Weakly Compressible AB Diblock and a C-Grafted Nanorod with Smearing Derivation

1 Canonical Ensemble Derivation (with w_+ and $w_{AC}^{(\pm)}$ fields)

The system is composed of n_D AB diblock chains and an explicit, neutral nanoparticle with n_G grafted chains of length N. Each diblock chain has $P_A + P_B = P$ segments. χ_{IJ} is the interaction strength between components I and J AB, AC, BC. Segment center densities are defined as

$$\hat{\rho}_{DA,c}(\mathbf{r}) = \sum_{i=1}^{n_D}\sum_{j=1}^{P_A}\delta(\mathbf{r}-\mathbf{r}_{i,j})$$

$$\hat{\rho}_{DB,c}(\mathbf{r}) = \sum_{i=1}^{n_D}\sum_{j=P_A+1}^{P}\delta(\mathbf{r}-\mathbf{r}_{i,j})$$

$$\hat{\rho}_{GC,c}(\mathbf{r}) = \sum_{i=1}^{n_G}\sum_{j=1}^{N}\delta(\mathbf{r}-\mathbf{r}_{i})$$

For all of the polymer segments, the full (smeared) segment densities are given by:

$$\hat{\rho}_K(\mathbf{r}) = (h * \hat{\rho}_{K,c})(\mathbf{r})$$

where $K \in \{DA, DB, GC\}$ and h is the segment density distribution function given by the Gaussian

$$h(\mathbf{r}) = \left(\frac{1}{2\pi a^2}\right)^{d/2}\exp\left(-\frac{|\mathbf{r}|^2}{2a^2}\right)$$

where a is the segment size and d is the number of dimensions. The nanoparticle density is given by

$$\hat{\rho}_P(\mathbf{r}) = \frac{\rho_0}{4}\mathrm{erfc}\left(\frac{|\mathbf{u}\cdot(\mathbf{r}-\mathbf{r}_c)| - L_P/2}{\xi}\right)\mathrm{erfc}\left(\frac{|\mathbf{u}\times(\mathbf{r}-\mathbf{r}_c)| - R_P}{\xi}\right)$$

where R_P is the nanoparticle radius, L_P is the nanoparticle length, ρ_0 is the bulk density, and ξ controls the nanoparticle interface width. The graft site distribution is defined as a thin shell at the surface of the nanoparticle defined as

$$\Gamma_\sigma(\mathbf{r}) = \frac{|\nabla\Gamma(\mathbf{r})|}{\int d\mathbf{r}'|\nabla\Gamma(\mathbf{r}')|}$$

where σ_0 to used to make this expression a probability density function.

Note that with this definition of Γ_σ, it's important to make sure to use odd numbers of grid points in each dimension to avoid Nyquist mode problems. The harmonic bond potential between connected segments is given by

$$\beta U_0 = \sum_{i=1}^{n_D}\sum_{j=1}^{P-1}\frac{3\left|\mathbf{r}_{i,j+1}-\mathbf{r}_{i,j}\right|^2}{2b^2} + \sum_{i=1}^{n_G}\sum_{j=1}^{N-1}\frac{3\left|\mathbf{r}_{i,j+1}-\mathbf{r}_{i,j}\right|^2}{2b^2} + \underbrace{\sum_{i=1}^{n_G}\frac{3}{2b^2}|\mathbf{r}_{i,1}-\mathbf{r}_{i,\perp}|^2}_{\substack{\text{contribution from bonding}\\ \text{the chain to the ghost site}}}$$

The non-bonded interaction potential is given by

$$\begin{aligned}\beta U_1 =& \frac{\chi_{AB}}{\rho_0}\int d\mathbf{r}\hat{\rho}_{DA}\hat{\rho}_{DB} + \frac{-\chi_{AC}}{\rho_0}\int d\mathbf{r}\hat{\rho}_{DA}\hat{\rho}_{GC} + \frac{\chi_{BC}}{\rho_0}\int d\mathbf{r}\hat{\rho}_{DB}\hat{\rho}_{GC}\\ &+ \frac{\chi_{AP}}{\rho_0}\int d\mathbf{r}\hat{\rho}_{DA}\hat{\rho}_P + \frac{\chi_{BP}}{\rho_0}\int d\mathbf{r}\hat{\rho}_{DB}\hat{\rho}_P + \frac{\chi_{CP}}{\rho_0}\int d\mathbf{r}\hat{\rho}_{GC}\hat{\rho}_P\\ =& \sum_{IJ,I\neq J}\frac{s_{IJ}\chi_{IJ}}{\rho_0}\int d\mathbf{r}\hat{\rho}_I\hat{\rho}_J\end{aligned}$$

where all $\chi_{IJ} > 0$ and s_{IJ} is either +1 (repulsive interaction) or -1 (attractive interaction). In the specific case we'll cover here, with a neutral particle, grafts that are attracted to A and repulsed by B, $s_{AC} = -1$ and $s_{AB} = s_{BC} = 1$, and $\chi_{IP} = 0$ for all I. A Helfand incompressibility potential penalizes deviations away from ρ_0, and is given by

$$\beta U_2 = \frac{\kappa}{2\rho_0} \int d\mathbf{r}\, [\hat{\rho}_+(\mathbf{r}) - \rho_0]^2$$

where

$$\hat{\rho}_+ = \hat{\rho}_{DA} + \hat{\rho}_{DB} + \hat{\rho}_{GC} + \hat{\rho}_P$$

is the local total density. This gives us a canonical partition function of

$$Z_C = \frac{1}{n_D! n_G! \left(\lambda_T^d\right)^{n_D+n_G}} \int d\mathbf{r}^{n_D P} \int d\mathbf{r}^{n_G N} \exp\left(-\beta U_0 - \beta U_1 - \beta U_2\right)$$

To prepare this for a particle-to-field transformation, let's define

$$\begin{aligned}
\hat{\rho}_{AB}^{(\pm)}(\mathbf{r}) =& \hat{\rho}_{DA}(\mathbf{r}) \pm \hat{\rho}_{DB}(\mathbf{r}) \\
\hat{\rho}_{AC}^{(\pm)}(\mathbf{r}) =& \hat{\rho}_{DA}(\mathbf{r}) \pm \hat{\rho}_{GC}(\mathbf{r}) \\
\hat{\rho}_{BC}^{(\pm)}(\mathbf{r}) =& \hat{\rho}_{DB}(\mathbf{r}) \pm \hat{\rho}_{GC}(\mathbf{r})
\end{aligned}$$

With these definitions, we can rewrite βU_1 as

$$\begin{aligned}
\beta U_1 =& \frac{\chi_{AB}}{4\rho_0} \int d\mathbf{r} \left(\hat{\rho}_{AB}^{(+)}(\mathbf{r})^2 - \hat{\rho}_{AB}^{(-)}(\mathbf{r})^2\right) + \frac{-\chi_{AC}}{4\rho_0} \int d\mathbf{r} \left(\hat{\rho}_{AC}^{(+)}(\mathbf{r})^2 - \hat{\rho}_{AC}^{(-)}(\mathbf{r})^2\right) + \frac{\chi_{BC}}{4\rho_0} \int d\mathbf{r} \left(\hat{\rho}_{BC}^{(+)}(\mathbf{r})^2 - \hat{\rho}_{BC}^{(-)}(\mathbf{r})^2\right) \\
&+ \frac{\chi_{AP}}{\rho_0} \int d\mathbf{r} \hat{\rho}_{DA}\hat{\rho}_P + \frac{\chi_{BP}}{\rho_0} \int d\mathbf{r} \hat{\rho}_{DB}\hat{\rho}_P + \frac{\chi_{CP}}{\rho_0} \int d\mathbf{r} \hat{\rho}_{GC}\hat{\rho}_P
\end{aligned}$$

From there, using the Gaussian functional integral (See Fredrickson eqns C.27 and C.28.), we get

$$\begin{aligned}
\exp(-\beta U_1) =& \frac{1}{\Omega_{AB}^{(+)}\Omega_{AB}^{(-)}\Omega_{AC}^{(+)}\Omega_{AC}^{(-)}\Omega_{BC}^{(+)}\Omega_{BC}^{(-)}} \int \mathcal{D}w_{AB}^{(+)} \int \mathcal{D}w_{AB}^{(-)} \int \mathcal{D}w_{AC}^{(+)} \int \mathcal{D}w_{AC}^{(-)} \int \mathcal{D}w_{BC}^{(+)} \int \mathcal{D}w_{BC}^{(-)} \\
&\times \exp\left(-\frac{\rho_0}{\chi_{AB}} \int d\mathbf{r} w_{AB}^{(+)}(\mathbf{r})^2 - i \int d\mathbf{r} \hat{\rho}_{AB}^{(+)}(\mathbf{r}) w_{AB}^{(+)}(\mathbf{r})\right) \exp\left(-\frac{\rho_0}{\chi_{AB}} \int d\mathbf{r} w_{AB}^{(-)}(\mathbf{r})^2 + \int d\mathbf{r} \hat{\rho}_{AB}^{(-)}(\mathbf{r}) w_{AB}^{(-)}(\mathbf{r})\right) \\
&\times \exp\left(-\frac{\rho_0}{\chi_{AC}} \int d\mathbf{r} w_{AC}^{(+)}(\mathbf{r})^2 + \int d\mathbf{r} \hat{\rho}_{AC}^{(+)}(\mathbf{r}) w_{AC}^{(+)}(\mathbf{r})\right) \exp\left(-\frac{\rho_0}{\chi_{AC}} \int d\mathbf{r} w_{AC}^{(-)}(\mathbf{r})^2 - i \int d\mathbf{r} \hat{\rho}_{AC}^{(-)}(\mathbf{r}) w_{AC}^{(-)}(\mathbf{r})\right) \\
&\times \exp\left(-\frac{\rho_0}{\chi_{BC}} \int d\mathbf{r} w_{BC}^{(+)}(\mathbf{r})^2 - i \int d\mathbf{r} \hat{\rho}_{BC}^{(+)}(\mathbf{r}) w_{BC}^{(+)}(\mathbf{r})\right) \exp\left(-\frac{\rho_0}{\chi_{BC}} \int d\mathbf{r} w_{BC}^{(-)}(\mathbf{r})^2 + \int d\mathbf{r} \hat{\rho}_{BC}^{(-)}(\mathbf{r}) w_{BC}^{(-)}(\mathbf{r})\right) \\
&\times \exp\left(-\frac{\chi_{AP}}{\rho_0} \int d\mathbf{r} \hat{\rho}_{DA}\hat{\rho}_P\right) \exp\left(-\frac{\chi_{BP}}{\rho_0} \int d\mathbf{r} \hat{\rho}_{DB}\hat{\rho}_P\right) \exp\left(-\frac{\chi_{CP}}{\rho_0} \int d\mathbf{r} \hat{\rho}_{GC}\hat{\rho}_P\right).
\end{aligned}$$

and

$$\exp(-\beta U_2) = \frac{1}{\Omega_+} \int \mathcal{D}w_+ \exp\left(-\frac{\rho_0}{2\kappa} \int d\mathbf{r} w_+(\mathbf{r})^2 + i \int d\mathbf{r} (\rho_0 - \hat{\rho}_+(\mathbf{r})) w_+(\mathbf{r})\right)$$

The $\exp(-\beta U_1)$ equation can generalize to

$$\begin{aligned}
\exp(-\beta U_1) = & \prod_{IJ, I\neq J, I\neq P} \left(\frac{1}{\Omega_{IJ}^{(+)}\Omega_{IJ}^{(-)}} \int \mathcal{D}w_{IJ}^{(+)} \int \mathcal{D}w_{IJ}^{(-)}\right) \exp\left(-\frac{\rho_0}{\chi_{IJ}} \int d\mathbf{r} \left(w_{IJ}^{(+)}(\mathbf{r})^2 + w_{IJ}^{(-)}(\mathbf{r})^2\right)\right) \\
&\times \exp\left(\left(\int d\mathbf{r} \left[-i\hat{\rho}_{IJ}^{(s_{IJ})} w_{IJ}^{(s_{IJ})} + \hat{\rho}_{IJ}^{(-s_{IJ})} w_{IJ}^{(-s_{IJ})}\right]\right)\right) \\
&\times \prod_{I, I\neq P} \exp\left(-\frac{s_{IP}\chi_{IP}}{\rho_0} \int d\mathbf{r} \hat{\rho}_I \hat{\rho}_P\right)
\end{aligned}$$

where, for example, $w_{IJ}^{(s_{IJ})}$ is $w_{IJ}^{(+)}$ if $s_{IJ}=+1$ and $w_{IJ}^{(-)}$ if $s_{IJ}=-1$. With this notation, $w_{IJ}^{(-s_{IJ})}$ is $w_{IJ}^{(-)}$ if $s_{IJ}=+1$ and $w_{IJ}^{(+)}$ if $s_{IJ}=-1$. Before moving on, to make our lives easier, let's define

$$\Omega = \Omega_+\Omega_{AB}^{(+)}\Omega_{AB}^{(-)}\Omega_{AC}^{(+)}\Omega_{AC}^{(-)}\Omega_{BC}^{(+)}\Omega_{BC}^{(-)}$$

Now the canonical partition function looks like

$$\begin{aligned}
Z_C =& \frac{1}{n_D! n_G! \left(\lambda_T^d\right)^{n_D+n_G}} \frac{1}{\Omega} \int \dots \int \mathcal{D}\{w\} \int d\mathbf{r}^{n_D P + n_G N} \\
&\times \exp\left(-\frac{\rho_0}{2\kappa}\int d\mathbf{r} w_+(\mathbf{r})^2 + i\rho_0 \int d\mathbf{r} w_+ + \sum_{IJ, I\neq J, I\neq P} -\frac{\rho_0}{\chi_{IJ}} \int d\mathbf{r}\left(w_{IJ}^{(+)}(\mathbf{r})^2 + w_{IJ}^{(-)}(\mathbf{r})^2\right)\right) \\
&\times \exp\left(\sum_{IP, I\neq P} -\frac{s_{IP}\chi_{IP}}{\rho_0}\int d\mathbf{r}\hat{\rho}_I\hat{\rho}_P - i\int d\mathbf{r} w_+\hat{\rho}_+\right) \\
&\times \exp\left(-\sum_{i=1}^{n_D}\sum_{j=1}^{P-1}\frac{3\left|\mathbf{r}_{i,j+1}-\mathbf{r}_{i,j}\right|^2}{2b^2} - \sum_{i=1}^{n_G}\sum_{j=1}^{N-1}\frac{3\left|\mathbf{r}_{i,j+1}-\mathbf{r}_{i,j}\right|^2}{2b^2} - \sum_{i=1}^{n_G}\frac{3|\mathbf{r}_{i,1}-\mathbf{r}_{i,\perp}|^2}{2b^2}\right) \\
&\times \exp\left(\sum_{IJ, I\neq J, I\neq P}\int d\mathbf{r}\left(-i\hat{\rho}_{IJ}^{(s_{IJ})} w_{IJ}^{(s_{IJ})} + \hat{\rho}_{IJ}^{(-s_{IJ})} w_{IJ}^{(-s_{IJ})}\right)\right)
\end{aligned}$$

Let's now rearrange all the terms with any $\hat{\rho}$ in them to determine what each w_I is:

$$\begin{aligned}
\hat{\rho}\text{ Terms} =& \exp\left(\int d\mathbf{r}\left[-iw_+\hat{\rho}_+ - \sum_{IP, I\neq P}\frac{s_{IP}\chi_{IJ}}{\rho_0}\hat{\rho}_I\hat{\rho}_P + \sum_{IJ, I\neq J, I\neq P}\left(-i\hat{\rho}_{IJ}^{(s_{IJ})} w_{IJ}^{(s_{IJ})} + \hat{\rho}_{IJ}^{(-s_{IJ})} w_{IJ}^{(-s_{IJ})}\right)\right]\right) \\
=& \exp\left(\int d\mathbf{r}\left[-iw_+\hat{\rho}_{DA} + -\frac{s_{AP}\chi_{AP}}{\rho_0}\hat{\rho}_{DA}\hat{\rho}_P + \left(-i\hat{\rho}_{DA}w_{AB}^{(+)} + \hat{\rho}_{DA}w_{AB}^{(-)} - i\hat{\rho}_{DA}w_{AC}^{(-)} + \hat{\rho}_{DA}w_{AC}^{(+)}\right)\right]\right) \\
&\times \exp\left(\int d\mathbf{r}\left[-iw_+\hat{\rho}_{DB} - \frac{s_{BP}\chi_{BP}}{\rho_0}\hat{\rho}_{DB}\hat{\rho}_P + \left(-i\hat{\rho}_{DB}w_{AB}^{(+)} - \hat{\rho}_{DB}w_{AB}^{(-)} - i\hat{\rho}_{DB}w_{BC}^{(+)} + \hat{\rho}_{DB}w_{BC}^{(-)}\right)\right]\right) \\
&\times \exp\left(\int d\mathbf{r}\left[-iw_+\hat{\rho}_{GC} - \frac{s_{CP}\chi_{CP}}{\rho_0}\hat{\rho}_{GC}\hat{\rho}_P + \left(+i\hat{\rho}_{GC}w_{AC}^{(-)} + \hat{\rho}_{GC}w_{AC}^{(+)} - i\hat{\rho}_{GC}w_{BC}^{(+)} - \hat{\rho}_{GC}w_{BC}^{(-)}\right)\right]\right) \\
&\times \exp\left(-i\int d\mathbf{r}\hat{\rho}_P w_+\right) \\
=& \exp\left(\int d\mathbf{r}\hat{\rho}_{DA}\left[-iw_+ - \frac{s_{AP}\chi_{AP}}{\rho_0}\hat{\rho}_P + \left(-iw_{AB}^{(+)} + w_{AB}^{(-)} - iw_{AC}^{(-)} + w_{AC}^{(+)}\right)\right]\right) \\
&\times \exp\left(\int d\mathbf{r}\hat{\rho}_{DB}\left[-iw_+ - \frac{s_{BP}\chi_{BP}}{\rho_0}\hat{\rho}_P + \left(-iw_{AB}^{(+)} - w_{AB}^{(-)} - iw_{BC}^{(+)} + w_{BC}^{(-)}\right)\right]\right) \\
&\times \exp\left(\int d\mathbf{r}\hat{\rho}_{GC}\left[-iw_+ - \frac{s_{CP}\chi_{CP}}{\rho_0}\hat{\rho}_P + \left(+iw_{AC}^{(-)} + w_{AC}^{(+)} - iw_{BC}^{(+)} - w_{BC}^{(-)}\right)\right]\right) \\
&\times \exp\left(-i\int d\mathbf{r}\hat{\rho}_P w_+\right) \\
=& \exp\left(-\int d\mathbf{r}\hat{\rho}_{DA}w_A - \int d\mathbf{r}\hat{\rho}_{DB}w_B - \int d\mathbf{r}\hat{\rho}_{GC}w_C - \int d\mathbf{r}\hat{\rho}_P w_+\right)
\end{aligned}$$

where

$$
\begin{aligned}
w_A &= i\left(w_+ + w_{AB}^{(+)} + w_{AC}^{(-)}\right) - w_{AB}^{(-)} - w_{AC}^{(+)} + \frac{s_{AP}\chi_{AP}}{\rho_0}\hat{\rho}_P \\
w_B &= i\left(w_+ + w_{AB}^{(+)} + w_{BC}^{(+)}\right) + w_{AB}^{(-)} - w_{BC}^{(-)} + \frac{s_{BP}\chi_{BP}}{\rho_0}\hat{\rho}_P \\
w_C &= i\left(w_+ - w_{AC}^{(-)} + w_{BC}^{(+)}\right) - w_{AC}^{(+)} + w_{BC}^{(-)} + \frac{s_{CP}\chi_{CP}}{\rho_0}\hat{\rho}_P
\end{aligned}
$$

Looking at these field definitions, we can generalize with a rule-based process. Here's how we could construct any w_X where X is A, B, or C; J and K are the other two of A, B, and C but K $\neq$ X:

1. Start with

$$
w_X = i\left(w_+ + w_{XJ}^{(+)} + w_{XK}^{(+)}\right) - w_{XJ}^{(-)} - w_{XJ}^{(-)} + \frac{s_{XP}\chi_{XP}}{\rho_0}\hat{\rho}_P
$$

   Note that, for example if X is B and J is A, then w_{XJ} is actually w_{AB}, not w_{BA}. As an example, let's go through the process for w_C. We start with:

$$
w_C = i\left(w_+ + w_{AC}^{(+)} + w_{BC}^{(+)}\right) - w_{AC}^{(-)} - w_{BC}^{(-)} + \frac{s_{CP}\chi_{CP}}{\rho_0}\hat{\rho}_P
$$

2. For any XJ where χ_{XJ} is attractive (s_{XJ} = -1), change any (+) to a (−) and vice versa. This turns w_C into:

$$
w_C = i\left(w_+ + w_{AC}^{(-)} + w_{BC}^{(+)}\right) - w_{AC}^{(+)} - w_{BC}^{(-)} + \frac{s_{CP}\chi_{CP}}{\rho_0}\hat{\rho}_P
$$

3. For any $w_{XJ}^{(-)}$ where $X > J$, multiply it by -1 (flip the sign). This gives us our final w_C:

$$
w_C = i\left(w_+ - w_{AC}^{(-)} + w_{BC}^{(+)}\right) - w_{AC}^{(+)} + w_{BC}^{(-)} + \frac{s_{CP}\chi_{CP}}{\rho_0}\hat{\rho}_P
$$

Using the definitions of $\hat{\rho}_{IJ}^{(\pm)}$, we can rewrite all the $\exp(\int d\mathbf{r} w\hat{\rho})$ type terms as

$$
\prod_{j}^{n_D P_A} \exp\left(-\omega_A(\mathbf{r}_j)\right) \prod_{k}^{n_D P_B} \exp\left(-\omega_B(\mathbf{r}_k)\right) \prod_{m}^{n_G N} \exp\left(-\omega_C(\mathbf{r}_m)\right)
$$

where ω_A, ω_B and ω_C are defined as

$$
\omega_K(\mathbf{r}) = (h * w_K)(\mathbf{r})
$$

Additionally, defining the bond transition probability Φ as

$$
\Phi(\mathbf{r} - \mathbf{r}') = \left(\frac{3}{2\pi b^2}\right)^{d/2} \exp\left(\frac{-3|\mathbf{r} - \mathbf{r}'|^2}{2b^2}\right),
$$

we can rewrite the canonical partition function equation as

$$
\begin{aligned}
Z_C =& \frac{1}{n_D! n_G! \left(\lambda_T^d\right)^{n_D+n_G}} \frac{1}{\Omega} \int \dots \int \mathcal{D}\{w\} \\
& \times \exp\left(-\frac{\rho_0}{2\kappa} \int d\mathbf{r} w_+(\mathbf{r})^2 + i \int d\mathbf{r} w_+ \left(\rho_0 - \hat{\rho}_P\right) + \sum_{IJ, I\neq J, I\neq P} -\frac{\rho_0}{\chi_{IJ}} \int d\mathbf{r} \left(w_{IJ}^{(+)}(\mathbf{r})^2 + w_{IJ}^{(-)}(\mathbf{r})^2 \right) \right) \\
& \times \int d\mathbf{r}^{n_D P} \int d\mathbf{r}^{n_G N} \left(\prod_j^{n_D} \left(\prod_k^{P-1} \Phi(\mathbf{r}_{j,k+1} - \mathbf{r}_{j,k}) \right) \right) \left(\prod_{\ell=1}^{n_G} \left(\prod_{m=1}^{N-1} \Phi(\mathbf{r}_{\ell,m+1} - \mathbf{r}_{\ell,m}) \right) \Phi\left(\mathbf{r}_{j,1} - \mathbf{r}_{j,\perp}\right) \right) \\
& \times \left(\frac{3}{2\pi b^2} \right)^{\left(\frac{d}{2}\right)\left(n_D(P-1) + n_G \cdot (N)\right)} \\
& \times \prod_j^{n_D P_A} \exp\left(-\omega_A(\mathbf{r}_j)\right) \prod_k^{n_D P_B} \exp\left(-\omega_B(\mathbf{r}_k)\right) \prod_m^{n_G N} \exp\left(-\omega_C(\mathbf{r}_m)\right)
\end{aligned}
$$

Then, we define Q_D as

$$Q_D = \frac{1}{V} \int d\mathbf{r} q_D(N_D, \mathbf{r})$$

where

$$q_D(j+1, \mathbf{r}) = \exp(-\omega_{X_{j+1}}(\mathbf{r})) \int d\mathbf{r}' \Phi(\mathbf{r} - \mathbf{r}') q(j, \mathbf{r}'`')$$

where X_{j+1} is either A or B depending on type of segment $j+1$ and $q_D(1, \mathbf{r}) = \exp(-\omega_A(\mathbf{r}))$.

The definition of the partition function for a grafted chain is.

$$q_G(j+1, \mathbf{r}) = \exp(-\omega_{g_{j+1}}(\mathbf{r})) \int d\mathbf{r}' \Phi(\mathbf{r} - \mathbf{r}') q_G(j, \mathbf{r})$$

for $j = 0, \cdots, N-2$. For $j = N-1$

$$q_G(N, \mathbf{r}) = \exp(-\omega_{g_{N_x}}(\mathbf{r})) \Phi(\mathbf{r}_N - \mathbf{r}_\perp)$$

With these definitions, we get

$$
\begin{aligned}
Z_C =& \frac{V^{n_D+n_G}}{n_D! n_G! \left(\lambda_T^d\right)^{n_D+n_G}} \frac{1}{\Omega} \left(\frac{2\pi b^2}{3} \right)^{\left(\frac{d}{2}\right)\left(n_D(P-1) + n_G \cdot (N)\right)} \int \dots \int \mathcal{D}\{w\} \\
& \times \exp\left(-\frac{\rho_0}{2\kappa} \int d\mathbf{r} w_+(\mathbf{r})^2 + i \int d\mathbf{r} w_+ \left(\rho_0 - \hat{\rho}_P\right) - i \int d\mathbf{r} \hat{\rho}_P w_+ \right) \\
& \times -\sum_{IJ, I\neq J, I\neq P} \frac{\rho_0}{\chi_{IJ}} \int d\mathbf{r} \left(w_{IJ}^{(+)}(\mathbf{r})^2 + w_{IJ}^{(-)}(\mathbf{r})^2 \right) \\
& \times Q_D^{n_D} \\
& \times -n_G \int d\mathbf{r} \sigma_G(\mathbf{r}) \ln q_G[\mathbf{r}; \omega_G]
\end{aligned}
$$

We can rewrite this as

$$
\begin{aligned}
Z_C =& \frac{V^{n_D+n_G}}{n_D! n_P! \left(\lambda_T^d\right)^{n_D+n_G}} \frac{1}{\Omega} \left(\frac{2\pi b^2}{3} \right)^{\left(\frac{d}{2}\right)\left(n_D(P-1) + n_G \cdot (N)\right)} \\
& \int \dots \int \mathcal{D}\{w\} \exp\left(-\mathcal{H}[\{w\}]\right)
\end{aligned}
$$

where

$$\mathcal{H}[w_+, w_{AB}^{(\pm)}, w_{BC}^{(\pm)}, w_{AC}^{(\pm)}] = \frac{\rho_0}{2\kappa}\int d\mathbf{r} w_+(\mathbf{r})^2 - i\int d\mathbf{r} w_+ (\rho_0 - \hat{\rho}_P) + \sum_{IJ, I\neq J, I\neq P} \frac{\rho_0}{\chi_{IJ}} \int d\mathbf{r} \left(w_{IJ}^{(+)}(\mathbf{r})^2 + w_{IJ}^{(-)}(\mathbf{r})^2 \right)$$
$$- n_D \log Q_D - n_G \int d\mathbf{r} \sigma_G(\mathbf{r}) \ln(q_G[\mathbf{r}; \omega_G])$$

Below is the derivation of the system for a variable version of graft chains and such.

$$\begin{aligned}
\frac{\delta H}{\delta w_{AB}^{(+)}} &= \frac{2\rho_0}{\chi_{AB}} w_{AB}^{(+)} + (\rho_{DA,c} * h)(\text{flag?} -1 : i) + (\rho_{DB,c} * h)(\text{flag?} -1 : i) \\
\frac{\delta H}{\delta w_{AB}^{(-)}} &= \frac{2\rho_0}{\chi_{AB}} w_{AB}^{(-)} + (\rho_{DA,c} * h)(\text{flag?} i : -1) + (\rho_{DB,c} * h)(\text{flag?} -i : +1) \\
\frac{\delta H}{\delta w_{AC}^{(+)}} &= \frac{2\rho_0}{\chi_{AC}} w_{AC}^{(+)} + (\rho_{DA,c} * h)(\text{flag?} -1 : i) + (\rho_{DC,c} * h)(\text{flag?} -1 : i) \\
\frac{\delta H}{\delta w_{AC}^{(-)}} &= \frac{2\rho_0}{\chi_{AC}} w_{AC}^{(-)} + (\rho_{DA,c} * h)(\text{flag?} i : -1) + (\rho_{DC,c} * h)(\text{flag?} -i : +1) \\
\frac{\delta H}{\delta w_{BC}^{(+)}} &= \frac{2\rho_0}{\chi_{BC}} w_{BC}^{(+)} + (\rho_{DB,c} * h)(\text{flag?} -1 : i) + (\rho_{DC,c} * h)(\text{flag?} -1 : i) \\
\frac{\delta H}{\delta w_{BC}^{(-)}} &= \frac{2\rho_0}{\chi_{BC}} w_{BC}^{(-)} + (\rho_{DB,c} * h)(\text{flag?} i : -1) + (\rho_{DC,c} * h)(\text{flag?} -i : +1)
\end{aligned}$$

2 Canonical 1S Update Derivation

2.1 w_+ Field

First let's do the w_+ update derivation for the Canonical Ensemble.

$$w_+^{t+1} = w_+^t - \lambda \left[\frac{\delta \mathcal{H}}{\delta w_+^t} + \left(\frac{\delta \mathcal{H}}{\delta w_+^{t+1}} \right)_{lin} - \left(\frac{\delta \mathcal{H}}{\delta w_+^t} \right)_{lin} \right]$$

Taking the Fourier Transform,

$$\hat{w}_+^{t+1} = \hat{w}_+^t - \lambda \left[\frac{\delta \hat{\mathcal{H}}}{\delta w_+^t} + \left(\frac{\delta \hat{\mathcal{H}}}{\delta w_+^{t+1}} \right)_{lin} - \left(\frac{\delta \hat{\mathcal{H}}}{\delta w_+^t} \right)_{lin} \right]$$

Then, after plugging in the correct expressions, we can solve for $\hat{w}_+^{t+1}$ and take the inverse Fourier Transform to get w_+^{t+1}.

$$\begin{aligned}
\frac{\delta \mathcal{H}}{\delta w_+^t} &= \frac{\rho_0}{\kappa} w_+^t - i\rho_0 + i[(\rho_{DA,c} * h)(\mathbf{r}) + (\rho_{DB,c} * h)(\mathbf{r}) + (\rho_{C,c} * h)(\mathbf{r})] \\
\frac{\delta \hat{\mathcal{H}}}{\delta w_+^t} &= \frac{\rho_0}{\kappa} \hat{w}_+^t - i\rho_0 \delta(\mathbf{k}) + i[\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}] \\
\left(\frac{\delta \hat{\mathcal{H}}}{\delta w_+^t} \right)_{lin} &= \frac{\rho_0}{\kappa} \hat{w}_+^t - i\hat{h}^2 \phi_D \rho_0 N_D (\hat{g}_{AA} + 2\hat{g}_{AB} + \hat{g}_{BB}) i\hat{w}_+^t - i\phi_g N_G \hat{g}_C \rho_0 \hat{h}^2 i\hat{w}_+^t \\
&= \frac{\rho_0}{\kappa} \hat{w}_+^t + \hat{h}^2 \phi_D \rho_0 N_D (\hat{g}_{AA} + 2\hat{g}_{AB} + \hat{g}_{BB}) \hat{w}_+^t + \phi_g N_G \hat{g}_C \rho_0 \hat{h}^2 \hat{w}_+^t
\end{aligned}$$

Assembling the pieces, we get

$$\hat{w}_+^{t+1} = \hat{w}_+^t - \lambda \left[\frac{\rho_0}{\kappa} \hat{w}_+^t - i\rho_0 \delta(\mathbf{k}) + i(\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{P,c}\hat{\Gamma}) + A(\hat{w}_+^{t+1} - \hat{w}_+^t) \right]$$

where

$$A = \frac{1}{w_+^t}\left(\frac{\delta\hat{\mathcal{H}}}{\delta w_+^t}\right)_{lin} = \frac{1}{w_+^{t+1}}\left(\frac{\delta\hat{\mathcal{H}}}{\delta w_+^{t+1}}\right)_{lin}$$
$$= \frac{\rho_0}{\kappa} + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA} + 2\hat{g}_{AB} + \hat{g}_{BB}) + \phi_g N_G\hat{g}_C\rho_0\hat{h}^2$$

If we also let B and F equal

$$B = A - \frac{\rho_0}{\kappa}$$
$$= \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA} + 2\hat{g}_{AB} + \hat{g}_{BB}) + \phi_g N_G\hat{g}_C\rho_0\hat{h}^2$$
$$F = -i\rho_0\delta(\mathbf{k}) + i(\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{C,c}\hat{h})$$

Then

$$\hat{w}_+^{t+1}(1 + \lambda A) = \hat{w}_+^t - \lambda\left(F - B\hat{w}_+^t\right)$$
$$\hat{w}_+^{t+1} = \frac{\hat{w}_+^t - \lambda\left(F - B\hat{w}_+^t\right)}{1 + \lambda A}$$

2.2 $w_{AB}^{(+)}$

2.2.1 Positive χ

For the $w_{AB}^{(+)}$ field, the relevant expressions are:

$$\left.\frac{\delta\mathcal{H}}{\delta w_{AB}^{(+)}}\right|_t = \frac{2\rho_0}{\chi_{AB}}\left. w_{AB}^{(+)}\right|_t + i[(\rho_{DA,c} * h)(\mathbf{r}) + (\rho_{DB,c} * h)(\mathbf{r})]$$
$$\left.\frac{\delta\hat{\mathcal{H}}}{\delta w_{AB}^{(+)}}\right|_t = \frac{2\rho_0}{\chi_{AB}}\left.\hat{w}_{AB}^{(+)}\right|_t + i[\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h}]$$
$$\left.\frac{\delta\hat{\mathcal{H}}}{\delta w_{AB}^{(+)}}\right|_t^{lin} = \frac{2\rho_0}{\chi_{AB}}\left.\hat{w}_{AB}^{(+)}\right|_t - i\hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA} + 2\hat{g}_{AB} + \hat{g}_{BB})i\left.\hat{w}_{AB}^{(+)}\right|_t$$
$$= \frac{2\rho_0}{\chi_{AB}}\left.\hat{w}_{AB}^{(+)}\right|_t + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA} + 2\hat{g}_{AB} + \hat{g}_{BB})\left.\hat{w}_{AB}^{(+)}\right|_t$$

This gives us

$$\left.\hat{w}_{AB}^{(+)}\right|_{t+1} = \left.\hat{w}_{AB}^{(+)}\right|_t - \lambda\left[\frac{2\rho_0}{\chi_{AB}}\left.\hat{w}_{AB}^{(+)}\right|_t + i(\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h}) + A(\left.\hat{w}_{AB}^{(+)}\right|_{t+1} - \left.\hat{w}_{AB}^{(+)}\right|_t)\right]$$

where

$$A = \frac{2\rho_0}{\chi_{AB}} + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA} + 2\hat{g}_{AB} + \hat{g}_{BB})$$

If we let B and F equal

$$B = A - \frac{2\rho_0}{\chi_{AB}}$$
$$= \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA} + 2\hat{g}_{AB} + \hat{g}_{BB})$$
$$F = +i(\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h})$$

Then

$$
\begin{aligned}
\hat{w}_{AB}^{(+)}\Big|_{t+1}(1+\lambda A) &= \hat{w}_{AB}^{(+)}\Big|_{t} - \lambda\left(F - B\,\hat{w}_{AB}^{(+)}\Big|_{t}\right)\\
\hat{w}_{AB}^{(+)}\Big|_{t+1} &= \frac{\hat{w}_{AB}^{(+)}\Big|_{t} - \lambda\left(F - B\,\hat{w}_{AB}^{(+)}\Big|_{t}\right)}{1+\lambda A}
\end{aligned}
$$

2.2.2 Negative χ

The changes in the signs come from the part of the code where there were flags of negaivity of chi. For the $w_{AB}^{(+)}$ field, the relevant expressions are:

$$
\begin{aligned}
\left.\frac{\delta\mathcal{H}}{\delta w_{AB}^{(+)}}\right|_{t} &= \frac{2\rho_0}{\chi_{AB}}\,w_{AB}^{(+)}\Big|_{t} - [(\rho_{DA,c} * h)(\mathbf{r}) + (\rho_{DB,c} * h)(\mathbf{r})]\\
\left.\frac{\delta\hat{\mathcal{H}}}{\delta w_{AB}^{(+)}}\right|_{t} &= \frac{2\rho_0}{\chi_{AB}}\,\hat{w}_{AB}^{(+)}\Big|_{t} - [\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h}]\\
\left.\frac{\delta\hat{\mathcal{H}}}{\delta w_{AB}^{(+)}}\right|_{t}^{lin} &= \frac{2\rho_0}{\chi_{AB}}\,\hat{w}_{AB}^{(+)}\Big|_{t}
\end{aligned}
$$

Note that we don't do the weak inhomogeneity expansion here because the $w_{AB}^{(+)}$ field tends to be much less stiff than the w_+ fields and so doesn't need the extra approximation. Now we get

$$
\begin{aligned}
\hat{w}_{AB}^{(+)}\Big|_{t+1} &= \hat{w}_{AB}^{(+)}\Big|_{t} - \lambda\left[\frac{2\rho_0}{\chi_{AB}}\,\hat{w}_{AB}^{(+)}\Big|_{t} - \hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h} + \frac{2\rho_0}{\chi_{AB}}(\,\hat{w}_{AB}^{(+)}\Big|_{t+1} - \hat{w}_{AB}^{(+)}\Big|_{t})\right]\\
\hat{w}_{AB}^{(+)}\Big|_{t+1}(1+\lambda\frac{2\rho_0}{\chi_{AB}}) &= \hat{w}_{AB}^{(+)}\Big|_{t} - \lambda\left(-\hat{\rho}_{DA,c}\hat{h} - \hat{\rho}_{DB,c}\hat{h}\right)\\
\hat{w}_{AB}^{(+)}\Big|_{t+1} &= \frac{\hat{w}_{AB}^{(+)}\Big|_{t} - \lambda\left(-\hat{\rho}_{DA,c}\hat{h} - \hat{\rho}_{DB,c}\hat{h}\right)}{\left(1+\lambda\frac{2\rho_0}{\chi_{AB}}\right)}
\end{aligned}
$$

2.3 $w_{AB}^{(-)}$ Field

2.3.1 Positive χ

For the $w_{AB}^{(-)}$ field, the relevant expressions are:

$$
\begin{aligned}
\left.\frac{\delta\mathcal{H}}{\delta w_{AB}^{(-)}}\right|_{t} &= \frac{2\rho_0}{\chi_{AB}}\,w_{AB}^{(-)}\Big|_{t} - (\rho_{DA,c} * h)(\mathbf{r}) + (\rho_{DB,c} * h)(\mathbf{r})\\
\left.\frac{\delta\hat{\mathcal{H}}}{\delta w_{AB}^{(-)}}\right|_{t} &= \frac{2\rho_0}{\chi_{AB}}\,\hat{w}_{AB}^{(-)}\Big|_{t} - \hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h}\\
\left.\frac{\delta\hat{\mathcal{H}}}{\delta w_{AB}^{(-)}}\right|_{t}^{lin} &= \frac{2\rho_0}{\chi_{AB}}\,\hat{w}_{AB}^{(-)}\Big|_{t}
\end{aligned}
$$

Note that we don't do the weak inhomogeneity expansion here because the $w_{AB}^{(-)}$ field tends to be much less stiff than the w_+ fields and so doesn't need the extra approximation. Now we get

$$\begin{aligned}
\hat{w}_{AB}^{(-)}\Big|_{t+1} &= \hat{w}_{AB}^{(-)}\Big|_{t} - \lambda\left[\frac{2\rho_0}{\chi_{AB}}\ \hat{w}_{AB}^{(-)}\Big|_{t} - \hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h} + \frac{2\rho_0}{\chi_{AB}}(\hat{w}_{AB}^{(-)}\Big|_{t+1} - \hat{w}_{AB}^{(-)}\Big|_{t})\right] \\
\hat{w}_{AB}^{(-)}\Big|_{t+1}(1+\lambda\frac{2\rho_0}{\chi_{AB}}) &= \hat{w}_{AB}^{(-)}\Big|_{t} - \lambda\left(-\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h}\right) \\
\hat{w}_{AB}^{(-)}\Big|_{t+1} &= \frac{\hat{w}_{AB}^{(-)}\Big|_{t} - \lambda\overbrace{\left(-\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{DB,c}\hat{h}\right)}^{F}}{\left(1+\lambda\frac{2\rho_0}{\chi_{AB}}\right)}
\end{aligned}$$

2.3.2 Negative χ

For the $w_{AB}^{(-)}$ field, the relevant expressions are:

$$\begin{aligned}
\frac{\delta\mathcal{H}}{\delta w_{AB}^{(-)}}\Bigg|_{t} &= \frac{2\rho_0}{\chi_{AB}}\ w_{AB}^{(-)}\Big|_{t} + i(\rho_{DA,c} * h)(\mathbf{r}) - i(\rho_{DB,c} * h)(\mathbf{r}) \\
\frac{\delta\hat{\mathcal{H}}}{\delta w_{AB}^{(-)}}\Bigg|_{t} &= \frac{2\rho_0}{\chi_{AB}}\ \hat{w}_{AB}^{(-)}\Big|_{t} + i\hat{\rho}_{DA,c}\hat{h} - i\hat{\rho}_{DB,c}\hat{h} \\
\frac{\delta\hat{\mathcal{H}}}{\delta w_{AB}^{(-)}}\Bigg|_{t}^{lin} &= \frac{2\rho_0}{\chi_{AB}}\ \hat{w}_{AB}^{(+)}\Big|_{t} - i\hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA} - \hat{g}_{BB})i\ \hat{w}_{AB}^{(-)}\Big|_{t} \\
&= \frac{2\rho_0}{\chi_{AB}}\ \hat{w}_{AB}^{(+)}\Big|_{t} + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA} - \hat{g}_{BB})\ \hat{w}_{AB}^{(-)}\Big|_{t}
\end{aligned}$$

This gives us

$$\hat{w}_{AB}^{(-)}\Big|_{t+1} = \hat{w}_{AB}^{(-)}\Big|_{t} - \lambda\left[\frac{2\rho_0}{\chi_{AB}}\ \hat{w}_{AB}^{(-)}\Big|_{t} + i(\hat{\rho}_{DA,c}\hat{h} - \hat{\rho}_{DB,c}\hat{h}) + A(\hat{w}_{AB}^{(-)}\Big|_{t+1} - \hat{w}_{AB}^{(-)}\Big|_{t})\right]$$

where

$$A = \frac{2\rho_0}{\chi_{AB}} + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA} - \hat{g}_{BB})$$

If we let B and F equal

$$\begin{aligned}
B &= A - \frac{2\rho_0}{\chi_{AB}} \\
&= \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA} - \hat{g}_{BB}) \\
F &= +i(\hat{\rho}_{DA,c}\hat{h} - \hat{\rho}_{DB,c}\hat{h})
\end{aligned}$$

Then

$$\begin{aligned}
\hat{w}_{AB}^{(-)}\Big|_{t+1}(1+\lambda A) &= \hat{w}_{AB}^{(-)}\Big|_{t} - \lambda\left(F - B\ \hat{w}_{AB}^{(-)}\Big|_{t}\right) \\
\hat{w}_{AB}^{(-)}\Big|_{t+1} &= \frac{\hat{w}_{AB}^{(-)}\Big|_{t} - \lambda\left(F - B\ \hat{w}_{AB}^{(-)}\Big|_{t}\right)}{1+\lambda A}
\end{aligned}$$

2.4 $w_{AC}^{(+)}$

2.4.1 Positive χ

For the $w_{AC}^{(+)}$ field, the relevant expressions are:

$$\left.\frac{\delta \mathcal{H}}{\delta w_{AC}^{(+)}}\right|_t = \frac{2\rho_0}{\chi_{AC}} \left. w_{AC}^{(+)}\right|_t + i[(\rho_{DA,c} * h)(\mathbf{r}) + (\rho_{C,c} * h)(\mathbf{r})]$$

$$\left.\frac{\delta \hat{\mathcal{H}}}{\delta w_{AC}^{(+)}}\right|_t = \frac{2\rho_0}{\chi_{AC}} \left. \hat{w}_{AC}^{(+)}\right|_t + i[\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}]$$

$$\begin{aligned}\left.\frac{\delta \hat{\mathcal{H}}}{\delta w_{AC}^{(+)}}\right|_t^{lin} &= \frac{2\rho_0}{\chi_{AC}} \left. \hat{w}_{AC}^{(+)}\right|_t - i\hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA})i \left. \hat{w}_{AC}^{(+)}\right|_t - i\hat{h}^2\rho_0\ \phi_G N_G(\hat{g}_C)i\left.\hat{w}_{AC}^{(+)}\right|_t \\ &= \frac{2\rho_0}{\chi_{AC}} \left. \hat{w}_{AC}^{(+)}\right|_t + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA}) \left. \hat{w}_{AC}^{(+)}\right|_t + \hat{h}^2\rho_0\ \phi_G N_G(\hat{g}_C)\left.\hat{w}_{AC}^{(+)}\right|_t\end{aligned}$$

This gives us

$$\left.\hat{w}_{AC}^{(+)}\right|_{t+1} = \left.\hat{w}_{AC}^{(+)}\right|_t - \lambda \left[\frac{2\rho_0}{\chi_{AC}} \left.\hat{w}_{AC}^{(+)}\right|_t + i(\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}) + A(\left.\hat{w}_{AC}^{(+)}\right|_{t+1} - \left.\hat{w}_{AC}^{(+)}\right|_t)\right]$$

where

$$A = \frac{2\rho_0}{\chi_{AC}} + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA}) + \phi_G\hat{h}^2\rho_0 N_G\hat{g}_C$$

If we let B and F equal

$$\begin{aligned}B &= A - \frac{2\rho_0}{\chi_{AC}} \\ &= \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA}) + \phi_G\hat{h}^2\rho_0 N_G\hat{g}_C \\ F &= +i(\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{C,c}\hat{h})\end{aligned}$$

Then

$$\begin{aligned}\left.\hat{w}_{AC}^{(+)}\right|_{t+1}(1+\lambda A) &= \left.\hat{w}_{AC}^{(+)}\right|_t - \lambda\left(F - B\left.\hat{w}_{AC}^{(+)}\right|_t\right) \\ \left.\hat{w}_{AC}^{(+)}\right|_{t+1} &= \frac{\left.\hat{w}_{AC}^{(+)}\right|_t - \lambda\left(F - B\left.\hat{w}_{AC}^{(+)}\right|_t\right)}{1+\lambda A}\end{aligned}$$

2.4.2 Negative χ

The changes in the signs come from the part of the code where there were flags of negaivity of chi. For the $w_{AC}^{(+)}$ field, the relevant expressions are:

$$\left.\frac{\delta \mathcal{H}}{\delta w_{AC}^{(+)}}\right|_t = \frac{2\rho_0}{\chi_{AC}} \left. w_{AC}^{(+)}\right|_t - [(\rho_{DA,c} * h)(\mathbf{r}) + (\rho_{C,c} * h)(\mathbf{r})]$$

$$\left.\frac{\delta \hat{\mathcal{H}}}{\delta w_{AC}^{(+)}}\right|_t = \frac{2\rho_0}{\chi_{AC}} \left. \hat{w}_{AC}^{(+)}\right|_t - [\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}]$$

$$\left.\frac{\delta \hat{\mathcal{H}}}{\delta w_{AC}^{(+)}}\right|_t^{lin} = \frac{2\rho_0}{\chi_{AC}} \left. \hat{w}_{AC}^{(+)}\right|_t$$

Note that we don't do the weak inhomogeneity expansion here because the $w_{AC}^{(+)}$ field tends to be much less stiff than the w_+ fields and so doesn't need the extra approximation. Now we get

$$\begin{aligned}
\hat{w}_{AC}^{(+)}\Big|_{t+1} &= \hat{w}_{AC}^{(+)}\Big|_{t} - \lambda\left[\frac{2\rho_0}{\chi_{AC}}\ \hat{w}_{AC}^{(+)}\Big|_{t} - (\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}) + \frac{2\rho_0}{\chi_{AC}}(\hat{w}_{AC}^{(+)}\Big|_{t+1} - \hat{w}_{AC}^{(+)}\Big|_{t})\right] \\
\hat{w}_{AC}^{(+)}\Big|_{t+1}(1+\lambda\frac{2\rho_0}{\chi_{AC}}) &= \hat{w}_{AC}^{(+)}\Big|_{t} - \lambda\left(-\hat{\rho}_{DA,c}\hat{h} - \hat{\rho}_{C,c}\hat{h}\right) \\
\hat{w}_{AC}^{(+)}\Big|_{t+1} &= \frac{\hat{w}_{AC}^{(+)}\Big|_{t} - \lambda\left(-\hat{\rho}_{DA,c}\hat{h} - \hat{\rho}_{C,c}\hat{h}\right)}{\left(1+\lambda\frac{2\rho_0}{\chi_{AC}}\right)}
\end{aligned}$$

2.5 $w_{AC}^{(-)}$ Field

2.5.1 Positive χ

For the $w_{AC}^{(-)}$ field, the relevant expressions are:

$$\begin{aligned}
\frac{\delta\mathcal{H}}{\delta w_{AC}^{(-)}}\Bigg|_{t} &= \frac{2\rho_0}{\chi_{AC}}\ w_{AC}^{(-)}\Big|_{t} - (\rho_{DA,c} * h)(\mathbf{r}) + (\rho_{C,c} * h)(\mathbf{r}) \\
\frac{\delta\hat{\mathcal{H}}}{\delta w_{AC}^{(-)}}\Bigg|_{t} &= \frac{2\rho_0}{\chi_{AC}}\ \hat{w}_{AC}^{(-)}\Big|_{t} - \hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{C,c}\hat{h} \\
\frac{\delta\hat{\mathcal{H}}}{\delta w_{AC}^{(-)}}\Bigg|_{t}^{lin} &= \frac{2\rho_0}{\chi_{AC}}\ \hat{w}_{AC}^{(-)}\Big|_{t}
\end{aligned}$$

Note that we don't do the weak inhomogeneity expansion here because the $w_{AC}^{(-)}$ field tends to be much less stiff than the w_+ fields and so doesn't need the extra approximation. Now we get

$$\begin{aligned}
\hat{w}_{AC}^{(-)}\Big|_{t+1} &= \hat{w}_{AC}^{(-)}\Big|_{t} - \lambda\left[\frac{2\rho_0}{\chi_{AC}}\ \hat{w}_{AC}^{(-)}\Big|_{t} - \hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{C,c}\hat{h} + \frac{2\rho_0}{\chi_{AC}}(\hat{w}_{AC}^{(-)}\Big|_{t+1} - \hat{w}_{AC}^{(-)}\Big|_{t})\right] \\
\hat{w}_{AC}^{(-)}\Big|_{t+1}(1+\lambda\frac{2\rho_0}{\chi_{AC}}) &= \hat{w}_{AC}^{(-)}\Big|_{t} - \lambda\left(-\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}\right) \\
\hat{w}_{AC}^{(-)}\Big|_{t+1} &= \frac{\hat{w}_{AC}^{(-)}\Big|_{t} - \lambda\left(-\hat{\rho}_{DA,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}\right)}{\left(1+\lambda\frac{2\rho_0}{\chi_{AC}}\right)}
\end{aligned}$$

2.5.2 Negative χ

For the $w_{AC}^{(-)}$ field, the relevant expressions are:

$$\begin{aligned}
\frac{\delta\mathcal{H}}{\delta w_{AC}^{(-)}}\Bigg|_{t} &= \frac{2\rho_0}{\chi_{AC}}\ w_{AC}^{(-)}\Big|_{t} + i(\rho_{DA,c} * h)(\mathbf{r}) - i(\rho_{C,c} * h)(\mathbf{r}) \\
\frac{\delta\hat{\mathcal{H}}}{\delta w_{AC}^{(-)}}\Bigg|_{t} &= \frac{2\rho_0}{\chi_{AC}}\ \hat{w}_{AC}^{(-)}\Big|_{t} + i\hat{\rho}_{DA,c}\hat{h} - i\hat{\rho}_{C,c}\hat{h} \\
\frac{\delta\hat{\mathcal{H}}}{\delta w_{AC}^{(-)}}\Bigg|_{t}^{lin} &= \frac{2\rho_0}{\chi_{AC}}\ \hat{w}_{AC}^{(-)}\Big|_{t} - i\hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA})i\ \hat{w}_{AC}^{(-)}\Big|_{t} + i\hat{h}^2\rho_0\ \phi_G N_G(\hat{g}_C)i\hat{w}_{AC}^{(-)}\Big|_{t} \\
&= \frac{2\rho_0}{\chi_{AC}}\ \hat{w}_{AC}^{(-)}\Big|_{t} + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA})\ \hat{w}_{AC}^{(-)}\Big|_{t} - \hat{h}^2\rho_0\ \phi_G N_G(\hat{g}_C)\hat{w}_{AC}^{(-)}\Big|_{t}
\end{aligned}$$

This gives us

$$\hat{w}_{AC}^{(-)}\Big|_{t+1} = \hat{w}_{AC}^{(-)}\Big|_{t} - \lambda\left[\frac{2\rho_0}{\chi_{AC}}\ \hat{w}_{AC}^{(-)}\Big|_{t} + i(\hat{\rho}_{DA,c}\hat{h} - \hat{\rho}_{C,c}\hat{h}) + A(\ \hat{w}_{AC}^{(-)}\Big|_{t+1} - \ \hat{w}_{AC}^{(-)}\Big|_{t})\right]$$

where

$$A = \frac{2\rho_0}{\chi_{AC}} + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA}) - \hat{h}^2\rho_0\phi_G N_G(\hat{g}_C)$$

If we let B and F equal

$$\begin{aligned} B &= A - \frac{2\rho_0}{\chi_{AC}} \\ &= \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{AA}) - \hat{h}^2\rho_0\phi_G N_G(\hat{g}_C) \\ F &= +i(\hat{\rho}_{DA,c}\hat{h} - \hat{\rho}_{C,c}\hat{h}) \end{aligned}$$

Then

$$\begin{aligned} \hat{w}_{AC}^{(-)}\Big|_{t+1}(1+\lambda A) &= \ \hat{w}_{AC}^{(-)}\Big|_{t} - \lambda\left(F - B\ \hat{w}_{AC}^{(-)}\Big|_{t}\right) \\ \hat{w}_{AC}^{(-)}\Big|_{t+1} &= \frac{\hat{w}_{AC}^{(-)}\Big|_{t} - \lambda\left(F - B\ \hat{w}_{AC}^{(-)}\Big|_{t}\right)}{1+\lambda A} \end{aligned}$$

2.6 $w_{BC}^{(+)}$

2.6.1 Positive χ

For the $w_{BC}^{(+)}$ field, the relevant expressions are:

$$\begin{aligned} \frac{\delta\mathcal{H}}{\delta w_{BC}^{(+)}}\Bigg|_t &= \frac{2\rho_0}{\chi_{BC}}\ w_{BC}^{(+)}\Big|_t + i[(\rho_{DB,c} * h)(\mathbf{r}) + (\rho_{C,c} * h)(\mathbf{r})] \\ \frac{\delta\hat{\mathcal{H}}}{\delta w_{BC}^{(+)}}\Bigg|_t &= \frac{2\rho_0}{\chi_{BC}}\ \hat{w}_{BC}^{(+)}\Big|_t + i[\hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}] \\ \frac{\delta\hat{\mathcal{H}}}{\delta w_{BC}^{(+)}}\Bigg|_t^{lin} &= \frac{2\rho_0}{\chi_{BC}}\ \hat{w}_{BC}^{(+)}\Big|_t - i\hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{BB})i\ \hat{w}_{BC}^{(+)}\Big|_t - i\hat{h}^2\rho_0\ \phi_G N_G(\hat{g}_C)i\hat{w}_{BC}^{(+)}\Big|_t \\ &= \frac{2\rho_0}{\chi_{BC}}\ \hat{w}_{BC}^{(+)}\Big|_t + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{BB})\ \hat{w}_{BC}^{(+)}\Big|_t + \hat{h}^2\rho_0\ \phi_G N_G(\hat{g}_C)\hat{w}_{BC}^{(+)}\Big|_t \end{aligned}$$

This gives us

$$\hat{w}_{BC}^{(+)}\Big|_{t+1} = \hat{w}_{BC}^{(+)}\Big|_{t} - \lambda\left[\frac{2\rho_0}{\chi_{BC}}\ \hat{w}_{BC}^{(+)}\Big|_{t} + i(\hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}) + A(\ \hat{w}_{BC}^{(+)}\Big|_{t+1} - \ \hat{w}_{BC}^{(+)}\Big|_{t})\right]$$

where

$$A = \frac{2\rho_0}{\chi_{BC}} + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{BB}) + \phi_G\hat{h}^2\rho_0 N_G\hat{g}_C$$

If we let B and F equal

$$\begin{aligned} B &= A - \frac{2\rho_0}{\chi_{BC}} \\ &= \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{BB}) + \phi_G\hat{h}^2\rho_0 N_G\hat{g}_C \\ F &= +i(\hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}) \end{aligned}$$

Then

$$\hat{w}_{BC}^{(+)}\Big|_{t+1}(1+\lambda A) = \hat{w}_{BC}^{(+)}\Big|_t - \lambda\left(F - B\,\hat{w}_{BC}^{(+)}\Big|_t\right)$$
$$\hat{w}_{BC}^{(+)}\Big|_{t+1} = \frac{\hat{w}_{BC}^{(+)}\Big|_t - \lambda\left(F - B\,\hat{w}_{BC}^{(+)}\Big|_t\right)}{1+\lambda A}$$

2.6.2 Negative χ

The changes in the signs come from the part of the code where there were flags of negaivity of chi.
For the $w_{BC}^{(+)}$ field, the relevant expressions are:

$$\left.\frac{\delta\mathcal{H}}{\delta w_{BC}^{(+)}}\right|_t = \frac{2\rho_0}{\chi_{BC}}\,w_{BC}^{(+)}\Big|_t - [(\rho_{DB,c} * h)(\mathbf{r}) + (\rho_{C,c} * h)(\mathbf{r})]$$
$$\left.\frac{\delta\hat{\mathcal{H}}}{\delta w_{BC}^{(+)}}\right|_t = \frac{2\rho_0}{\chi_{BC}}\,\hat{w}_{BC}^{(+)}\Big|_t - [\hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}]$$
$$\left.\frac{\delta\hat{\mathcal{H}}}{\delta w_{BC}^{(+)}}\right|_t^{lin} = \frac{2\rho_0}{\chi_{BC}}\,\hat{w}_{BC}^{(+)}\Big|_t$$

Note that we don't do the weak inhomogeneity expansion here because the $w_{BC}^{(+)}$ field tends to be much less stiff than the w_+ fields and so doesn't need the extra approximation. Now we get

$$\hat{w}_{BC}^{(+)}\Big|_{t+1} = \hat{w}_{BC}^{(+)}\Big|_t - \lambda\left[\frac{2\rho_0}{\chi_{BC}}\,\hat{w}_{BC}^{(+)}\Big|_t - (\hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}) + \frac{2\rho_0}{\chi_{BC}}(\,\hat{w}_{BC}^{(+)}\Big|_{t+1} - \hat{w}_{BC}^{(+)}\Big|_t)\right]$$
$$\hat{w}_{BC}^{(+)}\Big|_{t+1}(1+\lambda\frac{2\rho_0}{\chi_{BC}}) = \hat{w}_{BC}^{(+)}\Big|_t - \lambda\left(-\hat{\rho}_{DB,c}\hat{h} - \hat{\rho}_{C,c}\hat{h}\right)$$
$$\hat{w}_{BC}^{(+)}\Big|_{t+1} = \frac{\hat{w}_{BC}^{(+)}\Big|_t - \lambda\left(-\hat{\rho}_{DB,c}\hat{h} - \hat{\rho}_{C,c}\hat{h}\right)}{\left(1+\lambda\frac{2\rho_0}{\chi_{BC}}\right)}$$

2.7 $w_{BC}^{(-)}$ Field

2.7.1 Positive χ

For the $w_{BC}^{(-)}$ field, the relevant expressions are:

$$\left.\frac{\delta\mathcal{H}}{\delta w_{BC}^{(-)}}\right|_t = \frac{2\rho_0}{\chi_{BC}}\,w_{BC}^{(-)}\Big|_t - (\rho_{DB,c} * h)(\mathbf{r}) + (\rho_{C,c} * h)(\mathbf{r})$$
$$\left.\frac{\delta\hat{\mathcal{H}}}{\delta w_{BC}^{(-)}}\right|_t = \frac{2\rho_0}{\chi_{BC}}\,\hat{w}_{BC}^{(-)}\Big|_t - \hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}$$
$$\left.\frac{\delta\hat{\mathcal{H}}}{\delta w_{BC}^{(-)}}\right|_t^{lin} = \frac{2\rho_0}{\chi_{BC}}\,\hat{w}_{BC}^{(-)}\Big|_t$$

Note that we don't do the weak inhomogeneity expansion here because the $w_{BC}^{(-)}$ field tends to be much less stiff than the w_+ fields and so doesn't need the extra approximation. Now we get

$$\begin{aligned}
\hat{w}_{BC}^{(-)}\Big|_{t+1} &= \hat{w}_{BC}^{(-)}\Big|_t - \lambda\left[\frac{2\rho_0}{\chi_{BC}}\ \hat{w}_{BC}^{(-)}\Big|_t - \hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{C,c}\hat{h} + \frac{2\rho_0}{\chi_{BC}}(\ \hat{w}_{BC}^{(-)}\Big|_{t+1} - \hat{w}_{BC}^{(-)}\Big|_t)\right] \\
\hat{w}_{BC}^{(-)}\Big|_{t+1}(1+\lambda\frac{2\rho_0}{\chi_{BC}}) &= \hat{w}_{BC}^{(-)}\Big|_t - \lambda\left(-\hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}\right) \\
\hat{w}_{BC}^{(-)}\Big|_{t+1} &= \frac{\hat{w}_{BC}^{(-)}\Big|_t - \lambda\left(-\hat{\rho}_{DB,c}\hat{h} + \hat{\rho}_{C,c}\hat{h}\right)}{\left(1+\lambda\frac{2\rho_0}{\chi_{BC}}\right)}
\end{aligned}$$

2.7.2 Negative χ

For the $w_{BC}^{(-)}$ field, the relevant expressions are:

$$\begin{aligned}
\frac{\delta\mathcal{H}}{\delta w_{BC}^{(-)}}\bigg|_t &= \frac{2\rho_0}{\chi_{BC}}\ w_{BC}^{(-)}\Big|_t + i(\rho_{DB,c} * h)(\mathbf{r}) - i(\rho_{C,c} * h)(\mathbf{r}) \\
\frac{\delta\hat{\mathcal{H}}}{\delta w_{BC}^{(-)}}\bigg|_t &= \frac{2\rho_0}{\chi_{BC}}\ \hat{w}_{BC}^{(-)}\Big|_t + i\hat{\rho}_{DB,c}\hat{h} - i\hat{\rho}_{C,c}\hat{h} \\
\frac{\delta\hat{\mathcal{H}}}{\delta w_{BC}^{(-)}}\bigg|_t^{lin} &= \frac{2\rho_0}{\chi_{BC}}\ \hat{w}_{BC}^{(-)}\Big|_t - i\hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{BB})i\ \hat{w}_{BC}^{(-)}\Big|_t + i\hat{h}^2\rho_0\ \phi_G N_G(\hat{g}_C)i\hat{w}_{BC}^{(-)}\Big|_t \\
&= \frac{2\rho_0}{\chi_{BC}}\ \hat{w}_{BC}^{(-)}\Big|_t + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{BB})\ \hat{w}_{BC}^{(-)}\Big|_t - \hat{h}^2\rho_0\ \phi_G N_G(\hat{g}_C)\hat{w}_{BC}^{(-)}\Big|_t
\end{aligned}$$

This gives us

$$\hat{w}_{BC}^{(-)}\Big|_{t+1} = \hat{w}_{BC}^{(-)}\Big|_t - \lambda\left[\frac{2\rho_0}{\chi_{BC}}\ \hat{w}_{BC}^{(-)}\Big|_t + i(\hat{\rho}_{DB,c}\hat{h} - \hat{\rho}_{C,c}\hat{h}) + A(\ \hat{w}_{BC}^{(-)}\Big|_{t+1} - \hat{w}_{BC}^{(-)}\Big|_t)\right]$$

where

$$A = \frac{2\rho_0}{\chi_{BC}} + \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{BB}) - \hat{h}^2\rho_0\phi_G N_G(\hat{g}_C)$$

If we let B and F equal

$$\begin{aligned}
B &= A - \frac{2\rho_0}{\chi_{BC}} \\
&= \hat{h}^2\phi_D\rho_0 N_D(\hat{g}_{BB}) - \hat{h}^2\rho_0\phi_G N_G(\hat{g}_C) \\
F &= +i(\hat{\rho}_{DB,c}\hat{h} - \hat{\rho}_{C,c}\hat{h})
\end{aligned}$$

Then

$$\begin{aligned}
\hat{w}_{BC}^{(-)}\Big|_{t+1}(1+\lambda A) &= \hat{w}_{BC}^{(-)}\Big|_t - \lambda\left(F - B\ \hat{w}_{BC}^{(-)}\Big|_t\right) \\
\hat{w}_{BC}^{(-)}\Big|_{t+1} &= \frac{\hat{w}_{BC}^{(-)}\Big|_t - \lambda\left(F - B\ \hat{w}_{BC}^{(-)}\Big|_t\right)}{1+\lambda A}
\end{aligned}$$

2.8 Canonical Ensemble

In the Canonical Ensemble, the polymer densities are given by

$$\rho_{DA,c} = -n_D \frac{\delta \log Q_D}{\delta \omega_A(\mathbf{r})} = \frac{n_D}{VQ_D} \sum_{j=1}^{P_A} q_D(j,\mathbf{r}) e^{\omega_A(\mathbf{r})} q_D^{\dagger}(P-j,\mathbf{r})$$

$$\rho_{DB,c} = -n_D \frac{\delta \log Q_D}{\delta \omega_B(\mathbf{r})} = \frac{n_D}{VQ_D} \sum_{j=P_A+1}^{P} q_D(j,\mathbf{r}) e^{\omega_B(\mathbf{r})} q_D^{\dagger}(P-j,\mathbf{r})$$

and the particle density is given by

$$\rho_P(\mathbf{r}) = -n_P \frac{\delta \log Q_P}{\delta \omega_P(\mathbf{r})} = \frac{n_P}{VQ_P} e^{-\omega_P(\mathbf{r})}$$