

$$\mathbf{S}(\mathbf{r}) = \frac{4\pi}{Q}\int_f^1 ds\int d\mathbf{u}\, q_R(\mathbf{r},\mathbf{u},s)\left(\mathbf{uu}-\frac{1}{3}\mathbf{I}\right)q_R^\dagger(\mathbf{r},\mathbf{u},1-f-s). \tag{220}$$

The forward and inverse propagators satisfy the following PDEs

$$\frac{\partial}{\partial s}q_C(\mathbf{r},s) = \nabla_{\mathbf{r}}^2 q_C(\mathbf{r},s) - w_C(\mathbf{r})q_C(\mathbf{r},s), \quad 0\leqslant s\leqslant f, \tag{221}$$

$$q_C(\mathbf{r},0) = 1 \tag{222}$$

$$\tag{223}$$

$$\frac{\partial}{\partial s}q_R(\mathbf{r},\mathbf{u},s) = -\nu\mathbf{u}\cdot\nabla_{\mathbf{r}}q_R(\mathbf{r},\mathbf{u},s) - \Gamma(\mathbf{r},\mathbf{u})q_R(\mathbf{r},\mathbf{u},s), \quad 0\leqslant s\leqslant 1-f, \tag{224}$$

$$q_R(\mathbf{r},\mathbf{u},f) = \frac{1}{4\pi}. \tag{225}$$

$$\tag{226}$$

$$\frac{\partial}{\partial s}q_R^\dagger(\mathbf{r},\mathbf{u},s) = \nu\mathbf{u}\cdot\nabla_{\mathbf{r}}q_R^\dagger(\mathbf{r},\mathbf{u},s) - \Gamma(\mathbf{r},\mathbf{u})q_R^\dagger(\mathbf{r},\mathbf{u},s), \quad f\leqslant s\leqslant 1, \tag{227}$$

$$q_R^\dagger(\mathbf{r},\mathbf{u},f) = \frac{q_C(\mathbf{r},f)}{4\pi}. \tag{228}$$

$$\tag{229}$$

$$\frac{\partial}{\partial s}q_C^\dagger(\mathbf{r},s) = \nabla_{\mathbf{r}}^2 q_C^\dagger(\mathbf{r},s) - w_C(\mathbf{r})q_C^\dagger(\mathbf{r},s), \quad 1-f\leqslant s\leqslant 1, \tag{230}$$

$$q_C^\dagger(\mathbf{r},1-f) = \int d\mathbf{u}\, q_R(\mathbf{r},\mathbf{u},1-f). \tag{231}$$

Now let us analyse the mathematical structure of the PDE for the rod-subchain propagators, i.e.,

$$\frac{\partial}{\partial s}q_R(\mathbf{r},\mathbf{u},s) = -\nu\mathbf{u}\cdot\nabla_{\mathbf{r}}q_R(\mathbf{r},\mathbf{u},s) - \Gamma(\mathbf{r},\mathbf{u})q_R(\mathbf{r},\mathbf{u},s),$$

$$q_R(\mathbf{r},\mathbf{u},0) = \frac{1}{4\pi}.$$

Let $\mathbf{r} = \mathbf{r}+\nu s\mathbf{u}$*, the above PDE becomes an ODE*

$$\frac{d}{ds}q_R(\mathbf{r}+\nu s\mathbf{u},\mathbf{u},s) = \frac{\partial}{\partial s}q_R(\mathbf{r}+\nu s\mathbf{u},\mathbf{u},s) + \nu\mathbf{u}\cdot\nabla_{\mathbf{r}}q_R(\mathbf{r}+\nu s\mathbf{u},\mathbf{u},s) = -\Gamma(\mathbf{r}+\nu s\mathbf{u},\mathbf{u})q_R(\mathbf{r}+\nu s\mathbf{u},\mathbf{u},s)$$

One can solve it easily

$$q_R(\mathbf{r},\mathbf{u},s) = \frac{1}{4\pi}\exp\left[-\int_0^s d\tau\,\Gamma(\mathbf{r}+\nu\tau\mathbf{u},\mathbf{u})\right]$$

For backward propagator $q_R(\mathbf{r},\mathbf{u},s)$ *has the similar results.*

$$q_R^\dagger(\mathbf{r},\mathbf{u},s) = \frac{q_C(\mathbf{r},f)}{4\pi}\exp\left[-\int_f^s d\tau\,\Gamma(\mathbf{r}-\nu\tau\mathbf{u},\mathbf{u})\right]$$

Thanks to the analytical structures of PDEs for q_R and $q_R^\dagger$, these equations about Q and ρ_R, ρ_C can be written as

$$Q = \frac{1}{V}\frac{1}{4\pi}\int d\mathbf{u}\int d\mathbf{r}\,\exp\left[-\int_0^{1-f} ds\,\Gamma(\mathbf{r}+\nu s\mathbf{u},\mathbf{u})\right] q_C(\mathbf{r},f), \tag{232}$$

$$\rho_C(\mathbf{r}) = \frac{1}{Q}\int_0^f ds\, q_C(\mathbf{r},s)q_C^\dagger(\mathbf{r},f-s), \tag{233}$$

$$\rho_R(\mathbf{r}) = \frac{1}{Q}\frac{1}{4\pi}\int d\mathbf{u}\int_0^{1-f} ds\,\exp\left[-\int_0^{1-f} ds'\,\Gamma(\mathbf{r}-\nu s\mathbf{u}+\nu s'\mathbf{u},\mathbf{u})\right] q_C(\mathbf{r}-\nu s\mathbf{u},f), \tag{234}$$

$$\mathbf{S}(\mathbf{r}) = \frac{1}{Q}\frac{1}{4\pi}\int d\mathbf{u}\int_0^{1-f} ds\,\left(\mathbf{uu}-\frac{1}{3}\mathbf{I}\right)\exp\left[-\int_0^{1-f} ds'\,\Gamma(\mathbf{r}-\nu s\mathbf{u}+\nu s'\mathbf{u},\mathbf{u})\right] q_C(\mathbf{r}-\nu s\mathbf{u},f), \tag{235}$$

There possesses a simple physical interpretation: to compute the density or the orientational order parameter at a position $\mathbf{r}$, we consider the product of $q(\mathbf{r}-\nu s\mathbf{u},f)$, the probability that a link is present at the position $\mathbf{r}-\nu s\mathbf{u}$ ($s\in[0,1-f]$) with the probability that a coil-rod polymer whose link is at the position $\mathbf{r}-\nu s\mathbf{u}$ is also oriented at an angle $\mathbf{u}$ (the term in the exponential).

The propagator of coil subchain satisfies the following PDEs

$$\frac{\partial}{\partial s}q_C(\mathbf{r},s) = \nabla_{\mathbf{r}}^2 q_C(\mathbf{r},s) - w_C(\mathbf{r})q_C(\mathbf{r},s),\quad 0\leqslant s\leqslant f, \tag{236}$$

$$q_C(\mathbf{r},0) = 1, \tag{237}$$

The inverse propagator satisfies the MDEs

$$\frac{\partial}{\partial s}q_C^\dagger(\mathbf{r},s) = \nabla_{\mathbf{r}}^2 q_C^\dagger(\mathbf{r},s) - w_C(\mathbf{r})q_C^\dagger(\mathbf{r},s),\quad 1-f\leqslant s\leqslant 1, \tag{238}$$

$$q_C^\dagger(\mathbf{r},f) = \frac{1}{4\pi}\int d\mathbf{u}\exp\left[-\int_0^{1-f} ds\,\Gamma(\mathbf{r}+\nu s\mathbf{u},\mathbf{u})\right] \tag{239}$$

B. Numerical methods

Self-consistent iterative procedure

Step 1: Given initial estimations of fields w_C, w_R, and $\mathbf{M}$, and freeze computational box;

Step 2: Compute forward (back) propagator operators q and $q^\dagger$ (see Sec. X B 2);

Step 3: Obtain Q, ρ_C, ρ_R and $\mathbf{S}$ by integral equations (see Sec. X B 3), and calculate the value of effective Hamiltonian H;

Step 4: Update fields w_C, w_R and $\mathbf{M}$ using some iterative methods (see Sec. X B 4);

Step 5: Goto **Step 2** until the Hamiltonian does not change.

1. *Discrete Fourier transform*

We only consider the periodic crystals, therefore the Fourier psedospectral method is one of the most efficient numerical methods. For periodic functions, their discrete Fourier expansion can be written as

$$f(\mathbf{r}) = \sum_{\mathbf{k}} \hat{f}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{240}$$

Correspondingly, the Fourier coefficient is

$$\hat{f}_k = \frac{1}{N}\sum_{j=0}^{N-1} f(\mathbf{r}_j)e^{-i\mathbf{k}\cdot\mathbf{r}_j} \tag{241}$$

$$f(\mathbf{r}+\nu s\mathbf{u}) = \sum_{\mathbf{k}}(\hat{f}_{\mathbf{k}}e^{i\nu s\mathbf{k}\cdot\mathbf{u}})e^{i\mathbf{k}\cdot\mathbf{r}} := \sum_{\mathbf{k}}\tilde{f}_{\mathbf{k},s,\mathbf{u}}e^{i\mathbf{k}\cdot\mathbf{r}} \tag{242}$$

$\mathbf{u} = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta)^T, \phi \in [0, 2\pi), \theta \in [0, \pi]$.

2. *Numerical schemes for solving PDEs of coil chain*

The PDE of flexible chain, the propagator satisfies

$$\frac{\partial}{\partial s}q_C(\mathbf{r}, s) = \nabla^2_{\mathbf{r}}q_C(\mathbf{r}, s) - w_C(\mathbf{r})q_C(\mathbf{r}, s) \tag{243}$$

• Second-order operator-splitting scheme:
The propagator of coil subchain satisfies the following PDEs

$$\frac{\partial}{\partial s}q_C(\mathbf{r}, s) = \nabla^2_{\mathbf{r}}q_C(\mathbf{r}, s) - w_C(\mathbf{r})q_C(\mathbf{r}, s) := \mathcal{L}_1 q_C + \mathcal{L}_2 q_C \tag{244}$$

In each time step,

$$q(\mathbf{r}, s+h) = e^{\frac{h}{2}\mathcal{L}_1}e^{h\mathcal{L}_2}e^{\frac{h}{2}\mathcal{L}_1}q(\mathbf{r}, s) \tag{245}$$

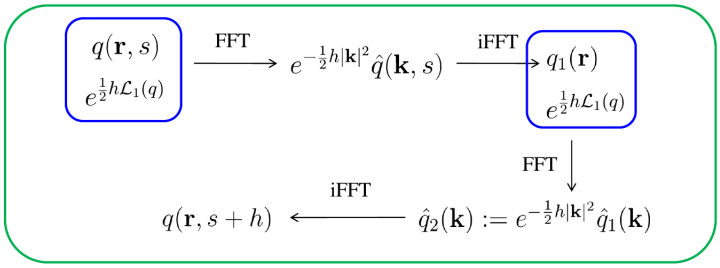

FIG. 2: Schematic plot of 2-order operator splitting method.

• Fourth-order Adams-Bashford scheme

$$\begin{aligned}\frac{25}{12}q^{j+1} - 4q^j + 3q^{j-1} - \frac{4}{3}q^{j-2} + \frac{1}{4}q^{j-3} = \\ \Delta s[\nabla^2 q^{j+1} - w(4q^j - 6q^{j-1} + 4q^{j-2} - q^{j-3})]\end{aligned} \tag{246}$$

This method also can be easily implemented using the psedospectral method. The initial values required to apply this formula are obtained using second-order operator-splitting scheme and Richardson's extrapolation. Assume that Q is the exact solution of the MDE, $Q(\Delta s)$ is the numerical solution of MDE by second-order operator-splitting scheme with s-step size Δs, then $Q - Q(\Delta s) = O(\Delta s^2)$. By Richardson's extrapolation, we have

$$Q - \Big(-\frac{1}{3}Q(\Delta s) + \frac{4}{3}Q\Big(\frac{\Delta s}{2}\Big)\Big) = O(\Delta s^4). \tag{247}$$

For a common scheme, the above extrapolation scheme usually has third order accuracy. However, making use of makes use of the feature of the second-order operator-splitting method, it has fourth-order accuracy.

3. Solving integral equations

In this subsection, integral formulas along three direction, s, $\mathbf{u}$ and $\mathbf{r}$ will firstly given. Then the part of parallel computing will be discussed.

- For s-direction, the fourth-order integral formula can be used to approximate the integral

$$\int_0^{T_s} ds\, f(s) \approx I_{n_s} = \Delta s \left\{ -\frac{5}{8}(f_0 + f_{n_s}) + \frac{1}{6}(f_1 + f_{n_s-1}) - \frac{1}{24}(f_2 + f_{n_s-2}) + \sum_{j=0}^{n_s} f_j \right\}. \tag{248}$$

- For the oriented variable $\mathbf{u}$,

$$\int d\mathbf{u} = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta$$

Along ϕ-direction, we can use the composite trapezoidal integral formula with the spectral accuracy.

$$\int_0^{T_\phi} d\phi\, f(\phi) \approx I_{n_\phi} = \frac{d\phi}{2}(f_0 + f_{n_\phi}) + \sum_{j=1}^{n_\phi - 1} f_j \tag{249}$$

Meanwhile, along θ-direction, we can use the Gaussian integral formula to achieve higher-order precision.

$$\int_0^{T_\theta} d\theta\, f(\theta) \approx I_{n_\theta} = \sum_{k=1}^{n_\theta} w_k f(\theta_k) \tag{250}$$

where w_k and θ_k $(k = 1, 2, \ldots, n_\theta)$ are the Gaussian weights, and Gaussian points.

- For spatial integral $\int d\mathbf{r}$, because of the periodic boundary conditions, the integral become very simple, i.e.,

$$\frac{1}{V} \int d\mathbf{r}\, f(\mathbf{r}) = \hat{f}\Big|_{\mathbf{k}=0} \tag{251}$$

Parallel Computing Part: For the rod system, the parallel computing mainly involves the integral approximation for order parameters ρ_R and $\mathbf{S}$, and the single chain partition functional Q.

---

4. Nonlinear iterative methods

Here we only give the gradient-type iterative methods to update fields $\mu_\pm$ and $\mathbf{M}$

$$\mu_+^{k+1} = \mu_+^k + \lambda_+(\rho_C^k + \rho_R^k - 1), \tag{252}$$

$$\mu_-^{k+1} = \mu_-^k - \lambda_- \left[\frac{2}{\chi N}\mu_-^k - (\rho_C^k - \rho_R^k) \right], \tag{253}$$

$$\mathbf{M}^{k+1} = \mathbf{M}^k - \lambda_{\mathbf{M}} \left[\frac{1}{\eta N}\mathbf{M}^k - \mathbf{S}^k \right], \tag{254}$$

where $\lambda_\pm, \lambda_{\mathbf{M}} > 0$.

X. AB ROD-COIL DIBLOCK COPOLYMER MELT - NUMERICAL VERSION

A. Self-consistent field theory

Within saddle-point approximation, the mean-field Hamiltonian functional is

$$H[\mu_+,\mu_-,\mathbf{M}]=\frac{n}{\chi NV}\int d\mathbf{r}\,\mu_-^2(\mathbf{r})-\frac{n}{V}\int d\mathbf{r}\,\mu_+(\mathbf{r})+\frac{n}{2\eta NV}\int d\mathbf{r}\,\mathbf{M}(\mathbf{r}):\mathbf{M}(\mathbf{r})-n\log Q. \tag{255}$$

The SCF equations system is composed of

$$\rho_C(\mathbf{r})+\rho_R(\mathbf{r})-1=0, \tag{256}$$

$$\frac{2}{\chi N}\mu_- -[\rho_C(\mathbf{r})-\rho_R(\mathbf{r})]=0, \tag{257}$$

$$\frac{1}{\eta N}\mathbf{M}(\mathbf{r})-\mathbf{S}(\mathbf{r})=0, \tag{258}$$

where $\mathbf{M},\mathbf{S}\in\mathbb{R}^{3\times3}$ are symmetric matrix.

Before going ahead, let us introduce some notations:

$$w_C=\mu_+-\mu_-,\quad w_R=\mu_++\mu_-,\quad \Gamma(\mathbf{u},\mathbf{r})=w_R(\mathbf{r})-\mathbf{M}(\mathbf{r}):\left(\mathbf{uu}-\frac{1}{3}\mathbf{I}\right) \tag{259}$$

The expressions of singe partition functional and order parameters are

$$Q=\frac{1}{V}\int d\mathbf{r}\int d\mathbf{u}\,q_R^\dagger(\mathbf{u},\mathbf{r},1-f)q_C(\mathbf{r},f), \tag{260}$$

$$\rho_C(\mathbf{r})=\frac{1}{Q}\int_0^f ds\,q_C(\mathbf{r},s)q_C^\dagger(\mathbf{r},f-s), \tag{261}$$

$$\rho_R(\mathbf{r})=\frac{4\pi}{Q}\int_0^{1-f} ds\int d\mathbf{u}\,q_R(\mathbf{u},\mathbf{r},s)q_R^\dagger(\mathbf{u},\mathbf{r},1-f-s), \tag{262}$$

$$\mathbf{S}(\mathbf{r})=\frac{4\pi}{Q}\int_0^{1-f} ds\int d\mathbf{u}\,q_R(\mathbf{u},\mathbf{r},s)\left(\mathbf{uu}-\frac{1}{3}\mathbf{I}\right)q_R^\dagger(\mathbf{u},\mathbf{r},1-f-s). \tag{263}$$

The forward and inverse propagators satisfy the following PDEs

$$\frac{\partial}{\partial s}q_C(\mathbf{r},s)=\nabla_{\mathbf{r}}^2q_C(\mathbf{r},s)-w_C(\mathbf{r})q_C(\mathbf{r},s),\quad 0\leqslant s\leqslant f, \tag{264}$$

$$q_C(\mathbf{r},0)=1 \tag{265}$$

$$\frac{\partial}{\partial s}q_R(\mathbf{u},\mathbf{r},s)=-\nu\mathbf{u}\cdot\nabla_{\mathbf{r}}q_R(\mathbf{u},\mathbf{r},s)-\Gamma(\mathbf{u},\mathbf{r})q_R(\mathbf{u},\mathbf{r},s),\quad f\leqslant s\leqslant 1, \tag{266}$$

$$q_R(\mathbf{u},\mathbf{r},f)=\frac{1}{4\pi}q_C(\mathbf{r},f). \tag{267}$$

$$\frac{\partial}{\partial s}q_R^\dagger(\mathbf{u},\mathbf{r},s)=\nu\mathbf{u}\cdot\nabla_{\mathbf{r}}q_R^\dagger(\mathbf{u},\mathbf{r},s)-\Gamma(\mathbf{r},\mathbf{u})q_R^\dagger(\mathbf{u},\mathbf{r},s),\quad 0\leqslant s\leqslant 1-f, \tag{268}$$

$$q_R^\dagger(\mathbf{u},\mathbf{r},f)=\frac{1}{4\pi}. \tag{269}$$

$$\frac{\partial}{\partial s}q_C^\dagger(\mathbf{r},s)=\nabla_{\mathbf{r}}^2q_C^\dagger(\mathbf{r},s)-w_C(\mathbf{r})q_C^\dagger(\mathbf{r},s),\quad 1-f\leqslant s\leqslant 1, \tag{270}$$

$$q_C^\dagger(\mathbf{r},1-f)=\int d\mathbf{u}\,q_R^\dagger(\mathbf{u},\mathbf{r},1-f). \tag{271}$$

B. Numerical methods

Self-consistent iterative procedure

Step 1: Given initial estimations of fields w_C, w_R, and $\mathbf{M}$, and freeze computational box;

Step 2: Compute forward (back) propagator operators q and $q^\dagger$ (see Sec. X B 2);

Step 3: Obtain Q, ρ_C, ρ_R and $\mathbf{S}$ by integral equations (see Sec. X B 3), and calculate the value of effective Hamiltonian H;

Step 4: Update fields w_C, w_R and $\mathbf{M}$ using some iterative methods (see Sec. X B 4);

Step 5: Goto **Step 2** until the Hamiltonian does not change.

1. *Discrete Fourier transform*

We only consider the periodic crystals, therefore the Fourier psedospectral method is one of the most efficient numerical methods. For periodic functions, their discrete Fourier expansion can be written as

$$f(\mathbf{r}) = \sum_{\mathbf{k}} \hat{f}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{272}$$

Correspondingly, the Fourier coefficient is

$$\hat{f}_k = \frac{1}{N}\sum_{j=0}^{N-1} f(\mathbf{r}_j) e^{-i\mathbf{k}\cdot\mathbf{r}_j} \tag{273}$$

- $\mathbf{u} = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta)^T, \phi \in [0, 2\pi), \theta \in [0, \pi]$.

2. *Numerical schemes for solving PDEs of coil chain*

The PDE of flexible chain, the propagator satisfies

$$\frac{\partial}{\partial s} q_C(\mathbf{r}, s) = \nabla^2_{\mathbf{r}} q_C(\mathbf{r}, s) - w_C(\mathbf{r}) q_C(\mathbf{r}, s) \tag{274}$$

- Second-order operator-splitting scheme for $q_C(\mathbf{r}, s)$ and $q^\dagger_C(\mathbf{r}, s)$

The propagator of coil subchain satisfies the following PDEs

$$\frac{\partial}{\partial s} q_C(\mathbf{r}, s) = \nabla^2_{\mathbf{r}} q_C(\mathbf{r}, s) - w_C(\mathbf{r}) q_C(\mathbf{r}, s) := \mathcal{L}_1 q_C + \mathcal{L}_2 q_C \tag{275}$$

In each time step,

$$q_C(\mathbf{r}, s + \Delta s) = e^{\Delta s \mathcal{L}_2/2} e^{\Delta s \mathcal{L}_1} e^{\Delta s \mathcal{L}_2/2} q_C(\mathbf{r}, s) \tag{276}$$

- Second-order operator-splitting scheme for $q_R(\mathbf{u}, \mathbf{r}, s)$ and $q^\dagger_R(\mathbf{u}, \mathbf{r}, s)$ The propagator of rod subchain satisfies the following PDEs

$$\frac{\partial}{\partial s} q^\dagger_R(\mathbf{u}, \mathbf{r}, s) = \nu\mathbf{u}\cdot\nabla_{\mathbf{r}} q^\dagger_R(\mathbf{u}, \mathbf{r}, s) - \Gamma(\mathbf{u}, \mathbf{r}) q^\dagger_R(\mathbf{u}, \mathbf{r}, s) := \mathcal{L}_1 q_R + \mathcal{L}_2 q_R$$

In particular, the second-order operator-splitting scheme is

$$q_R(\mathbf{u}, \mathbf{r}, s + \Delta s) = e^{\Delta s \mathcal{L}_2/2} e^{\Delta s \mathcal{L}_1} e^{\Delta s \mathcal{L}_2/2} q_R(\mathbf{u}, \mathbf{r}, s). \tag{277}$$

By psedospectral technology, the operator in the right term of PDE in each s step can be split into three parts,

$$\begin{array}{ccccc} q(\mathbf{u}, \mathbf{r}) & \to & \hat{q}(\mathbf{u}, \mathbf{k}) & \to & q(\mathbf{u}, \mathbf{r}) \\ & e^{\Delta s \mathcal{L}_2/2} & & e^{\Delta s \mathcal{L}_1} & \quad e^{\Delta s \mathcal{L}_2/2} \end{array}$$

3. Solving integral equations

In this subsection, integral formulas along three direction, s, $\mathbf{u}$ and $\mathbf{r}$ will firstly given. Then the part of parallel computing will be discussed.

- For s-direction, the fourth-order integral formula can be used to approximate the integral

$$\int_0^{T_s} ds\, f(s) \approx I_{n_s} = \Delta s \left\{ -\frac{5}{8}(f_0 + f_{n_s}) + \frac{1}{6}(f_1 + f_{n_s-1}) - \frac{1}{24}(f_2 + f_{n_s-2}) + \sum_{j=0}^{n_s} f_j \right\}. \tag{278}$$

- For the oriented variable $\mathbf{u}$,

$$\int d\mathbf{u} = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta$$

Along ϕ-direction, we can use the composite trapezoidal integral formula with the spectral accuracy.

$$\int_0^{T_\phi} d\phi\, f(\phi) \approx I_{n_\phi} = \frac{d\phi}{2}(f_0 + f_{n_\phi}) + \sum_{j=1}^{n_\phi - 1} f_j \tag{279}$$

Meanwhile, along θ-direction, we can use the Gaussian integral formula to achieve higher-order precision.

$$\int_0^{T_\theta} d\theta\, f(\theta) \approx I_{n_\theta} = \sum_{k=1}^{n_\theta} w_k f(\theta_k) \tag{280}$$

where w_k and θ_k $(k = 1, 2, \ldots, n_\theta)$ are the Gaussian weights, and Gaussian points.

- For spatial integral $\int d\mathbf{r}$, because of the periodic boundary conditions, the integral become very simple, i.e.,

$$\frac{1}{V} \int d\mathbf{r}\, f(\mathbf{r}) = \hat{f}\Big|_{\mathbf{k}=0} \tag{281}$$

Parallel Computing Part: For the rod system, the parallel computing mainly involves the integral approximation for order parameters ρ_R and $\mathbf{S}$, and the single chain partition functional Q.

4. Nonlinear iterative methods

Here we only give the gradient-type iterative methods to update fields $\mu_\pm$ and $\mathbf{M}$

$$\mu_+^{k+1} = \mu_+^k + \lambda_+(\rho_C^k + \rho_R^k - 1), \tag{282}$$

$$\mu_-^{k+1} = \mu_-^k - \lambda_- \left[\frac{2}{\chi N}\mu_-^k - (\rho_C^k - \rho_R^k) \right], \tag{283}$$

$$\mathbf{M}^{k+1} = \mathbf{M}^k - \lambda_{\mathbf{M}} \left[\frac{1}{\eta N}\mathbf{M}^k - \mathbf{S}^k \right], \tag{284}$$

where $\lambda_\pm, \lambda_{\mathbf{M}} > 0$.

XI. SCFT OF T-SHAPED LIQUID-CRYSTAL BLOCK COPOLYMER SYSTEM

A. T-shaped liquid-crystal block copolymer

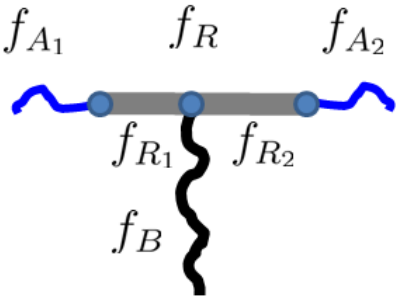

FIG. 3: Schematic diagram of T-shaped liquid-crystal block copolymer composed of a rod-like core, tethered with the same flexible units at both ends and flexible chain in lateral position.

Notations	Physical meanings
V	volume of the system
b_A	statistical segment length of coil A
b_B	statistical segment length of coil B
b_R	statistical segment length of stiff subchain
d_R	diameter of stiff subchain
$\varepsilon = b_A/b_B$	conformationally asymmetries between coils A and B
$\nu = (b_R/b_B)(6N)^{1/2}$	size asymmetry ratio between B coil and rod R
η	Maier-Saupe interaction parameter
λ	stiff parameter of semiflexible chain

TABLE I: Notations used in the context.

B. Modeling with wormlike chain model

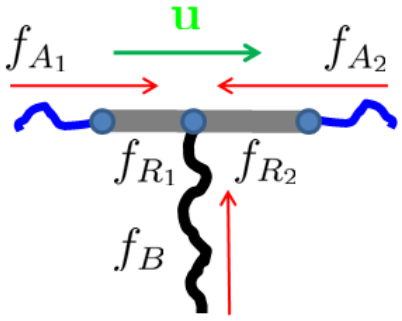

FIG. 4: Schematic diagram of T-shaped liquid-crystal block copolymer. In this subsection, we will use wormlike chain to model the liquid-crystal-part subchain. The green arrow denotes the unique forward direction of orientation. Red arrows denote the forward direction when calculating propagators of coil blocks.

To develop a statistical mechanical description of the self-assembly behavior, we consider an incompressible melt of n T-shaped liquid-crystal block copolymers in a volume V. The flexible (coil) part of the polymer is modeled as

a Gaussian chain where the conformation of the polymers are represented by continuous space curves $\mathbf{R}_\alpha(s)$, where $\alpha = 1, \ldots, n$ indexes the different polymers and s is an arc length variable running from 0 to N_{A_1}, from 0 to N_{A_2}, and from 0 to N_B, the number of coil segments along each chain contour. It is not continuous in this T-shaped molecule. The stiffer block of the T-shaped liquid-crystal block copolymer is modeled by a wormlike chain. As figure 4 shows, two unit orientation vectors $\mathbf{u}_1$ and $\mathbf{u}_1$ are used to character its conformation, from N_{A_1} to $N_{A_1} + N_{R_1}$, and N_{A_2} to $N_{A_2} + N_{R_2}$, respectively. The monomeric units of the flexible coil are characterized by statistical segment length b_A and b_B, while the diameter of the rod's monomers are denoted as d_R. For simplicity, we define the statistical segment length of the rod, b_R, by assuming equal monomeric volumes ρ_0 for the coil and rods. In this notation the block copolymer is assumed to be characterized by $N_{A_1} + N_{A_2} + N_B$ coil segments and N_R rod segments. The total polymerization degree is $N = N_{A_1} + N_{A_2} + N_B + N_{R_1} + N_{R_2}$.

The physics of our model is encapsulated within the repulsive enthalpic interactions between the rod and coil elements which favors their microphase separation, along with the repulsive orientational interactions between the rods which favors their alignment. In this work, we adopt a coarse-grained formalism where both these interactions are modeled through energetic penalties ascribed to the spatial variations of the order parameters characterizing the distributions of rod and coil segments and the orientational order of the rod segments. We begin by defining the following microscopic order parameters to characterize the self-assembly morphologies:

$$\text{densities of coils:} \quad \hat{\rho}_A(\mathbf{r}) = \frac{1}{\rho_0} \sum_{\alpha=1}^{n} \Big(\int_0^{N_{A_1}} + \int_0^{N_{A_2}} \Big) ds\, \delta(\mathbf{r} - \mathbf{R}_\alpha(s)) \tag{285}$$

$$\hat{\rho}_B(\mathbf{r}) = \frac{1}{\rho_0} \sum_{\alpha=1}^{n} \int_0^{N_B} ds\, \delta(\mathbf{r} - \mathbf{R}_\alpha(s)) \tag{286}$$

$$\text{density of rods:} \quad \hat{\rho}_R(\mathbf{r}) = \frac{1}{\rho_0} \sum_{\alpha=1}^{n} \int_{N_{A_1}}^{N_{A_1}+N_B} ds\, \delta\left\{\mathbf{r} - [\mathbf{R}_\alpha(N_{A_1}) + b_R s \mathbf{u}_\alpha]\right\} \tag{287}$$

$$\text{orientational order parameter:} \quad \hat{\mathbf{S}}(\mathbf{r}) = \frac{1}{\rho_0} \sum_{\alpha=1}^{n} \int_{N_{A_1}}^{N_{A_1}+N_B} ds\, \delta\left\{\mathbf{r} - [\mathbf{R}_\alpha(N_{A_1}) + b_R s \mathbf{u}_\alpha]\right\} \Big(\mathbf{uu} - \frac{1}{3}\mathbf{I} \Big) \tag{288}$$

The incompressibility constraint is provided by enforcing that

$$\hat{\rho}_A(\mathbf{r}) + \hat{\rho}_B(\mathbf{r}) + \hat{\rho}_R(\mathbf{r}) = 1 \tag{289}$$

The conformations of noninteracting flexible components are ascribed a Gaussian statistical weight, $\exp(-H_0)$, with a harmonic stretching (free) energy given by (units of $k_B T$)

$$H_0[\mathbf{r}] = \frac{3}{2b_A^2} \sum_{\alpha=1}^{n} \Big(\int_0^{N_{A_1}} + \int_0^{N_{A_1}} \Big) ds \left| \frac{d\mathbf{R}_\alpha(s)}{ds} \right|^2 + \frac{3}{2b_B^2} \sum_{\alpha=1}^{n} \int_0^{N_B} ds \left| \frac{d\mathbf{R}_\alpha(s)}{ds} \right|^2 \tag{290}$$

The conformations of noninteracting semiflexible components are ascribed a wormlike statistical weight, $\exp(-H_1)$, with a bending (free) energy given by

$$H_1[\mathbf{r}] = \frac{\lambda}{2b_R^2} \sum_{\alpha=1}^{n} \int_{N_{A_1}}^{N_{A_1}+N_B} ds \left| \frac{d\mathbf{u}_\alpha(s)}{ds} \right|^2 \tag{291}$$

Interactions between monomers on the same or different polymers are usually modeled by pseudopotentials in the monomer densities, e.g., a local quadratic form in the microscopic monomer densities. In the case of the three different species melt considered here, we adopt the following form for this pseudopotential

$$H_F = \rho_0 \int d\mathbf{r} \left[\chi_{AB} \hat{\rho}_A(\mathbf{r}) \hat{\rho}_B(\mathbf{r}) + \chi_{AR} \hat{\rho}_A(\mathbf{r}) \hat{\rho}_R(\mathbf{r}) + \chi_{BR} \hat{\rho}_B(\mathbf{r}) \hat{\rho}_R(\mathbf{r}) \right] \tag{292}$$

where $\chi_{\alpha\beta}$ represents the Flory-Huggins interaction parameter between the α and β blocks. The Maier-Saupe-type orentational interaction is adopted to describe the excluded volume interactions between the rods

$$H_S = -\frac{\eta \rho_0}{2} \int d\mathbf{r}\, \hat{\mathbf{S}}(\mathbf{r}) : \hat{\mathbf{S}}(\mathbf{r}) \tag{293}$$

with η representing the strength of the orientational interaction favoring the alignment of the rods.

The particle-based partition function is

$$\mathcal{Z} = \int D\mathbf{R}_\alpha(s) d\mathbf{u}_\alpha(s) \delta[\hat{\rho}_A(\mathbf{r}) + \hat{\rho}_B(\mathbf{r}) + \hat{\rho}_R(\mathbf{r}) - 1] \exp[-H_0 - H_1 - H_F - H_S] \tag{294}$$

where the functional delta constraint imposes the local incompressibility condition. There are three differently chemical species in the T-shaped liquid-crystal block copolymer melt system. A typical starting point is to decouple the quadratic density and orientational interactions through a Hubbard-Stratanovich transformation leading to a representation wherein independent polymer chains are coupled to fluctuating potential fields. In our recent work, we have extend this decouple technology to multi-species systems. By this new approach, the derived field-based theory has good mathematical feature that shows the equilibrium states are saddle-points. Moreover, the descent and ascent directions of saddle-points of the effective field-based energy have been shown explicitly. The method can be also extended to multi-species liquid-crystal block copolymer systems straightforwardly. For our considered system, the field-based theory is

$$\mathcal{Z} \propto \int D\mu_+ \int D\mu_1 \int D\mu_2 \, \exp(-H[\mu_+, \mu_1, \mu_2]) \tag{295}$$

where

$$H = \frac{n}{V} \int d\mathbf{r} \left(\frac{1}{4N\zeta_1} \mu_1^2 + \frac{1}{4N\zeta_1} \mu_2^2 - \mu_+ \right) + \frac{n}{2\eta NV} \int d\mathbf{r} \, \mathbf{M}(\mathbf{r}) : \mathbf{M}(\mathbf{r}) - n \log Q[\mu_+, \mu_1, \mu_2] \tag{296}$$

$$\omega_\alpha = \mu_+ - \sigma_{1\alpha}\mu_1 - \sigma_{2\alpha}\mu_2, \quad \alpha \in \{A, R, B\}. \tag{297}$$

In this expression, these coefficients are

$$\begin{aligned}
&\zeta_1 = \frac{-\Delta}{4\chi_{AB}}, \qquad \Delta = \chi_{AB}^2 + \chi_{AR}^2 + \chi_{BR}^2 - 2\chi_{AB}\chi_{AR} - 2\chi_{AB}\chi_{BR} - 2\chi_{AR}\chi_{BR} \\
&\zeta_2 = \chi_{AB}, \\
&\sigma_{1A} = \frac{1}{3}, \qquad \sigma_{1R} = -\frac{2}{3}, \qquad \sigma_{1B} = \frac{1}{3}, \\
&\sigma_{2A} = \frac{1+\alpha}{3}, \quad \sigma_{2R} = \frac{1-2\alpha}{3}, \quad \sigma_{2B} = \frac{\alpha - 2}{3}, \quad \alpha = \frac{\chi_{AB} + \chi_{AR} - \chi_{RB}}{2\chi_{AB}}.
\end{aligned} \tag{298}$$

The descent and ascent directions of the saddle-points are dependent on the sign of ζ_1 and ζ_2. For simplicity, we assume that $\chi_{AB} > 0$. When $\Delta > 0$, the equilibrium solutions of the energy functional (296) shall be maximized with respect to the potential field μ_+ and μ_1, and minimized with respect to potential fields μ_2 and $\mathbf{M}$. When $\Delta < 0$, the equilibrium states of the energy functional (296) are the maxima along the potential field μ_+, and minima along other potential fields μ_1, μ_2, $\mathbf{M}$. When $\Delta = 0$, the "exchange chemical field" μ_1 disappears. The field-based energy functional degenerates to

$$H = \frac{n}{V} \int d\mathbf{r} \left(\frac{1}{4N\zeta_2} \mu_2^2 - \mu_+ \right) + \frac{n}{2\eta NV} \int d\mathbf{r} \, \mathbf{M}(\mathbf{r}) : \mathbf{M}(\mathbf{r}) - n \log Q[\mu_+, \mu_1, \mu_2] \tag{299}$$

$$\omega_\alpha = \mu_+ - \sigma_{2\alpha}\mu_2, \quad \alpha \in \{A, B, C\}. \tag{300}$$

In this case, the physical solutions of the incompressible block copolymer system are saddle points in which the energy functional (299) shall be maximized along field μ_+, and minimized along fields μ_2 and $\mathbf{M}$.

The following representation is nondimensionalized in units of by $R_{gB} = b_B(N/6)^{1/2}$, and the contour variable s in units of the degree of polymerization N

$$f_{A_1} = N_{A_1}/N, \; f_{A_2} = N_{A_2}/N, \; f_B = N_B/N, \; f_{R_1} = N_{R_1}/N, \; f_{R_2} = N_{R_2}/N, \; f_{A_1} + f_{A_2} + f_B + f_R = 1 \tag{301}$$

We also define

$$\Gamma(\mathbf{r}, \mathbf{u}) = w_R(\mathbf{r}) - \mathbf{M}(\mathbf{r}) : \left(\mathbf{u}\mathbf{u} - \frac{1}{3}\mathbf{I} \right) \tag{302}$$

For the sake of brevity, we often use $\Gamma(\mathbf{r})$ to instead $\Gamma(\mathbf{r}, \mathbf{u})$ in the subsequent modeling process.

In this present research, we focus on the mean-field approximation, commonly referred to in this context as self-consistent field theory (SCFT). In SCFT, the above exact Hamiltonian $H[\mu_+, \mu_1, \mu_2, \mathbf{M}]$ is approximated by its value $H[\mu_+^*, \mu_1^*, \mu_2^*, \mathbf{M}^*]$ which is evaluated at the saddle points of H.

$$\frac{\delta H}{\delta \mu_1}\Big|_{\mu_+^*,\mu_1^*,\mu_2^*,\mathbf{M}^*} = 0 \tag{303}$$

$$\frac{\delta H}{\delta \mu_2}\Big|_{\mu_+^*,\mu_1^*,\mu_2^*,\mathbf{M}^*} = 0 \tag{304}$$

$$\frac{\delta H}{\delta \mu_+}\Big|_{\mu_+^*,\mu_1^*,\mu_2^*,\mathbf{M}^*} = 0 \tag{305}$$

$$\frac{\delta H}{\delta \mathbf{M}}\Big|_{\mu_+^*,\mu_1^*,\mu_2^*,\mathbf{M}^*} = 0 \tag{306}$$

For brevity, we will omit the asterisk in the subsequent description. The above conditions yield the following self-consistent equations for the potentials fields

$$\rho_A + \rho_B + \rho_R - 1 = 0, \tag{307}$$

$$\frac{1}{2N\zeta_1}\mu_1 - \sigma_{1A}\rho_A - \sigma_{1R}\rho_R - \sigma_{1B}\rho_B = 0, \tag{308}$$

$$\frac{1}{2N\zeta_2}\mu_2 - \sigma_{2A}\rho_A - \sigma_{2R}\rho_R - \sigma_{2B}\rho_B = 0, \tag{309}$$

$$\frac{1}{\eta N}\mathbf{M} - \mathbf{S} = 0. \tag{310}$$

In the above equations, ρ_A, ρ_B and ρ_R represent the volume fractions of the flexible and the semiflexible, respectively, and $\mathbf{S}$ the averaged orientational order parameter. These fields can be computed as

$$Q = \frac{1}{V}\int d\mathbf{r} q_B(\mathbf{r}, 0) q_B^\dagger(\mathbf{r}, f_B), \tag{311}$$

$$\rho_A(\mathbf{r}) = \frac{1}{Q}\left(\int_0^{f_{A_1}} ds\, q_{A,1}(\mathbf{r}, s) q_{A,1}^\dagger(\mathbf{r}, f_{A_1} - s) + \int_0^{f_{A_2}} ds\, q_{A,2}(\mathbf{r}, s) q_{A,2}^\dagger(\mathbf{r}, f_{A_2} - s)\right), \tag{312}$$

$$\rho_B(\mathbf{r}) = \frac{1}{Q}\int_0^{f_B} ds\, q_B(\mathbf{r}, s) q_B^\dagger(\mathbf{r}, f_B - s), \tag{313}$$

$$\begin{aligned}\rho_R(\mathbf{r}) = \frac{4\pi}{Q}\Bigg(&\int_0^{f_{R_1}} ds \int d\mathbf{u}\, q_{R,1}(\mathbf{r}, \mathbf{u}, s) q_{R,1}^\dagger(\mathbf{r}, \mathbf{u}, f_{R_1} - s) \\ &+ \int_0^{f_{R_2}} ds \int d\mathbf{u}\, q_{R,2}(\mathbf{r}, \mathbf{u}, s) q_{R,2}^\dagger(\mathbf{r}, \mathbf{u}, f_{R_2} - s)\Bigg),\end{aligned} \tag{314}$$

$$\begin{aligned}\mathbf{S}(\mathbf{r}) = \frac{4\pi}{Q}\Bigg[&\int_0^{f_{R_1}} ds \int d\mathbf{u}\, q_{R,1}(\mathbf{r}, \mathbf{u}, s)\Big(\mathbf{u}\mathbf{u} - \frac{1}{3}\mathbf{I}\Big) q_{R,1}^\dagger(\mathbf{r}, \mathbf{u}, f_{R_1} - s) \\ &+ \int_0^{f_{R_2}} ds \int d\mathbf{u}\, q_{R,2}(\mathbf{r}, \mathbf{u}, s)\Big(\mathbf{u}\mathbf{u} - \frac{1}{3}\mathbf{I}\Big) q_{R,2}^\dagger(\mathbf{r}, \mathbf{u}, f_{R_2} - s)\Bigg]\end{aligned} \tag{315}$$

These propagators satisfy the following PDEs

$$\begin{aligned}&\frac{\partial}{\partial s} q_{A,1}(\mathbf{r}, s) = \varepsilon^2 \nabla_{\mathbf{r}}^2 q_{A,1}(\mathbf{r}, s) - w_A(\mathbf{r}) q_{A,1}(\mathbf{r}, s), \quad 0 \leqslant s \leqslant f_{A_1}, \\ &\quad q_{A,1}(\mathbf{r}, 0) = 1\end{aligned} \tag{316}$$

$$\begin{aligned}&\frac{\partial}{\partial s} q_{R,1}(\mathbf{r}, \mathbf{u}, s) = -\nu \mathbf{u} \cdot \nabla_{\mathbf{r}} q_{R,1}(\mathbf{r}, \mathbf{u}, s) - \Gamma(\mathbf{r}, \mathbf{u}) q_{R,1}(\mathbf{r}, \mathbf{u}, s) + \frac{1}{2\lambda}\nabla_{\mathbf{u}}^2 q_{R,1}(\mathbf{r}, \mathbf{u}, s), \\ &\quad q_{R,1}(\mathbf{r}, \mathbf{u}, 0) = \frac{q_{A,1}(\mathbf{r}, f_{A_1})}{4\pi}, \quad 0 \leqslant s \leqslant f_{R_1},\end{aligned} \tag{317}$$

$$\begin{aligned}\frac{\partial}{\partial s}q_{A,2}(\mathbf{r},s) &= \varepsilon^2\nabla^2_{\mathbf{r}}q_{A,2}(\mathbf{r},s) - w_A(\mathbf{r})q_{A,2}(\mathbf{r},s), \quad 0 \leqslant s \leqslant f_{A_2},\\ q_{A,2}(\mathbf{r},0) &= 1\end{aligned} \tag{318}$$

$$\begin{aligned}&\frac{\partial}{\partial s}q_{R,2}(\mathbf{r},\mathbf{u},s) = \nu\mathbf{u}\cdot\nabla_{\mathbf{r}}q_{R,2}(\mathbf{r},\mathbf{u},s) - \Gamma(\mathbf{r},\mathbf{u})q_{R,2}(\mathbf{r},\mathbf{u},s) + \frac{1}{2\lambda}\nabla^2_{\mathbf{u}}q_{R,2}(\mathbf{r},\mathbf{u},s),\\ &q_{R,2}(\mathbf{r},\mathbf{u},f_{A_2}) = \frac{q_{A,2}(\mathbf{r},f_{A_2})}{4\pi}, \quad 0 \leqslant s \leqslant f_{R_2},\end{aligned} \tag{319}$$

$$\begin{aligned}\frac{\partial}{\partial s}q_{B}(\mathbf{r},s) &= \nabla^2_{\mathbf{r}}q_{B}(\mathbf{r},s) - w_B(\mathbf{r})q_{B}(\mathbf{r},s), \quad 0 \leqslant s \leqslant f_{B},\\ q_{B}(\mathbf{r},0) &= 1\end{aligned} \tag{320}$$

$$\begin{aligned}\frac{\partial}{\partial s}q^{\dagger}_{B}(\mathbf{r},s) &= \nabla^2_{\mathbf{r}}q^{\dagger}_{B}(\mathbf{r},s) - w_B(\mathbf{r})q^{\dagger}_{B}(\mathbf{r},s), \quad 0 \leqslant s \leqslant f_{B},\\ q^{\dagger}_{B}(\mathbf{r},0) &= \int d\mathbf{u}\, q_{R,1}(\mathbf{r},\mathbf{u},f_{R_1})q_{R,2}(\mathbf{r},\mathbf{u},f_{R_2})\end{aligned} \tag{321}$$

$$\begin{aligned}&\frac{\partial}{\partial s}q^{\dagger}_{R,1}(\mathbf{r},\mathbf{u},s) = \nu\mathbf{u}\cdot\nabla_{\mathbf{r}}q^{\dagger}_{R,1}(\mathbf{r},\mathbf{u},s) - \Gamma(\mathbf{r},\mathbf{u})q^{\dagger}_{R,1}(\mathbf{r},\mathbf{u},s) + \frac{1}{2\lambda}\nabla^2_{\mathbf{u}}q^{\dagger}_{R,1}(\mathbf{r},\mathbf{u},s), \quad 0 \leqslant s \leqslant f_{R_1},\\ &q^{\dagger}_{R,1}(\mathbf{r},\mathbf{u},0) = \frac{1}{4\pi}q_B(\mathbf{r},f_B)q_{R,2}(\mathbf{r},\mathbf{u},f_{R_2})\end{aligned} \tag{322}$$

$$\begin{aligned}&\frac{\partial}{\partial s}q^{\dagger}_{R,2}(\mathbf{r},\mathbf{u},s) = -\nu\mathbf{u}\cdot\nabla_{\mathbf{r}}q^{\dagger}_{R,2}(\mathbf{r},\mathbf{u},s) - \Gamma(\mathbf{r},\mathbf{u})q^{\dagger}_{R,2}(\mathbf{r},\mathbf{u},s) + \frac{1}{2\lambda}\nabla^2_{\mathbf{u}}q^{\dagger}_{R,2}(\mathbf{r},\mathbf{u},s), \quad 0 \leqslant s \leqslant f_{R_2},\\ &q^{\dagger}_{R,2}(\mathbf{r},\mathbf{u},0) = \frac{1}{4\pi}q_B(\mathbf{r},f_B)q_{R,1}(\mathbf{r},\mathbf{u},f_{R_1})\end{aligned} \tag{323}$$

$$\begin{aligned}\frac{\partial}{\partial s}q^{\dagger}_{A,1}(\mathbf{r},s) &= \varepsilon^2\nabla^2_{\mathbf{r}}q^{\dagger}_{A,1}(\mathbf{r},s) + w_A(\mathbf{r})q^{\dagger}_{A,1}(\mathbf{r},s), \quad 0 \leqslant s \leqslant f_{A_1},\\ q^{\dagger}_{A,1}(\mathbf{r},0) &= \int d\mathbf{u}\, q^{\dagger}_{R,1}(\mathbf{r},\mathbf{u},f_{R_1})\end{aligned} \tag{324}$$

$$\begin{aligned}\frac{\partial}{\partial s}q^{\dagger}_{A,2}(\mathbf{r},s) &= \varepsilon^2\nabla^2_{\mathbf{r}}q^{\dagger}_{A,2}(\mathbf{r},s) + w_A(\mathbf{r})q^{\dagger}_{A,2}(\mathbf{r},s), \quad 0 \leqslant s \leqslant f_{A_2},\\ q^{\dagger}_{A,2}(\mathbf{r},0) &= \int d\mathbf{u}\, q^{\dagger}_{R,2}(\mathbf{r},\mathbf{u},f_{R_2})\end{aligned} \tag{325}$$

C. Modeling with rod system

In the sequel, we consider that liquid-crystal part is rod rather than semiflexible. Then the rod part of the polymer is modeled as a rod of finite thickness with a unit orientation vector $\mathbf{u}_\alpha$ characterizing its conformation. Note that in this case we define unique forward direction of orientation as figure 5 shown. For this case, $(\lambda \to +\infty)$, the propagators $q_{R,1}(\mathbf{r},\mathbf{u},s)$, $q_{R,2}(\mathbf{r},\mathbf{u},s)$, $q^{\dagger}_{R,1}(\mathbf{r},\mathbf{u},s)$, and $q^{\dagger}_{R,2}(\mathbf{r},\mathbf{u},s)$ of rod block parts can be calculated analytically. The propagators of coils can be computed in the same way

$$\begin{aligned}\frac{\partial}{\partial s}q_{A,1}(\mathbf{r},s) &= \varepsilon^2\nabla^2_{\mathbf{r}}q_{A,1}(\mathbf{r},s) - w_A(\mathbf{r})q_{A,1}(\mathbf{r},s), \quad 0 \leqslant s \leqslant f_{A_1},\\ q_{A,1}(\mathbf{r},0) &= 1\end{aligned} \tag{326}$$

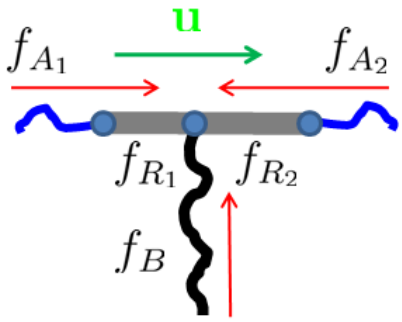

FIG. 5: Schematic diagram of T-shaped liquid-crystal block copolymer. In this subsection, we will use rod-like chain model to describe the liquid-crystal-part subchain. The green arrow denotes the unique forward direction of orientation. Red arrows denote the forward direction when calculating propagators of coil blocks.

$$\begin{aligned}\frac{\partial}{\partial s}q_{A,2}(\mathbf{r},s) &= \varepsilon^2\nabla^2_{\mathbf{r}}q_{A,2}(\mathbf{r},s) - w_A(\mathbf{r})q_{A,2}(\mathbf{r},s), \quad 0\leqslant s\leqslant f_{A_2},\\ q_{A,2}(\mathbf{r},0) &= 1\end{aligned} \tag{327}$$

$$\begin{aligned}\frac{\partial}{\partial s}q_{B}(\mathbf{r},s) &= \nabla^2_{\mathbf{r}}q_{B}(\mathbf{r},s) - w_B(\mathbf{r})q_{B}(\mathbf{r},s), \quad 0\leqslant s\leqslant f_{B},\\ q_{B}(\mathbf{r},0) &= 1\end{aligned} \tag{328}$$

$$\begin{aligned}&\frac{\partial}{\partial s}q^\dagger_{B}(\mathbf{r},s) = -\nabla^2_{\mathbf{r}}q^\dagger_{B}(\mathbf{r},s) + w_B(\mathbf{r})q^\dagger_{B}(\mathbf{r},s), \quad 0\leqslant s\leqslant f_{B},\\ &q^\dagger_B(\mathbf{r},0) = \int d\mathbf{u}\left\{\exp\Big[-\int_0^{f_{R_1}} ds\,\Gamma(\mathbf{r}+\nu s\mathbf{u})\Big]q_{A,1}(\mathbf{r}-\nu f_{R_1}\mathbf{u},f_{A_1})\right.\\ &\qquad\left.\exp\Big[-\int_0^{f_{R_2}} ds\,\Gamma(\mathbf{r}-\nu s\mathbf{u})\Big]q_{A,2}(\mathbf{r}+\nu f_{R_2}\mathbf{u},f_{A_2})\right\}\end{aligned} \tag{329}$$

$$\begin{aligned}&\frac{\partial}{\partial s}q^\dagger_{A,1}(\mathbf{r},s) = -\varepsilon^2\nabla^2_{\mathbf{r}}q^\dagger_{A,1}(\mathbf{r},s) + w_A(\mathbf{r})q^\dagger_{A,1}(\mathbf{r},s), \quad 0\leqslant s\leqslant f_{A_1},\\ &q^\dagger_{A,1}(\mathbf{r},f_{R_1}) = \int d\mathbf{u}\left\{q_B(\mathbf{r}+\nu f_{R_1}\mathbf{u},f_B)q_{A,2}\big[\mathbf{r}+\nu(f_{R_1}+f_{R_2})\mathbf{u},f_{A_2}\big]\right.\\ &\qquad\left.\exp\Big[-\int_0^{f_{R_2}} ds\,\Gamma(\mathbf{r}+\nu(f_{R_1}+f_{R_2})\mathbf{u}-\nu s\mathbf{u}\Big]\exp\Big[-\int_0^{f_{R_1}} ds\,\Gamma(\mathbf{r}+\nu f_{R_1}\mathbf{u}-\nu s\mathbf{u})\Big]\right\}\end{aligned} \tag{330}$$

$$\begin{aligned}&\frac{\partial}{\partial s}q^\dagger_{A,2}(\mathbf{r},s) = -\varepsilon^2\nabla^2_{\mathbf{r}}q^\dagger_{A,2}(\mathbf{r},s) + w_A(\mathbf{r})q^\dagger_{A,2}(\mathbf{r},s), \quad 0\leqslant s\leqslant f_{A_2},\\ &q^\dagger_{A,2}(\mathbf{r},f_{R_2}) = \int d\mathbf{u}\left\{q_B(\mathbf{r}-\nu f_{R_2}\mathbf{u},f_B)q_{A,1}(\mathbf{r}-\nu(f_{R_1}+f_{R_2})\mathbf{u},f_{A_1})\right.\\ &\qquad\left.\exp\Big[-\int_0^{f_{R_1}} ds\,\Gamma(\mathbf{r}-\nu f_{R_2}\mathbf{u}+\nu s\mathbf{u})\Big]\exp\Big[-\int_0^{f_{R_2}} ds\,\Gamma(\mathbf{r}-\nu(f_{R_1}+f_{R_2})\mathbf{u}+\nu s\mathbf{u})\Big]\right\}\end{aligned} \tag{331}$$

Furthermore, the partition function Q for an unconstrained chain can be evaluated in terms of the chain propagator $q(\mathbf{r},s)$

$$Q = \frac{1}{V}\int d\mathbf{r}q_B(\mathbf{r},0)q^\dagger_B(\mathbf{r},f_B), \tag{332}$$

The segement densities ρ_A, ρ_B and ρ_R along with the orientational order $\mathbf{S}(\mathbf{r})$ follows that

$$\rho_A(\mathbf{r}) = \frac{1}{Q}\left(\int_0^{f_{A_1}} ds\, q_{A,1}(\mathbf{r},s)q^\dagger_{A,1}(\mathbf{r},f_A-s) + \int_0^{f_A} ds\, q_{A,2}(\mathbf{r},s)q^\dagger_{A,2}(\mathbf{r},f_{A_2}-s)\right) \tag{333}$$

$$\rho_B(\mathbf{r}) = \frac{1}{Q}\int_0^{f_B} ds\, q_B(\mathbf{r},s)q^\dagger_B(\mathbf{r},f_B-s), \tag{334}$$

$$\begin{aligned}\rho_R(\mathbf{r}) = \frac{1}{Q}\Bigg\{ &\int_0^{f_{R_1}} ds \int d\mathbf{u}\,\Big[q_{A,1}(\mathbf{r}-\nu s\mathbf{u},f_{A_1})q_{A,2}(\mathbf{r}-\nu s\mathbf{u}+\nu(f_{R_1}+f_{R_2})\mathbf{u},f_{A_2}) \\ &\qquad\times q_B(\mathbf{r}+\nu(f_{R_1}-s)\mathbf{u},f_B)\exp\big(-\int_0^{f_{R_1}+f_{R_2}} ds'\,\Gamma(\mathbf{r}-\nu s\mathbf{u}+\nu s'\mathbf{u})\big)\Big] \\ &+\int_0^{f_{R_1}} ds \int d\mathbf{u}\,\Big[q_{A,2}(\mathbf{r}+\nu s\mathbf{u},f_{A_2})q_{A,1}(\mathbf{r}+\nu s\mathbf{u}-\nu(f_{R_1}+f_{R_2})\mathbf{u},f_{A_1}) \\ &\qquad\times q_B(\mathbf{r}-\nu(f_{R_1}-s)\mathbf{u},f_B)\exp\big(-\int_0^{f_{R_1}+f_{R_2}} ds'\,\Gamma(\mathbf{r}+\nu s\mathbf{u}-\nu s'\mathbf{u})\big)\Big]\Bigg\},\end{aligned} \tag{335}$$

$$\begin{aligned}\mathbf{S}(\mathbf{r}) = \frac{1}{Q}\Bigg\{ &\int_0^{f_{R_1}} ds \int d\mathbf{u}\,\Big[\big(\mathbf{uu}-\frac{1}{3}\mathbf{I}\big)q_{A,1}(\mathbf{r}-\nu s\mathbf{u},f_{A_1})q_{A,2}(\mathbf{r}-\nu s\mathbf{u}+\nu(f_{R_1}+f_{R_2})\mathbf{u},f_{A_2}) \\ &\qquad\times q_B(\mathbf{r}+\nu(f_{R_1}-s)\mathbf{u},f_B)\exp\big(-\int_0^{f_{R_1}+f_{R_2}} ds'\,\Gamma(\mathbf{r}-\nu s\mathbf{u}+\nu s'\mathbf{u})\big)\Big] \\ &+\int_0^{f_{R_1}} ds \int d\mathbf{u}\,\Big[\big(\mathbf{uu}-\frac{1}{3}\mathbf{I}\big)q_{A,2}(\mathbf{r}+\nu s\mathbf{u},f_{A_2})q_{A,1}(\mathbf{r}+\nu s\mathbf{u}-\nu(f_{R_1}+f_{R_2})\mathbf{u},f_{A_1}) \\ &\qquad\times q_B(\mathbf{r}-\nu(f_{R_1}-s)\mathbf{u},f_B)\exp\big(-\int_0^{f_{R_1}+f_{R_2}} ds'\,\Gamma(\mathbf{r}+\nu s\mathbf{u}-\nu s'\mathbf{u})\big)\Big]\Bigg\}.\end{aligned} \tag{336}$$

XII. NUMERICAL METHODS

Self-consistent field iterative procedure

Step 1: Given initial estimations of fields w_α, $\alpha = A, B, C$, and fixed computational box;

Step 2: Compute forward (back) propagator operators q and $q^\dagger$ (see Sec. XII B);

Step 3: Obtain Q and ρ_α by integral equations (see Sec. XII C), and calculate the value of effective Hamiltonian H;

Step 4: Update fields w_α using some mixing methods (see Sec. XII D);

Step 5: Goto **Step 2** until the Hamiltonian does not change.

A. Discretization scheme

1. Spatial discretization

The projection method can be chosen to solve self-consistent field equations to study the quasicrystals as well as periodic structures. Using the projection method, a quasiperiodic or periodic function can be expanded as

$$f(\mathbf{r}) = \sum_{\{\mathbf{H}\}} \hat{f}_{\mathbf{H}} e^{i[(\mathcal{S}\cdot\mathbf{H})^T\cdot\mathbf{r}]}. \tag{337}$$

More details about this numerical method can be found in Ref. [4].

2. Spherical harmonic series

Spherical harmonic– The spherical harmonic $Y_{lm}(\phi,\theta)$, $-l \leqslant m \leqslant l$ is a function of two coordinates ϕ, θ on the surface of a sphere. The spherical harmonics are orthogonal for different l and m, and they are normalized so that their integrated square over the spherical surface is unity:

$$\int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) Y^*_{l'm'}(\phi,\theta) Y_{lm}(\phi,\theta) = \delta_{l'l}\delta_{m'm} \tag{338}$$

Here the asterisk denotes complex conjugation. In particular, the spherical harmonics are related to *associated Legendre polynomials* by the equation

$$Y_{lm}(\phi,\theta) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\phi} \tag{339}$$

By using the relation

$$Y_{l,-m}(\phi,\theta) = (-1)^m Y^*_{lm}(\phi,\theta) \tag{340}$$

With $x = \cos\theta$, the associated Legendre polynomials are

$$P_l^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x), \quad l, m \geqslant 0 \tag{341}$$

where P_l is the ordinary Legendre polynomials

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l, \quad l \geqslant 0. \tag{342}$$

The associated Legendre polynomials can be generated by the following stable recurrence on l

$$(l-m)P_l^m = x(2l-1)P_{l-1}^m - (l+m-1)P_{l-2}^m \tag{343}$$

For convenience of the following computations, we define

$$\tilde{P}_l^m = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m \tag{344}$$

Then the recurrence relation becomes

$$\tilde{P}_l^m = \sqrt{\frac{4l^2-1}{l^2-m^2}}\left[x\tilde{P}_{l-1}^m - \sqrt{\frac{(l-1)^2-m^2}{4(l-1)^2-1}}\tilde{P}_{l-2}^m\right] \tag{345}$$

We start the recurrence with the closed-form expression for the $l=m$ function,

$$\tilde{P}_m^m = (-1)^m\sqrt{\frac{2m+1}{4\pi(2m)!}}(2m-1)!!(1-x^2)^{m/2} \tag{346}$$

Using Eq.(345) with $l=m+1$, and setting $\tilde{P}_{m-1}^m = 0$, we find

$$\tilde{P}_{m+1}^m = x\sqrt{2m+3}\tilde{P}_m^m \tag{347}$$

The above two equations provide the two starting values required for Eq.(345) for general l.

Fast spherical harmonic transforms– Any smooth function on the surface of a sphere can be written as an expansion in spherical harmonics.

$$g(\mathbf{u}) = g(\phi,\theta) = \sum_{l=0}^{+\infty}\sum_{m=-l}^{l} g_{lm}Y_{lm}(\phi,\theta). \tag{348}$$

where $\mathbf{u} = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta)^T, \phi\in[0,2\pi), \theta\in[0,\pi]$.

Suppose the function can be well-approximated by truncating the expansion at $l = l_{\max}$:

B. Solving modified diffusion equation (MDE)

1. *Continuous Gaussian chain*

For brevity, we consider that the value of field w in Eqn. (193) is the same to demonstrate discretization schemes.

- Second-order operator-splitting scheme:
  In each time step $j\Delta s \to (j+1)\Delta s$

$$\begin{aligned}
&\frac{dq}{ds} = \nabla^2 q, \qquad j\Delta s \leqslant s \leqslant (j+\frac{1}{2})\Delta s\\
&\frac{dq}{ds} = -w(\mathbf{r})q, \quad j\Delta s \leqslant s \leqslant (j+1)\Delta s\\
&\frac{dq}{ds} = \nabla^2 q, \qquad (j+\frac{1}{2})\Delta s \leqslant s \leqslant (j+1)\Delta s
\end{aligned}$$

- Fourth-order Adams-Bashford scheme [6]:

$$\begin{aligned}
&\frac{25}{12}q^{j+1} - 4q^j + 3q^{j-1} - \frac{4}{3}q^{j-2} + \frac{1}{4}q^{j-3} =\\
&\qquad \Delta s[\nabla^2 q^{j+1} - w(4q^j - 6q^{j-1} + 4q^{j-2} - q^{j-3})]
\end{aligned} \tag{349}$$

This method also can be implemented using the psedospectral method. The initial values required to apply this formula are obtained using second-order operator-splitting scheme and Richardson's extrapolation. Assume that Q is the exact solution of the MDE, $Q(\Delta s)$ is the numerical solution of MDE by second-order operator-splitting scheme with s-step size Δs, then $Q - Q(\Delta s) = O(\Delta s^2)$. By Richardson's extrapolation, we have

$$Q - \Big(\frac{1}{21}Q(\Delta s) - \frac{4}{7}Q\Big(\frac{\Delta s}{2}\Big) + \frac{32}{21}Q\Big(\frac{\Delta s}{4}\Big)\Big) = O(\Delta s^4) \tag{350}$$

A more simper extrapolation scheme is proposed by Ranjan et. al [5]

$$Q - \Big(-\frac{1}{3}Q(\Delta s) + \frac{4}{3}Q\Big(\frac{\Delta s}{2}\Big)\Big) = O(\Delta s^4). \tag{351}$$

For a common scheme, the above extrapolation scheme usually has three order accuracy. However, making use of makes use of the feature of the second-order operator-splitting method, it has fourth-order accuracy.

- Certainly, one can obtain any high-order schemes using any one of the above schemes with Richardson's extrapolation.

2. Wormlike chain

The operator splitting scheme can be also used to solve MDEs of wormlike chain model. The right term of equation 206 can be decomposed into three terms

$$\begin{aligned}\mathcal{L} &= -\beta\mathbf{u}\cdot\nabla_{\mathbf{r}} - \Big[w(\mathbf{r}) - \mathbf{M}(\mathbf{r}) : \Big(\mathbf{uu} - \frac{1}{3}\mathbf{I}\Big)\Big] + \frac{1}{2\lambda}\nabla^2_{\mathbf{u}} \\ &= \mathcal{L}_\nabla + \mathcal{L}_{WM} + \mathcal{L}_\Delta.\end{aligned} \tag{352}$$

In particular, the second-order operator-splitting scheme is

$$q^{(n+1)}(\mathbf{r},\mathbf{u}) = e^{\Delta s\mathcal{L}_{WM}/2}e^{\Delta s\mathcal{L}_\nabla/2}e^{\Delta s\mathcal{L}_\Delta}e^{\Delta s\mathcal{L}_\nabla/2}e^{\Delta s\mathcal{L}_{WM}/2}q^{(n)}(\mathbf{r},\mathbf{u}). \tag{353}$$

By psedospectral technology, the operator in the right term of Eq.(206) in each s step can be split into five parts,

$$\begin{array}{ccccccccc} q(\mathbf{r},\mathbf{u}) & \to & \hat{q}(\mathbf{k},\mathbf{u}) & \to & \hat{q}_{lm}(\mathbf{k}) & \to & \hat{q}(\mathbf{k},\mathbf{u}) & \to & q(\mathbf{r},\mathbf{u}) \\ e^{\Delta s\mathcal{L}_{WM}/2} & & e^{\Delta s\mathcal{L}_\nabla/2} & & e^{\Delta s\mathcal{L}_\Delta} & & e^{\Delta s\mathcal{L}_\nabla/2} & & e^{\Delta s\mathcal{L}_{WM}/2} \end{array}$$

C. Numerical approximate to integral equations

A fourth-order integral formula is (see Ref. [7], P.134)

$$\int_0^{n_s} ds\, f(s) = \Delta s\left\{-\frac{5}{8}(f_0 + f_{n_s}) + \frac{1}{6}(f_1 + f_{n_s-1}) - \frac{1}{24}(f_2 + f_{n_s-2}) + \sum_{j=0}^{n_s} f_j\right\}. \tag{354}$$

D. Iterative method

1. Simple mixing method

Simple Mixing Algorithm
The conjugate field w_α can be updated through

$$w_{\alpha,j}^{(k+1)} = w_{\alpha,j}^{(k)} + \lambda\left(\frac{\delta H}{\delta\rho_\alpha}\right)_j^{(k)}, \tag{355}$$

where α is a parameter, usually ≤ 0.1. The incompressible field w_+ can be updated by Eqns. (185-188).

2. Andersion mixing method

Anderson Mixing Algorithm (Expression I)

- The k-th iteration begins with the evaluation of temp fields $\bar{w}_{\alpha,j}^{(k)}$, $\alpha = A, B, C$, from Eqns. (185-188) where $\rho_{\alpha,j}^{(k)}$ are evaluated from the old fields $w_{\alpha,j}^{(k)}$, and

$$w_{+,j}^{(k)} = \frac{\sum_\alpha w_{\alpha,j}^{(k)} X_\alpha}{\sum_\alpha X_\alpha}, \quad j \neq 0, \tag{356}$$

$$w_{+,0}^{(k)} = \frac{\sum_\alpha w_{\alpha,j}^{(k)} X_\alpha - 2N\chi_{AB}\chi_{BC}\chi_{AC}}{\sum_\alpha X_\alpha}, \tag{357}$$

  where $X_A = \chi_{BC}(\chi_{AB} + \chi_{AC} - \chi_{BC})$, $X_B = \chi_{AC}(\chi_{BC} + \chi_{AB} - \chi_{AC})$, $X_C = \chi_{AB}(\chi_{AC} + \chi_{BC} - \chi_{AB})$. (*Note that the SCFT is unaffected by additive constants to the fields, and therefore we adjust all the fields so that their spatial averages are zero.*)

- Define the deviation:

$$d_{\alpha,j}^{(k)} = \bar{w}_{\alpha,j}^{(k)} - w_{\alpha,j}^{(k)}, \tag{358}$$

  and error tolerance

$$\text{Error} = \left[\frac{\sum_{\alpha,j} (d_{\alpha,j}^{(k)})^2}{\sum_{\alpha,j} (w_{\alpha,j}^{(k)})^2} \right]^{1/2} \tag{359}$$

  as a measure of the numerical inaccuracy in the field Eqns (185)-(187).

- If the error exceeds some tolerance (Error > tol), then $w_{\alpha,j}^{(k+1)}$ are obtained from the proceeding n_r iterations. This is done by evaluating the symmetric matrix,

$$U_{mn}^{(k)} = \sum_{\alpha,j} (d_{\alpha,j}^{(k)} - d_{\alpha,j}^{(k-m)},\ d_{\alpha,j}^{(k)} - d_{\alpha,j}^{(k-n)}) \tag{360}$$

  for $m, n = 1, 2, \ldots, n_r$, and vector

$$V_m^{(k)} = \sum_{\alpha,j} (d_{\alpha,j}^{(k)} - d_{\alpha,j}^{(k-m)},\ d_{\alpha,j}^{(k)}). \tag{361}$$

  From these, we calculate the coefficients

$$C_n = \sum_m (U^{-1})_{nm} V_m, \tag{362}$$

  and combine the previous histories as

$$T_{\alpha,j}^{(k)} = w_{\alpha,j}^{(k)} + \sum_{n=1}^{n_r} C_n (w_{\alpha,j}^{(k-n)} - w_{\alpha,j}^{(k)}), \tag{363}$$

$$D_{\alpha,j}^{(k)} = d_{\alpha,j}^{(k)} + \sum_{n=1}^{n_r} C_n (d_{\alpha,j}^{(k-n)} - d_{\alpha,j}^{(k)}). \tag{364}$$

  Finally, the new fields are obtained from

$$w_{\alpha,j}^{(k+1)} = T_{\alpha,j}^{(k)} + \lambda D_{\alpha,j}^{(k)}, \tag{365}$$

  where $0 < \lambda = 1.0 - 0.9^k < 1$.

Anderson Mixing Algorithm The Anderson mixing algorithm can be represented in the following way [8]

[1] K. Hayashida, T. Dotera, A. Takano, and Y. Matsushita, Phys. Rev. Lett. **98**, 195502 (2007).
[2] J. Zhang and F. S. Bates, J. Am. Chem. Soc. **134**, 7636 (2012).
[3] G. H. Fredrickson, *The Equilibrium Theory of Inhomogeneous Polymers*, Oxford University Press, USA, 2006.
[4] K. Jiang and P. Zhang, arXiv:1212.3326 (2012).
[5] A. Ranjan, J. Qin, D. C. Morse, Linear response and stability of ordered phases of block copolymer melts, *Macromolecules*, **41**, 942 (2008).
[6] E. W. Cochran, C. J. Garcia-Cervera, and G. H. Fredrickson, *Macromolecules*, **39**, 2449 (2006).
[7] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical recipes in C*, Cambridge University Press, New York, 1992.
[8] H. F. Walker and P. Ni *SIAM J. Numer. Analy.*, **49**, 1715 (2011).