

Supplemental Material: Transport of partially active polymers in chemical gradients

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1 The Langevin equations, Rouse modes and the Fokker-Planck equation

The set of overdamped Langevin equations describing the motion of the polymer is

$$\dot{\mathbf{X}}_i(t) = -\mu \nabla_{\mathbf{X}_i} \mathcal{H} + \mu \alpha_i f_s(\mathbf{X}_i) \mathbf{p}_i + \boldsymbol{\xi}_i(t), \quad (1)$$

$$\dot{\mathbf{p}}_i(t) = \mathbf{p}_i \times \boldsymbol{\eta}_i(t), \quad (2)$$

where $i = \{0, 1, 2, \dots, N-1\}$, N being the number of monomers in the polymer chain, μ is the mobility of the monomers, f_s is the active force, which is a function of the spatial coordinates and it acts along the orientation vector $\{\mathbf{p}_i\}$, which evolves in time due to rotational diffusion. The nature of monomers are taken care by the parameters $\{\alpha_i\}$, with $\alpha_i = 1$ and 0 corresponding to active and passive monomers, respectively. $\{\boldsymbol{\xi}_i(t)\}$ and $\{\boldsymbol{\eta}_i(t)\}$ are zero-mean white Gaussian noises such that

$$\langle \boldsymbol{\xi}_i(t) \otimes \boldsymbol{\xi}_j(s) \rangle = 2D\mathbf{I} \delta_{ij} \delta(t-s), \quad (3)$$

$$\langle \boldsymbol{\eta}_i(t) \otimes \boldsymbol{\eta}_j(s) \rangle = 2D_r \mathbf{I} \delta_{ij} \delta(t-s), \quad (4)$$

where D is the thermal diffusivity and D_r is the rotational diffusivity, and \mathbf{I} is the $d \times d$ identity matrix (d denotes the number of dimensions). The interactions between monomers are modeled by a harmonic potential and are governed by the Hamiltonian \mathcal{H} ,

$$\mathcal{H} = \frac{\zeta}{2} \sum_{ij} M_{ij} \mathbf{X}_i \cdot \mathbf{X}_j, \quad (5)$$

where M_{ij} is the connectivity matrix of the polymer and ζ is the spring constant.

As done frequently in polymer physics, we obtain the Rouse modes from the physical coordinates of the monomers via the linear transformation

$$\boldsymbol{\chi}_i = \sum_j \varphi_{ij} \mathbf{X}_j, \quad (6)$$

where φ_{ij} is a matrix that diagonalizes the connectivity matrix \mathbf{M} such that $\sum_{jk} \varphi_{ij} M_{jk} \varphi_{kl}^{-1} = \frac{\gamma_i}{\gamma} \delta_{il}$, $\gamma = \mu\zeta$ being an inverse timescale due to the spring relaxation. Applying this linear transformation to Eq. (1), we

get the time evolution of the Rouse modes:

$$\dot{\boldsymbol{\chi}}_i = \gamma_i \boldsymbol{\chi}_i + \sum_j \varphi_{ij} \alpha_j v(\mathbf{X}_j) \mathbf{p}_j + \tilde{\boldsymbol{\xi}}_i(t), \quad (7)$$

where $v(\mathbf{X}_j) = \mu f_s(\mathbf{X}_j)$ is the swim speed of the monomers and $\{\tilde{\boldsymbol{\xi}}_i(t)\}$ are Gaussian white noises with the same statistical properties as $\{\boldsymbol{\xi}_i(t)\}$.

The corresponding Fokker-Planck equation for Eq. (2) and Eq. (7) is given by

$$\partial_t \mathcal{P} = (\mathcal{L}_0 + \mathcal{L}_a + \mathcal{L}_p) \mathcal{P}, \quad (8)$$

where $\mathcal{P}(\{\boldsymbol{\chi}\}, \{\mathbf{p}\}, t)$ is the joint probability density. The operators in Eq. (8) are defined as

$$\begin{aligned} \mathcal{L}_0 &\equiv \sum_{i=0}^{N-1} \nabla_i \cdot [\gamma_i \boldsymbol{\chi}_i + D \nabla_i], \\ \mathcal{L}_a &\equiv - \sum_{i=0}^{N-1} \nabla_i \cdot \left[\sum_j \varphi_{ij} \alpha_j v(\mathbf{X}_j) \mathbf{p}_j \right], \\ \mathcal{L}_p &\equiv \sum_{i=0}^{N-1} D_r \tilde{\nabla}_i^2, \end{aligned} \quad (9)$$

where $\nabla_i \equiv \nabla_{\boldsymbol{\chi}_i}$ and $\tilde{\nabla}_i \equiv \nabla_{\mathbf{p}_i}$.

2 Coarse-graining of the Fokker-Planck Equation

Since we are only interested in the spatial distribution of these polymers, we look for a probability density ρ that is only a function of the center of mass of the polymer $\mathbf{X}_{\text{COM}} = \boldsymbol{\chi}_0 / \sqrt{N}$. To obtain this we carry out two steps of coarse graining : (i) integrating out all the orientation vectors to obtain a marginal density

$$\varrho = (\{\boldsymbol{\chi}\}, t) = \int \prod_i d\mathbf{p}_i P(\{\boldsymbol{\chi}\}, \{\mathbf{p}\}, t), \quad (10)$$

and (ii) integrating out the rest of the Rouse modes to obtain the probability distribution function ρ_0

$$\rho_0(\boldsymbol{\chi}_0, t) = \int \prod_{i \neq 0} d\boldsymbol{\chi}_i \varrho(\{\boldsymbol{\chi}\}, t). \quad (11)$$

To carry out the first step of coarse-graining, we expand the joint probability distribution function using spherical harmonics:

$$P(\{\boldsymbol{\chi}\}, \{\mathbf{p}\}, t) = \frac{1}{\Omega_d^N} \left(\phi + \sum_i \boldsymbol{\sigma}_i \cdot \mathbf{p}_i + \sum_{i \neq j} \boldsymbol{\sigma}_{ij} : \mathbf{p}_i \mathbf{p}_j + \sum_i \boldsymbol{\omega}_i : (\mathbf{p}_i \mathbf{p}_i - \mathbf{I}/d) + \Theta \right), \quad (12)$$

constructed using the eigenfunctions 1 , $\{\mathbf{p}_i\}$, $\{\mathbf{p}_i \mathbf{p}_i - \mathbf{I}/d\}$, with the eigenvalues 0 , $-(d-1)$, and $-2d$, respectively. ϕ , $\boldsymbol{\sigma}_i$, $\boldsymbol{\sigma}_{ij}$, and $\boldsymbol{\omega}_i$ are the modes of the expansion and are functions of $\{\boldsymbol{\chi}\}, t$. ϕ is the marginal density ϱ , $\{\boldsymbol{\sigma}_i\}$ are related to the average orientations, while $\boldsymbol{\omega}$ contains information about the nematic order. The function Θ takes into account all the higher order modes and eigenfunctions. We are interested

the steady state distribution of the density in small gradients, and hence we ignore the $\{\boldsymbol{\omega}_i\}$, $\{\boldsymbol{\sigma}_{ij}\}$, and Θ terms that lead to $\mathcal{O}(\nabla^2)$ terms after coarse-graining. More details about this can be found in Ref. [1, 2]. The truncated expansion for P thus reads -

$$P(\{\boldsymbol{\chi}\}, \{\boldsymbol{p}\}, t) = \frac{1}{\Omega_d^N} \left(\phi + \sum_i \boldsymbol{\sigma}_i \cdot \boldsymbol{p}_i \right). \quad (13)$$

Before integrating out the orientation vectors, we define the scalar product

$$\langle f, g \rangle = \int \prod_i d\boldsymbol{p}_i f(\{\boldsymbol{p}\}) g(\{\boldsymbol{p}\}), \quad (14)$$

and list out the following identities that will be useful while integrating -

$$\langle 1, \mathcal{P} \rangle = \phi = \varrho, \quad (15)$$

$$\langle \boldsymbol{p}_j, \mathcal{P} \rangle = \frac{1}{d} \boldsymbol{\sigma}_j, \quad (16)$$

$$\langle \boldsymbol{p}_j \boldsymbol{p}_j, \mathcal{P} \rangle = \frac{1}{d} \phi \mathbf{I}, \quad (17)$$

$$\langle \boldsymbol{p}_j \boldsymbol{p}_k, \mathcal{P} \rangle = 0, \quad (18)$$

$$\langle 1, \sum_i \tilde{\nabla}_i^2 \mathcal{P} \rangle = 0, \quad (19)$$

$$\langle \boldsymbol{p}_j, \sum_i \tilde{\nabla}_i^2 \mathcal{P} \rangle = -\frac{1}{d} \boldsymbol{\sigma}_j, \quad (20)$$

$$\langle \boldsymbol{p}_j \boldsymbol{p}_k, \sum_i \tilde{\nabla}_i^2 \mathcal{P} \rangle = 0. \quad (21)$$

Taking the scalar product of Eq. (8) with 1 and \boldsymbol{p}_j gives us the coarse grained dynamics of the first two modes of the expansion-

$$\partial_t \varrho = \sum_i \nabla_i \left[\gamma_i \boldsymbol{\chi}_i \varrho + D \nabla_i \varrho - \sum_j \varphi_{ij} \alpha_j v(\boldsymbol{X}_j) \frac{\boldsymbol{\sigma}_j}{d} \right], \quad (22)$$

$$\partial_t \boldsymbol{\sigma}_j = -\tau^{-1} \boldsymbol{\sigma}_j + \sum_l \nabla_l \cdot [\gamma_l \boldsymbol{\chi}_l \boldsymbol{\sigma}_j + D \nabla_l \boldsymbol{\sigma}_j - \varphi_{lj} \alpha_j v(\boldsymbol{X}_j) \varrho], \quad (23)$$

where $\tau^{-1} = (d-1)D_r$. The equation for the dynamics of ϱ can be written as a continuity equation

$$\partial_t \varrho = - \sum_i \nabla_i \cdot \boldsymbol{J}_i, \quad (24)$$

where the fluxes are given by

$$\boldsymbol{J}_i = -\gamma_i \boldsymbol{\chi}_i \varrho + \sum_j \varphi_{ij} \alpha_j v(\boldsymbol{X}_j) \frac{\boldsymbol{\sigma}_j}{d} - D \nabla_i \varrho. \quad (25)$$

Proceeding with the second step of coarse-graining, using the definition in Eq. (11), we get

$$\partial_t \rho_0 = -\nabla_0 \cdot \boldsymbol{\mathcal{J}}_0, \quad (26)$$

where

$$\mathcal{J}_0 = \sum_j \frac{\varphi_{0j}}{d} \int \prod_{h \neq 0} d\chi_h \alpha_j v(\mathbf{X}_j) \boldsymbol{\sigma}_j - D \nabla_0 \rho_0, \quad (27)$$

where we have used the fact that $\gamma_0 = 0$ (see Sec. 3 for more details).

Since ϱ satisfies a conserved equation (Eq. (24)), it is the slowest mode [1]. Therefore the time derivative terms in the time-evolution equation for $\{\boldsymbol{\sigma}_j\}$'s can be neglected in Eq. (23) as they decay on a much faster timescale compared to ϱ . Thus, we get -

$$\boldsymbol{\sigma}_j = \sum_l \tau \nabla_l \cdot [\gamma_l \chi_l \boldsymbol{\sigma}_j + D \nabla_l \boldsymbol{\sigma}_j - \varphi_{lj} \alpha_j v(\mathbf{X}_j) \varrho]. \quad (28)$$

Plugging this into Eq. (27), and isolating the contribution by the active term we get

$$\begin{aligned} \mathcal{J}_0^{act} &= \sum_j \frac{\varphi_{0j}}{d} \int \prod_{h \neq 0} d\chi_h \alpha_j v(\mathbf{X}_j) \boldsymbol{\sigma}_j, \\ &= - \underbrace{\sum_j \frac{\varphi_{0j} \tau}{d} \int \prod_{h \neq 0} d\chi_h \alpha_j v(\mathbf{X}_j) \sum_l \nabla_l \cdot [\varphi_{lj} \alpha_j v(\mathbf{X}_j) \varrho]}_{\mathcal{J}_0^{act,1}} \\ &\quad + \underbrace{\sum_j \frac{\varphi_{0j} \tau}{d} \int \prod_{h \neq 0} d\chi_h \alpha_j v(\mathbf{X}_j) \sum_l \nabla_l \cdot [\gamma_l \chi_l \boldsymbol{\sigma}_j]}_{\mathcal{J}_0^{act,2}} + \mathcal{O}(\nabla_0^2), \end{aligned} \quad (29)$$

where the $\mathcal{O}(\nabla_0^2)$ term is the contribution from the $\nabla_l \boldsymbol{\sigma}_j$ term in Eq. (28) [3]. To solve for the probability distribution function ρ_0 analytically, we consider a small gradient approximation, in which the contribution of the $\mathcal{O}(\nabla_0^2)$ or higher terms to the expression of the flux \mathcal{J}_0 can be neglected. Therefore, we shall ignore such terms in the rest of our calculations.

To calculate $\mathcal{J}_0^{act,1}$, we split the summation over l into terms with $l = 0$ and $l \neq 0$. The latter gives

$$- \sum_j \frac{\varphi_{0j} \tau}{d} \int \prod_{h \neq 0} d\chi_h \alpha_j v(\mathbf{X}_j) \sum_{l \neq 0} \nabla_l \cdot [\varphi_{lj} \alpha_j v(\mathbf{X}_j) \varrho], \quad (30)$$

$$= \frac{\tau}{2d} \sum_{j,l \neq 0} \varphi_{0j} \int \prod_{h \neq 0} d\chi_h \sqrt{N} \alpha_j^2 \varphi_{lj} \varphi_{lj} \varrho \nabla_0 (v^2(\mathbf{X}_j)), \quad (31)$$

$$= \frac{\tau}{2d} \underbrace{\left[\sum_{j,l \neq 0} \alpha_j^2 \varphi_{lj}^2 \right]}_{S_1^l} \rho_0 \nabla_0 \left(v^2 \left(\frac{\mathbf{x}_0}{\sqrt{N}} \right) \right) + \mathcal{O}(\nabla_0^2), \quad (32)$$

where we have used integration by parts and

$$\nabla_l v(\mathbf{X}_j) = \sqrt{N} \varphi_{lj} \nabla_0 v(\mathbf{X}_j), \quad (33)$$

$$\nabla_0 v^2(\mathbf{X}_j) = \nabla_0 v^2(\varphi_{lj} \chi_l) = \nabla_0 v^2(\varphi_{0j} \chi_0) + \mathcal{O}(\nabla_0^2), \quad (34)$$

$$\varphi_{0j} = \frac{1}{\sqrt{N}}. \quad (35)$$

The $l = 0$ term is simplified as

$$-\sum_j \frac{\varphi_{0j}\tau}{d} \int \prod_{h \neq 0} d\chi_h \alpha_j v(\mathbf{X}_j) \nabla_0 \cdot [\varphi_{0j} \alpha_j v(\mathbf{X}_j) \varrho], \quad (36)$$

$$= -\frac{\tau}{2d} \underbrace{\left[\sum_j \alpha_j^2 \varphi_{0j}^2 \right]}_{S_2} \rho_0 \nabla_0 \left(v^2 \left(\frac{\chi_0}{\sqrt{N}} \right) \right) - \frac{\tau}{d} \left[\sum_j \alpha_j^2 \varphi_{0j}^2 \right] v^2 \left(\frac{\chi_0}{\sqrt{N}} \right) \nabla_0 \rho_0 + \mathcal{O}(\nabla_0^2), \quad (37)$$

where the summation S_2 can be simplified using Eq. (35) to obtain -

$$S_2 = \frac{1}{N} \sum_{j=0}^{N-1} \alpha_j^2 = \frac{1}{N} \sum_{j=0}^{N-1} \alpha_j. \quad (38)$$

Combining the two terms we get

$$\mathcal{J}_0^{act,1} = \frac{\tau}{2d} (S_1' - S_2) \rho_0 \nabla_0 \left(v^2 \left(\frac{\chi_0}{\sqrt{N}} \right) \right) - \frac{\tau}{d} S_2 v^2 \left(\frac{\chi_0}{\sqrt{N}} \right) \nabla_0 \rho_0 + \mathcal{O}(\nabla_0^2). \quad (39)$$

Representing $\mathcal{J}_0^{act,2}$ as

$$\mathcal{J}_0^{act,2} = \sum_l \mathcal{I}_l, \quad (40)$$

we have

$$\mathcal{I}_l = \sum_j \frac{\varphi_{0j}\tau}{d} \int \prod_{h \neq 0} d\chi_h \alpha_j v(\mathbf{X}_j) [\nabla_l \cdot (\gamma_l \chi_l \boldsymbol{\sigma}_j)], \quad (41)$$

$$= \sum_j -\frac{\varphi_{0j}\tau}{d} \int \prod_{h \neq 0} d\chi_h [\nabla_l (\alpha_j v(\mathbf{X}_j))] \cdot \gamma_l \chi_l \boldsymbol{\sigma}_j. \quad (42)$$

Substituting the expression for $\boldsymbol{\sigma}_j$ using Eq. (28) -

$$\mathcal{I}_l = \sum_j \frac{\varphi_{0j}\tau^2}{d} \sum_m \int \prod_{h \neq 0} d\chi_h [\nabla_l (\alpha_j v(\mathbf{X}_j))] \cdot \gamma_l \chi_l [\nabla_m (\varphi_{mj} \alpha_j v(\mathbf{X}_j) \varrho) - \nabla_m \cdot (\gamma_m \chi_m \boldsymbol{\sigma}_j)] + \mathcal{O}(\nabla_0^2). \quad (43)$$

The first term is simplified as

$$\sum_j \frac{\varphi_{0j}\tau^2}{d} \sum_m \int \prod_{h \neq 0} d\chi_h [\nabla_l (\alpha_j v(\mathbf{X}_j))] \cdot \gamma_l \chi_l [\nabla_m (\varphi_{mj} \alpha_j v(\mathbf{X}_j) \varrho)], \quad (44)$$

$$= -\sum_j \frac{\varphi_{0j}\tau^2}{d} \int \prod_{h \neq 0} d\chi_h [\nabla_l (\alpha_j v(\mathbf{X}_j))] \gamma_l \varphi_{lj} \alpha_j v(\mathbf{X}_j) \varrho + \mathcal{O}(\nabla_0^2), \quad (45)$$

$$= -\frac{\gamma_l \tau^2}{2d} \sqrt{N} \left[\sum_j \varphi_{0j} \varphi_{lj} \varphi_{lj} \alpha_j^2 \right] \rho_0 \nabla_0 \left(v^2 \left(\frac{\chi_0}{\sqrt{N}} \right) \right) + \mathcal{O}(\nabla_0^2), \quad (46)$$

$$= -\frac{\gamma_l \tau^2}{2d} \left[\sum_j \varphi_{lj}^2 \alpha_j^2 \right] \rho_0 \nabla_0 \left(v^2 \left(\frac{\chi_0}{\sqrt{N}} \right) \right) + \mathcal{O}(\nabla_0^2). \quad (47)$$

The second term simplifies to

$$-\sum_j \frac{\varphi_{0j}\tau^2}{d} \sum_m \int \prod_{h \neq 0} d\boldsymbol{\chi}_h [\nabla_l (\alpha_j v(\boldsymbol{X}_j))] \cdot \gamma_l \boldsymbol{\chi}_l [\nabla_m \cdot (\gamma_m \boldsymbol{\chi}_m \boldsymbol{\sigma}_j)], \quad (48)$$

$$= \sum_j \frac{\varphi_{0j}\tau^2}{d} \int \prod_{h \neq 0} d\boldsymbol{\chi}_h [\nabla_l (\alpha_j v(\boldsymbol{X}_j))] \cdot \gamma_l \boldsymbol{\chi}_l \boldsymbol{\sigma}_j + \mathcal{O}(\nabla_0^2), \quad (49)$$

$$= -\tau \gamma_l \boldsymbol{\mathcal{I}}_l + \mathcal{O}(\nabla_0^2). \quad (50)$$

Combining the two terms and substituting in Eq. (40), we get

$$\mathcal{J}_0^{act,2} = -\frac{\tau}{2d} \underbrace{\left[\sum_{lj} \frac{\tau \gamma_l}{1 + \tau \gamma_l} \varphi_{lj}^2 \alpha_j^2 \right]}_{S_1^*} \rho_0 \nabla_0 \left(v^2 \left(\frac{\boldsymbol{\chi}_0}{\sqrt{N}} \right) \right). \quad (51)$$

Therefore the complete expression for the flux \mathcal{J}_0 (Eq. (27)) is

$$\mathcal{J}_0 = \frac{\tau}{2d} (S_1 - S_2) \rho_0 \nabla_0 \left(v^2 \left(\frac{\boldsymbol{\chi}_0}{\sqrt{N}} \right) \right) - \left[D + \frac{\tau}{d} S_2 v^2 \left(\frac{\boldsymbol{\chi}_0}{\sqrt{N}} \right) \right] \nabla_0 \rho_0, \quad (52)$$

where $S_1 = S_1' - S_1^*$,

$$S_1 = \sum_{l=1, j=0}^{N-1} \frac{1}{1 + \tau \gamma_l} \varphi_{lj}^2 \alpha_j^2. \quad (53)$$

We now change the variable to $\boldsymbol{X}_{\text{COM}} = \boldsymbol{\chi}_0/\sqrt{N}$ and rewrite the coarse-grained Fokker-Planck equation in terms of the function $\rho(\boldsymbol{X}_{\text{COM}}, t) = \rho_0(\boldsymbol{\chi}_0, t)$. Dropping subscripts and the arguments, the flux in Eq. (52) can be written as

$$\mathcal{J} = \rho \boldsymbol{\mathcal{V}} - \nabla(\mathcal{D}\rho), \quad (54)$$

where the gradients are with respect to the centre of mass coordinates and $\boldsymbol{\mathcal{V}}$ and \mathcal{D} are the effective drift and effective diffusion coefficient, respectively, given by

$$\begin{aligned} \boldsymbol{\mathcal{V}}(\boldsymbol{X}_{\text{COM}}) &= \frac{\tau}{dN} \left(\frac{S_1 + S_2}{2} \right) \nabla (v^2(\boldsymbol{X}_{\text{COM}})), \\ \mathcal{D}(\boldsymbol{X}_{\text{COM}}) &= \frac{1}{N} \left(D + \frac{\tau}{d} S_2 v^2(\boldsymbol{X}_{\text{COM}}) \right). \end{aligned} \quad (55)$$

The two terms are related by $\boldsymbol{\mathcal{V}} = (1 - \frac{\epsilon}{2}) \nabla \mathcal{D}$, where

$$\epsilon = \frac{S_2 - S_1}{S_2}, \quad (56)$$

3 Eigenvectors and eigenvalues for a linear chain

The eigenvector matrix for a linear chain can be obtained as [4]-

$$\varphi_{lj} = \begin{cases} \sqrt{\frac{1}{N}}, & (l = 0) \\ \sqrt{\frac{2}{N}} \cos\left(\frac{l\pi}{N} \left(j + \frac{1}{2}\right)\right), & (l \neq 0) \end{cases} \quad (57)$$

and the normalized eigenvalues are given by -

$$\gamma_l = 4\gamma \sin^2 \left(\frac{l\pi}{2N} \right). \quad (58)$$

It can be easily verified that $|\varphi_{lj}|$ or φ_{lj}^2 is invariant for $j \rightarrow N - 1 - j$. Consider a polymer whose active monomers are distributed symmetrically along the chain (ex - both end monomers active). It can now be shown, using the invariance of ϕ_{lj}^2 under the aforementioned transformation, that the values of S_1 (Eq. (53)) and S_2 (the fraction of active monomers in the polymer) are twice their values for the corresponding case when only one half of the polymer has active monomers (ex - only one end monomer active). This gives us the same value of epsilon (Eq. (56)) for both cases.

3.1 Comparison between end monomer active and central monomer active

For a polymer with one end monomer active, we have:

$$S_1^{end} = \sum_{l=1}^{N-1} \frac{1}{1 + \tau\gamma_l} \phi_{l0}^2 = \frac{2}{N} \sum_{l=1}^{N-1} \frac{\cos^2 \left(\frac{l\pi}{2N} \right)}{1 + 4\tau\gamma \sin^2 \left(\frac{l\pi}{2N} \right)}, \quad (59)$$

while for a polymer with the central monomer active:

$$S_1^{mid} = \sum_{l=1}^{N-1} \frac{1}{1 + \tau\gamma_l} \phi_{l\frac{N}{2}}^2 = \frac{2}{N} \sum_{l=1}^{N-1} \frac{\cos^2 \left(\frac{l(N+1)\pi}{2N} \right)}{1 + 4\tau\gamma \sin^2 \left(\frac{l\pi}{2N} \right)}. \quad (60)$$

For both cases

$$S_2 = \frac{1}{N}. \quad (61)$$

In the limit of $N \gg 1$ we can rewrite S_1^{mid} as

$$S_1^{mid} = \frac{2}{N} \sum_{l=2,4,\dots}^{N-1} \frac{1}{1 + 4\tau\gamma \sin^2 \left(\frac{l\pi}{2N} \right)} \simeq \frac{1}{N} \sum_{l=1}^{N-1} \frac{1}{1 + 4\tau\gamma \sin^2 \left(\frac{l\pi}{2N} \right)}. \quad (62)$$

In this limiting case we can introduce the continuous limit according to

$$q = \frac{l\pi}{2N}, \quad dq = \frac{\pi}{2N}, \quad q \in \{0, \pi/2\}. \quad (63)$$

Then we obtain

$$S_1^{end} = \frac{1}{\pi} \int_0^{\frac{\pi}{2}} dq \frac{\cos^2 q}{1 + 4\kappa \sin^2 q} = \frac{\sqrt{1 + 4\kappa} - 1}{8\kappa} \simeq \frac{1}{4\kappa^{1/2}}, \quad (64)$$

and

$$S_1^{mid} = \frac{1}{2\pi} \int_0^{\frac{\pi}{2}} dq \frac{1}{1 + 4\kappa \sin^2 q} = \frac{1}{4\sqrt{1 + 4\kappa}} \simeq \frac{1}{8\kappa^{1/2}}. \quad (65)$$

Here, we have introduced the activity parameter

$$\kappa = \tau\gamma = \frac{\tau}{\tau_m}, \quad (66)$$

which is the ratio of the persistence time of the direction of the active force and the diffusive monomer relaxation time, τ_m . Since active motion of the monomers should be always dominant we can safely assume

$\kappa \gg 1$ which leads to the asymptotic expressions in Eq. (64) and (65). In this limit the exponent $\epsilon = (S_2 - S_1)/S_2$ which determines the degree of stationary anti-chemotactic behavior reads

$$-\epsilon_{end} = \frac{N}{4\sqrt{\kappa}} - 1 \simeq -2\epsilon_{mid}. \quad (67)$$

For chemotactic behavior ($\epsilon < 0$), we require $N^2 \gg \kappa$, or $\tau \ll \tau_m N^2 = \tau_R$, which means that the active persistence time should be much smaller than the diffusive relaxation time, or Rouse time, of the whole chain. We note that the relation $|\epsilon_{end}| > |\epsilon_{mid}|$ holds generally using the exact results in Eq.(64) and (65) for $\kappa > 1$.

Within the same limit can consider the result for the all-active chain, i.e. $\forall \alpha_l = 1$, For this case obtain

$$S_1^{all} = \sum_{l=1}^{N-1} \frac{1}{1 + \tau\gamma \sin^2\left(\frac{l\pi}{2N}\right)} = N \cdot S_1^{end} \quad \text{and} \quad S_2^{all} = 1 = N \cdot S_2^{end,mid}, \quad (68)$$

where we have used the normalization condition of the eigenfunctions in Eq.(53). Thus, we obtain the large N limit:

$$|\epsilon_{end}| \simeq 2|\epsilon_{mid}| \simeq 2|\epsilon_{all}|. \quad (69)$$

4 Semiflexible polymers

We can extend our study to semiflexible polymers by incorporating bending interactions in the Hamiltonian as -

$$\mathcal{H} = \sum \frac{\zeta}{2} (\mathbf{X}_{i+1} - \mathbf{X}_i)^2 + \sum \frac{\zeta_b}{2} (\mathbf{R}_{i+1} - \mathbf{R}_i)^2, \quad (70)$$

where ζ_b is the bending stiffness. This quadratic bending term [5, 6] allows us to use our theoretical framework to solve for the probability density function ρ analytically. The Hamiltonian can then be written as -

$$\mathcal{H} = \frac{1}{2} \sum_{i,j} M_{ij}^{\text{eff}} \mathbf{X}_i \cdot \mathbf{X}_j, \quad (71)$$

where \mathbf{M}^{eff} is

$$\mathbf{M}^{\text{eff}} = \zeta \mathbf{M} + \zeta_b \mathbf{M}_b. \quad (72)$$

Here \mathbf{M} and \mathbf{M}_b are the Rouse connectivity matrix and the bending connectivity matrix (which can be derived from Eq. (70)), respectively.

The expressions for ρ , ϵ , and S_2 remain unchanged from the flexible case. However, S_1 now becomes -

$$S_1 = \sum_{l=1, j=0}^{N-1} \frac{1}{1 + \tau\gamma_l^{\text{eff}}} \varphi_{lj}^{\text{eff}2} \alpha_j^2, \quad (73)$$

where φ^{eff} is the diagonalizing matrix of \mathbf{M}^{eff} : $\sum_{jk} \varphi_{ij}^{\text{eff}} M_{jk}^{\text{eff}} \varphi_{kl}^{\text{eff}} = \lambda_i \delta_{il}$, λ_i being the eigenvalues, and γ_i^{eff} s are the rescaled eigenvalues $\gamma_i^{\text{eff}} = \mu \lambda_i$.

The results for the semiflexible case are presented in Fig. 1. The left panel presents the results for the most chemotactic chain of length $N = 6$ - only the leading monomer is active, for different values of ζ_b . We see that as we increase ζ_b , the degree of self-localization at the region of maximum activity reduces. This effect of the bending stiffness can be exploited to reverse the accumulation behavior of flexible chemotactic chains as shown in the right panel of Fig. 1, which is the semiflexible counterpart of Fig. 2 of the main text with $\zeta_b = 32$. In the flexible case, one can see that all polymer configurations are chemotactic (Fig. 2 of the main text). However, for $\zeta_b = 32$, we observe that apart from the polymers with either or both end monomers active, the other configurations show anti-chemotactic behavior.

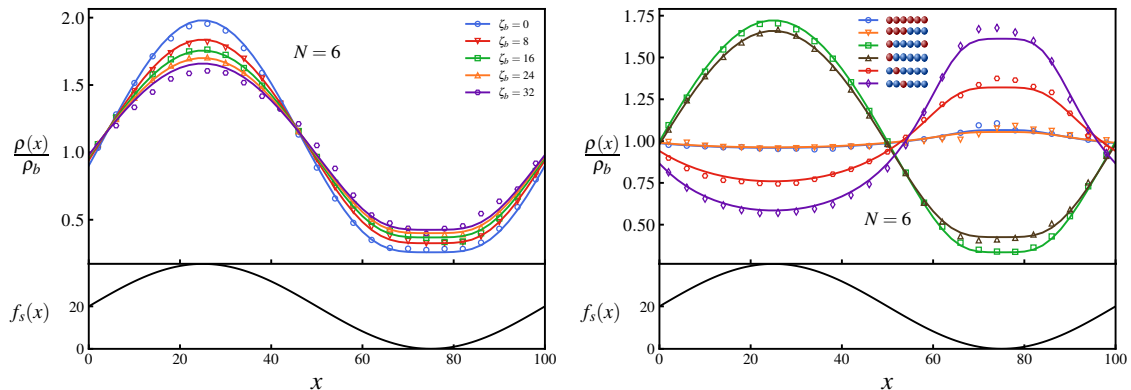


Figure 1: The steady state density profiles for (left) various values of the bending stiffness ζ_b of a polymer with only the leading monomer active, and (right) various configurations of a polymer with bending stiffness $\zeta_b = 32$. For both cases, chain length $N = 6$, $\zeta = 8$, $D_r = 5$, $\mu = 1$, and $D = 1$ in a box of length $L = 100$ that has a sinusoidally varying activity profile in the x -direction: $f_s(x) = 20 \left(1 + \sin\left(\frac{2\pi x}{L}\right)\right)$ as depicted. The densities are normalized by $\rho_b = 1/L$. The solid lines represent analytical predictions and the symbols represent Langevin dynamics simulation results.

5 Mean first passage time (MFPT)

The coarse grained Fokker-Planck Equation can be rewritten as

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \left(\left(1 - \frac{\epsilon}{2}\right) \nabla \mathcal{D} \rho \right) + \nabla^2 (\mathcal{D} \rho). \quad (74)$$

Following the procedure in Sec 5.2 in [7], the equation of the mean first passage time $T(x)$ for a one dimensional problem with absorbing barriers at a and b , and x being the initial position of the polymer's center of mass is

$$\left(\left(1 - \frac{\epsilon}{2}\right) \partial_x \mathcal{D} \right) \partial_x T(x) + \mathcal{D} \partial_x^2 T(x) = -1, \quad (75)$$

which can be solved analytically to yield,

$$T(x) = \frac{\int_a^x \frac{dy}{\psi(y)} \int_x^b \frac{dy'}{\psi(y')} \int_a^{y'} \frac{dz \psi(z)}{\mathcal{D}(z)} - \int_x^b \frac{dy}{\psi(y)} \int_a^x \frac{dy'}{\psi(y')} \int_a^{y'} \frac{dz \psi(z)}{\mathcal{D}(z)}}{\int_a^b \frac{dy}{\psi(y)}}, \quad (76)$$

where $\psi(x)$ is the integrating factor, given by -

$$\psi(x) = \exp \left(\int_a^x dx' \frac{\left(1 - \frac{\epsilon}{2}\right) \partial_x \mathcal{D}(x')}{\mathcal{D}(x')} \right). \quad (77)$$

We are interested in calculating the MFPT for a polymer in reaching the location of maximum activity starting from the center of a box with length $L = 100$. Since we consider a periodically varying activity field $f_s(x) = 20(1 + \sin(2\pi x/L))$, we apply absorbing boundary conditions at $x = 25$ and 125 i.e $a = 25$ and $b = 125$. Setting $t_m = T(50)$, we get the required MFPT.

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