

# Weakly Compressible AB Diblock + Bare C-like Nanoparticles with Negative $\chi_{AC}$ and Smearing Derivation

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

The system is composed of  $n_D$  AB diblock chains and  $n_P$  bare, A-like nanoparticles. Each diblock chain has  $P_A + P_B = P$  segments.  $\chi_{IJ}$  is the interaction strength between components  $I$  and  $J$  AB, AC, BC. Segment center densities are defined as

$$\begin{aligned}\hat{\rho}_{DA,c}(\mathbf{r}) &= \sum_{i=1}^{n_D} \sum_{j=1}^{P_A} \delta(\mathbf{r} - \mathbf{r}_{i,j}) \\ \hat{\rho}_{DB,c}(\mathbf{r}) &= \sum_{i=1}^{n_D} \sum_{j=P_A+1}^P \delta(\mathbf{r} - \mathbf{r}_{i,j}) \\ \hat{\rho}_{P,c}(\mathbf{r}) &= \sum_{i=1}^{n_P} \delta(\mathbf{r} - \mathbf{r}_i)\end{aligned}$$

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  $K \in \{DA, DB\}$  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 full nanoparticle density distribution is given by

$$\hat{\rho}_P = (\Gamma * \hat{\rho}_{P,c})(\mathbf{r})$$

where

$$\Gamma(\mathbf{r}) = \frac{\rho_0}{2} \text{erfc}\left(\frac{|\mathbf{r}| - R_P}{\xi}\right)$$

where  $R_P$  is the nanoparticle radius,  $\rho_0$  is the bulk density, and  $\xi$  controls the nanoparticle interface width. The harmonic bond potential between connected segments is given by

$$\beta U_0 = \sum_{i=1}^{n_D} \sum_{j=1}^{P-1} \frac{3|\mathbf{r}_{i,j+1} - \mathbf{r}_{i,j}|^2}{2b^2}$$

The nonbonded interaction potential is given by

$$\beta U_1 = \frac{\chi_{AB}}{\rho_0} \int d\mathbf{r} \hat{\rho}_{DA} \hat{\rho}_{DB} + \frac{-\chi_{AC}}{\rho_0} \int d\mathbf{r} \hat{\rho}_{DA} \hat{\rho}_P + \frac{\chi_{BC}}{\rho_0} \int d\mathbf{r} \hat{\rho}_{DB} \hat{\rho}_P$$

A Helfand incompressibility potential penalizes deviations away from  $\rho_0$ , and is given by

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

where  $\hat{\rho}_+ = \hat{\rho}_{DA} + \hat{\rho}_{DB} + \hat{\rho}_P$  is the local total density.

This gives us a canonical partition function of

$$Z_C = \frac{1}{n_D!n_P!(\lambda_T^3)^{n_D+n_P}} \int d\mathbf{r}^{n_D N_D} \int d\mathbf{r}^{n_P} \exp(-\beta U_0 - \beta U_1 - \beta U_2)$$

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

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

With these definitions, we can rewrite  $\beta U_1$  as

$$\beta U_1 = \frac{\chi_{AB}}{4\rho_0} \int d\mathbf{r} \left( \hat{\rho}_{AB}^{(+)}(\mathbf{r})^2 - \hat{\rho}_{AB}^{(-)}(\mathbf{r})^2 \right) + \frac{-\chi_{AC}}{4\rho_0} \int d\mathbf{r} \left( \hat{\rho}_{AC}^{(+)}(\mathbf{r})^2 - \hat{\rho}_{AC}^{(-)}(\mathbf{r})^2 \right) + \frac{\chi_{BC}}{4\rho_0} \int d\mathbf{r} \left( \hat{\rho}_{BC}^{(+)}(\mathbf{r})^2 - \hat{\rho}_{BC}^{(-)}(\mathbf{r})^2 \right)$$

From there, using the Gaussian functional integral, we get

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

and

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

Notice that since  $\chi_{AC} < 0$ , the prefactors of +1 and  $-i$  on the second terms in the exponentials with  $\chi_{AC}$  are switched. (See Fredrickson eqns C.27 and C.28.) 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

$$\begin{aligned}Z_C &= \frac{1}{n_D!n_P!(\lambda_T^3)^{n_D+n_P}} \frac{1}{\Omega} \int \dots \int \mathcal{D}\{w\} \\ &\times \exp\left(-\frac{\rho_0}{2\kappa} \int d\mathbf{r} w_+(\mathbf{r})^2 + i\rho_0 \int d\mathbf{r} w_+ - \sum_{IJ \in \{AB, AC, BC\}} \frac{\rho_0}{\chi_{IJ}} \int d\mathbf{r} \left( w_{IJ}^{(+)}(\mathbf{r})^2 + w_{IJ}^{(-)}(\mathbf{r})^2 \right)\right) \\ &\times \int d\mathbf{r}^{n_D N_D} \int d\mathbf{r}^{n_P} \exp\left(-\sum_{i=1}^{n_D} \sum_{j=1}^{P-1} \frac{3|\mathbf{r}_{i,j+1} - \mathbf{r}_{i,j}|^2}{2b^2} - i \int d\mathbf{r} w_+ \hat{\rho}_+\right) \\ &\times \exp\left(\int d\mathbf{r} \left(-i\hat{\rho}_{AB}^{(+)} w_{AB}^{(+)} + \hat{\rho}_{AB}^{(-)} w_{AB}^{(-)} + \hat{\rho}_{AC}^{(+)} w_{AC}^{(+)} - i\hat{\rho}_{AC}^{(-)} w_{AC}^{(-)} - i\hat{\rho}_{BC}^{(+)} w_{BC}^{(+)} + \hat{\rho}_{BC}^{(-)} w_{BC}^{(-)}\right)\right)\end{aligned}$$

Using the definitions of  $\hat{\rho}_{IJ}^{(\pm)}$ , and defining

$$\begin{aligned}w_A &= i \left( w_+ + w_{AB}^{(+)} + w_{AC}^{(-)} \right) - w_{AB}^{(-)} - w_{AC}^{(+)} \\ w_B &= i \left( w_+ + w_{AB}^{(+)} + w_{BC}^{(-)} \right) - w_{AB}^{(-)} - w_{BC}^{(+)} \\ w_C &= i \left( w_+ + w_{AC}^{(-)} + w_{BC}^{(+)} \right) - w_{AC}^{(+)} - w_{BC}^{(-)},\end{aligned}$$

we can rewrite all the  $\exp(\int d\mathbf{r} w \hat{\rho})$  type terms as

$$\prod_j^{n_D N_{DA}} \exp(-\omega_A(\mathbf{r}_j)) \prod_k^{n_D N_{DB}} \exp(-\omega_B(\mathbf{r}_k)) \cdot \prod_l^{n_P} \exp(-\omega_P(\mathbf{r}_l)).$$

where  $\omega_A$  and  $\omega_B$  are defined as

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

and  $\omega_P$  is defined as

$$\omega_P(\mathbf{r}) = (\Gamma * w_C)(\mathbf{r})$$

Additionally, defining the bond transition probability  $\Phi$  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

$$\begin{aligned} Z_C = & \frac{1}{n_D! n_P! (\lambda_T^3)^{n_D + n_P}} \frac{1}{\Omega} \int \dots \int \mathcal{D}\{w\} \\ & \times \exp\left( -\frac{\rho_0}{2\kappa} \int d\mathbf{r} w_+(\mathbf{r})^2 + i\rho_0 \int d\mathbf{r} w_+ - \sum_{IJ} \frac{\rho_0}{\chi_{IJ}} \int d\mathbf{r} \left( w_{IJ}^{(+)}(\mathbf{r})^2 + w_{IJ}^{(-)}(\mathbf{r})^2 \right) \right) \\ & \times \int d\mathbf{r}^{n_D N_D} \int d\mathbf{r}^{n_P} \prod_j^{n_D} \prod_k^{N_D-1} \Phi(\mathbf{r}_{j,k+1} - \mathbf{r}_{j,k}) \\ & \times \prod_j^{n_D N_{DA}} \exp(-\omega_A(\mathbf{r}_j)) \prod_k^{n_D N_{DB}} \exp(-\omega_B(\mathbf{r}_k)) \cdot \prod_l^{n_P} \exp(-\omega_P(\mathbf{r}_l)) \end{aligned}$$

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  $q_D(1, \mathbf{r}) = \exp(-\omega_A(\mathbf{r}))$ . We also define  $Q_P$  as

$$Q_P = \frac{1}{V} \int d\mathbf{r} \exp(-\omega_P)$$

With these definitions, we get

$$\begin{aligned} Z_C = & \frac{V^{n_D + n_P}}{n_D! n_P! (\lambda_T^3)^{n_D + n_P}} \frac{1}{\Omega} \left( \frac{2\pi b^2}{3} \right)^{(d/2)n_D(N_D-1)} \int \dots \int \mathcal{D}\{w\} \\ & \times \exp\left( -\frac{\rho_0}{2\kappa} \int d\mathbf{r} w_+(\mathbf{r})^2 + i\rho_0 \int d\mathbf{r} w_+ - \sum_{IJ} \frac{\rho_0}{\chi_{IJ}} \int d\mathbf{r} \left( w_{IJ}^{(+)}(\mathbf{r})^2 + w_{IJ}^{(-)}(\mathbf{r})^2 \right) \right) \\ & \times Q_D^{n_D} Q_P^{n_P} \end{aligned}$$

We can rewrite this as

$$Z_C = \frac{V^{n_D+n_P}}{n_D!n_P! (\lambda_T^3)^{n_D+n_P}} \frac{1}{\Omega} \left( \frac{2\pi b^2}{3} \right)^{(d/2)n_D(N_D-1)} \int \dots \int \mathcal{D}\{w\} \exp(-\mathcal{H}[\{w\}])$$

where

$$\mathcal{H}[w_+, w_{AB}^{(\pm)}] = \frac{\rho_0}{2\kappa} \int d\mathbf{r} w_+(\mathbf{r})^2 - i\rho_0 \int d\mathbf{r} w_+ + \sum_{IJ} \frac{\rho_0}{\chi_{IJ}} \int d\mathbf{r} \left( w_{IJ}^{(+)}(\mathbf{r})^2 + w_{IJ}^{(-)}(\mathbf{r})^2 \right) - n_D \log Q_D - n_P \log Q_P$$

## 2 Grand Canonical Derivation

The grand canonical partition function is then given by

$$Z_G(\mu_D, \mu_P, V, T) = \sum_{n_D}^{\infty} \exp(\beta\mu_D n_D) \sum_{n_P}^{\infty} \exp(\beta\mu_P n_P) Z_C(n_D, n_P, V, T)$$

Now let's define activities  $z_D$  and  $z_P$  as

$$z_K = z_{K0} \exp(\beta\mu_K)$$

where

$$z_{D0} = \frac{1}{\lambda_T^3} \left( \frac{2\pi b^2}{3} \right)^{d/2(N_D-1)}$$

and

$$z_{P0} = \frac{1}{\lambda_T^3}$$

Now we can rewrite equation  $Z_G$  as

$$\begin{aligned} Z_G(\mu_D, \mu_P, V, T) &= \frac{1}{\Omega} \int \dots \int \mathcal{D}\{w\} \\ &\times \exp \left( -\frac{\rho_0}{2\kappa} \int d\mathbf{r} w_+(\mathbf{r})^2 + i\rho_0 \int d\mathbf{r} w_+ - \frac{\rho_0}{\chi} \int d\mathbf{r} w_{AB}^{(+)}(\mathbf{r})^2 - \frac{\rho_0}{\chi} \int d\mathbf{r} w_{AB}^{(-)}(\mathbf{r})^2 \right) \\ &\times \sum_{n_D}^{\infty} \frac{(z_D V Q_D)^{n_D}}{n_D!} \sum_{n_P}^{\infty} \frac{(z_P V Q_P)^{n_P}}{n_P!} \\ &= \frac{1}{\Omega} \int \dots \int \mathcal{D}\{w\} \\ &\times \exp \left( -\frac{\rho_0}{2\kappa} \int d\mathbf{r} w_+(\mathbf{r})^2 + i\rho_0 \int d\mathbf{r} w_+ - \sum_{IJ} \frac{\rho_0}{\chi_{IJ}} \int d\mathbf{r} \left( w_{IJ}^{(+)}(\mathbf{r})^2 + w_{IJ}^{(-)}(\mathbf{r})^2 \right) \right) \\ &\times \exp(z_D V Q_D) \exp(z_P V Q_P) \end{aligned}$$

And finally, we get

$$Z_G(\mu_D, \mu_P, V, T) = \frac{1}{\Omega} \int \dots \int \mathcal{D}\{w\} \exp(-\mathcal{H}_G[\{w\}])$$

where

$$\mathcal{H}_G[\{w\}] = \frac{\rho_0}{2\kappa} \int d\mathbf{r} w_+(\mathbf{r})^2 - i\rho_0 \int d\mathbf{r} w_+ + \sum_{IJ} \frac{\rho_0}{\chi_{IJ}} \int d\mathbf{r} \left( w_{IJ}^{(+)}(\mathbf{r})^2 + w_{IJ}^{(-)}(\mathbf{r})^2 \right) - z_D V Q_D - z_P V Q_P$$

### 3 Canonical 1S Update Derivation

#### 3.1 $w_+$ 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,

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

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

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

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

$$\begin{aligned} A &= \frac{1}{w_+^t} \left( \frac{\delta \hat{\mathcal{H}}}{\delta \hat{w}_+^t} \right)_{lin} = \frac{1}{w_+^{t+1}} \left( \frac{\delta \hat{\mathcal{H}}}{\delta \hat{w}_+^{t+1}} \right)_{lin} \\ &= \frac{\rho_0}{\kappa} + \hat{h}^2 \phi_D \rho_0 N_D (\hat{g}_{AA} + 2\hat{g}_{AB} + \hat{g}_{BB}) + \phi_P \rho_0 \hat{\Gamma}^2 \end{aligned}$$

If we also let  $B$  and  $F$  equal

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

Then

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

### 3.2 $w_{AB}^{(+)}$

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

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

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

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

If we let  $B$  and  $F$  equal

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

Then

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

### 3.3 $w_{AB}^{(-)}$ Field

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

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

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

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

### 3.4 $w_{AC}^{(-)}$

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

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

This gives us

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

where

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

If we let  $B$  and  $F$  equal

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

Then

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

### 3.5 $w_{AC}^{(+)}$ Field

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

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

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

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

### 3.6 $w_{BC}^{(+)}$

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

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

This gives us

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

where

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

If we let  $B$  and  $F$  equal

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



Then

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

### 3.7 $w_{BC}^{(-)}$ Field

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

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

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

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

## 4 Calculating Densities

### 4.1 Canonical Ensemble

In the Canonical Ensemble, the polymer densities are given by

$$\begin{aligned}\rho_{DA,c} &= -n_D \frac{\delta \log Q_D}{\delta \omega_A(\mathbf{r})} = \frac{n_D}{V Q_D} \sum_{j=1}^{P_A} q_D(j, \mathbf{r}) e^{\omega_A(\mathbf{r})} q_D^\dagger(P-j, \mathbf{r}) \\ \rho_{DB,c} &= -n_D \frac{\delta \log Q_D}{\delta \omega_B(\mathbf{r})} = \frac{n_D}{V Q_D} \sum_{j=P_A+1}^P q_D(j, \mathbf{r}) e^{\omega_B(\mathbf{r})} q_D^\dagger(P-j, \mathbf{r})\end{aligned}$$

and the particle density is given by

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

## 4.2 Grand Canonical Ensemble

In the Grand Canonical Ensemble, the polymer densities are given by

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

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

and the particle density is given by

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

## 5 Comparing $z_D$ values with 2 Field Model

From the 2-field model derivation,

$$z_{D0,2} = \frac{1}{\lambda_T^3} \exp\left(-\frac{N_D \chi}{4}\right) \left(\frac{2\pi b^2}{3}\right)^{d/2(N_D-1)}$$

And from the 3-field model derivation, (this document)

$$z_{D0,3} = \frac{1}{\lambda_T^3} \left(\frac{2\pi b^2}{3}\right)^{d/2(N_D-1)}$$

Therefore, to compare 2-field and 3-field simulations, we need to take this into account to make sure  $\mu_D$  matches between them. Thus, given a 3-field model using  $z_{D,3}$ , the corresponding value of  $z_{D,2}$  necessary to match a 2-field model is

$$z_{D,2} = \exp\left(-\frac{N_D \chi}{4}\right) z_{D,3}$$

## 6 Simplification for Homogeneous System

In a homogeneous system, the fields  $w_+$ ,  $w_{AB}^{(+)}$ , and  $w_{AB}^{(-)}$  are all constants. To simplify solving the equations, it is convenient to use only real numbers by solving for  $iw_+$ ,  $iw_{AB}^{(+)}$ , and  $w_{AB}^{(-)}$ . With this in mind, we can rewrite the Grand Canonical Hamiltonian as

$$H_G = -\frac{\rho_0 V}{2\kappa} (iw_+)^2 - \rho_0 V (iw_+) - \frac{\rho_0 V}{\chi} (iw_{AB}^{(+)})^2 + \frac{\rho_0 V}{\chi} (w_{AB}^{(-)})^2 - z_D V Q_D - z_P V Q_P$$

If we solve with simple Euler equations, we get

$$\begin{aligned}
iw_+^{t+1} &= iw_+^t - i\lambda_+ \frac{\partial H_G/V}{\partial w_+^t} \\
&= iw_+^t + \lambda_+ \frac{\partial H_G/V}{\partial iw_+^t} \\
iw_{AB}^{(+)} \Big|_{t+1} &= iw_{AB}^{(+)} \Big|_t - i\lambda_+ \frac{\partial H_G/V}{\partial w_{AB}^{(+)} \Big|_t} \\
&= iw_{AB}^{(+)} \Big|_t + \lambda_+ \frac{\partial H_G/V}{\partial iw_{AB}^{(+)} \Big|_t} \\
w_{AB}^{(-)} \Big|_{t+1} &= w_{AB}^{(-)} \Big|_t - \lambda_- \frac{\partial H_G/V}{\partial w_{AB}^{(-)} \Big|_t}
\end{aligned}$$

With this in mind, we can rewrite the partition functions as

$$\begin{aligned}
Q_D &= \exp(-P_A w_A - P_B w_B) \\
Q_P &= \exp(-\rho_0 V_P w_A)
\end{aligned}$$

Let's note that

$$\begin{aligned}
\rho_D &= \rho_{DA} + \rho_{DB} \\
&= -z_D \frac{\partial Q_D}{\partial \omega_A} - z_D \frac{\partial Q_D}{\partial \omega_B} \\
&= -z_D \frac{\partial Q_D}{\partial w_A} - z_D \frac{\partial Q_D}{\partial w_B} \\
&= z_D P \exp(-P_A w_A - P_B w_B) \\
&= z_D P Q_D
\end{aligned}$$

and

$$\begin{aligned}
\rho_{P,c} &= -z_P \frac{\partial Q_P}{\partial \omega_P} \\
&= z_P \exp(-\rho_0 V_P w_A) \\
\rho_{P,c} &= z_P Q_P \\
\rho_P &= \rho_0 V_P z_P Q_P
\end{aligned}$$

with the following derivatives:

$$\frac{\partial H_G/V}{\partial iw_+} = -\frac{\rho_0}{\kappa} (iw_+) - \rho_0 - \frac{2\rho_0}{\chi} (iw_{AB}^{(+)}) + \frac{2\rho_0}{\chi} (w_{AB}^{(-)}) - z_D \frac{\partial Q_D}{\partial iw_+} - z_P \frac{\partial Q_P}{\partial iw_+}$$

With this in mind, we can rewrite the partition functions as

$$\begin{aligned}
Q_D &= \exp(-f P w_A - (1-f) P w_B) \\
&= \exp(-f P (iw_+ + iw_{AB}^{(+)} - w_{AB}^{(-)}) - (1-f) P (iw_+ + iw_{AB}^{(+)} + w_{AB}^{(-)})) \\
&= \exp(-P (iw_+ + iw_{AB}^{(+)} + (2f-1) w_{AB}^{(-)}))
\end{aligned}$$

and

$$\begin{aligned} Q_P &= \exp(-\rho_0 V_P w_A) \\ &= \exp(-\rho_0 V_P (i w_+ + i w_{AB}^{(+)} - w_{AB}^{(-)})) \end{aligned}$$

Then we can rewrite the Grand Canonical Hamiltonian as

$$\begin{aligned} H_G &= -\frac{\rho_0 V}{2\kappa} (i w_+)^2 - \rho_0 V (i w_+) - \frac{\rho_0 V}{\chi} (i w_{AB}^{(+)})^2 + \frac{\rho_0 V}{\chi} (w_{AB}^{(-)})^2 \\ &\quad - z_D V \exp(-P(i w_+ + i w_{AB}^{(+)})) + (2f - 1) P w_{AB}^{(-)} \\ &\quad - z_P V \exp(-\rho_0 V_P (i w_+ + i w_{AB}^{(+)} - w_{AB}^{(-)})) \end{aligned}$$

If we solve with simple Euler equations, we get

$$\begin{aligned} w_+^{t+1} &= w_+^t - \lambda_+ \frac{\partial H_G / V}{\partial w_+^t} \\ w_{AB}^{(+)} \Big|_{t+1} &= w_{AB}^{(+)} \Big|_t - \lambda_+ \frac{\partial H_G / V}{\partial w_{AB}^{(+)} \Big|_t} \\ w_{AB}^{(-)} \Big|_{t+1} &= w_{AB}^{(-)} \Big|_t - \lambda_- \frac{\partial H_G / V}{\partial w_{AB}^{(-)} \Big|_t} \end{aligned}$$

with the following derivatives:

$$\frac{\partial H}{\partial w_+^t} = -\frac{\rho_0}{\kappa} (i w_+) - \rho_0 - \frac{2\rho_0}{\chi} (i w_{AB}^{(+)}) + \frac{2\rho_0}{\chi} (w_{AB}^{(-)})$$