

## Supporting Information

### Active Brownian Polymers with Hydrodynamic Interactions: Conformations and Dynamics

Aitor Martín-Gómez, Thomas Eisenstecken, Gerhard Gompper, and Roland G. Winkler  
*Theoretical Soft Matter and Biophysics, Institute of Complex Systems and Institute for Advanced Simulation,  
Forschungszentrum Jülich, D-52425 Jülich, Germany*

#### S-I. INTERMOLECULAR DISTANCE

Figure S.1(a) displays the mean square distance  $a^2(s, s')$  (Eq. (27)). It increases nonlinearly with the separation  $|s - s'|$ . There is a quantitative difference between the exact expression (27) and the approximation (30), but the later captures the essence of the distance and Péclet-number dependence. The difference between the two expressions vanishes for  $Pe \rightarrow 0$  and is small for  $Pe \gg 1$ , as illustrated in Fig. S.1(b). There,  $\Delta a^2$  is the ratio of the magnitude of the difference between  $a^2$  determined via Eq. (27) and (30), respectively, divided by the expression Eq. (27). Within the applied simplified theoretical approach, the quantitative agreement between the  $a^2(s, s')$  of Eq. (27) and (30) suffices and justifies the use of Eq. (30).

#### S-II. MODE-NUMBER DEPENDENCE OF OSSEN TENSOR

The mode-number dependence of the Oseen tensor  $\Omega_{nn}$  (31), with the approximation (30) for  $a^2(s)$ , is illustrated in Fig. S.2 for various Péclet numbers and  $pL = 10^3$  and  $10^5$ . In the limit  $Pe \rightarrow 0$ , our approach is equivalent with the Zimm model for  $pL \rightarrow \infty$ , and we correspondingly find  $\Omega_{nn} \sim 1/\sqrt{n}$  [1–3]. The Oseen tensor  $\Omega_{nn}$  drops abruptly below unity above a length-dependent mode number  $n_m$ , where  $\zeta_{n_m}/p = n_m\pi/pL \lesssim 1$ . Hence, the hydrodynamic contribution  $1 + 3\pi\eta\Omega_{nn}$  becomes irrelevant for modes  $n \gtrsim n_m$  and the relaxation times are equal to those of an ABPO-HI. Activity changes the mode-number dependence of  $\Omega_{nn}$  in a non-monotonic manner, and the values of  $\Omega_{11}$  at nonzero  $Pe$  can be larger than those of the passive polymer. However, with increasing  $Pe$ ,  $\Omega_{11}$  is reduced and also  $\Omega_{nn}$  decrease more slowly with increasing  $n$  compared to the passive polymer. Together, this leads to a weaker dependence of the polymer dynamics on hydrodynamics with increasing activity. The length-dependence of  $\Omega_{nn}$  at small mode numbers is roughly given by Eq. (34). Moreover, also the Péclet-number dependence is approximately captured by Eq. (34) for  $pL = 10^5$  and  $Pe \gtrsim 10$ .

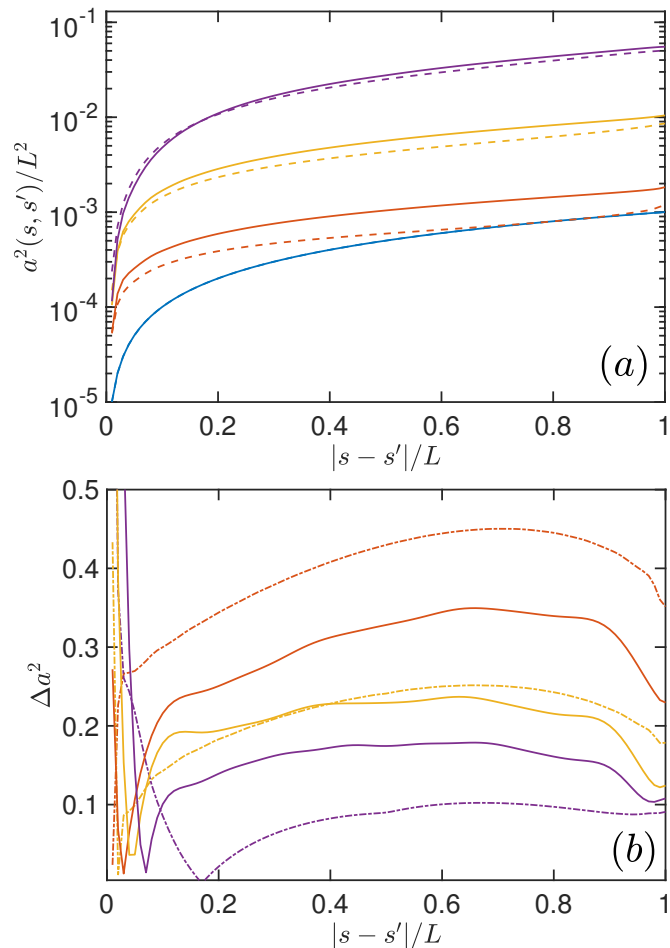


FIG. S.1: (a) Mean square distance between two points along the polymer contour as a function of their separation for  $pL = 10^2$  and the Péclet numbers  $Pe = 10^{-2}$  (blue),  $2 \times 10^1$  (orange),  $1.5 \times 10^2$  (yellow), and  $10^3$  (purple). The solid line is obtained by Eq. (27) and the dashed line by the approximation (30). In the valuation of Eq. (27),  $s' = -L/2$ . (b) Ratio  $\Delta a^2$  of the magnitude of the difference between  $a^2$  determined via Eq. (27) and (30) divided by the expression Eq. (27) for  $pL = 2 \times 10^2$  (solid) and  $pL = 5 \times 10^1$  (dashed-dotted). The colors correspond to the same Péclet numbers as in (a).

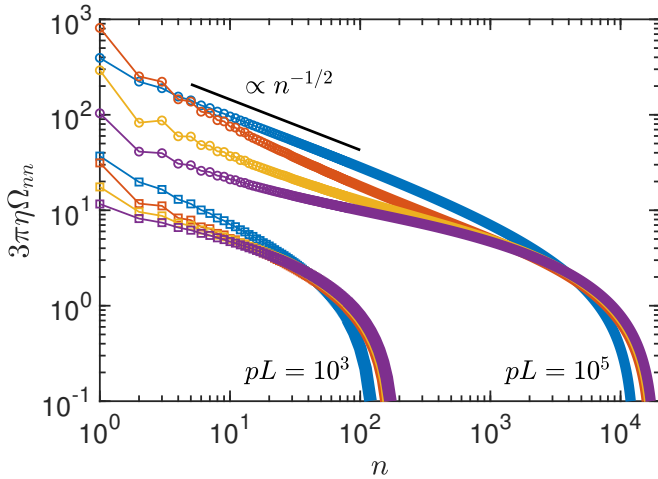


FIG. S.2: Mode-number dependence of the Oseen tensor  $\Omega_{nn}$  (Eq. (31)) for polymers of length  $pL = 10^5$  (circles) and  $pL = 10^3$  (squares) and the Péclet numbers  $Pe = 10^{-2}$  (blue),  $2 \times 10^1$  (orange),  $1.5 \times 10^2$  (yellow), and  $10^3$  (purple). The black line indicates the power law  $\Omega_{nn} \sim 1/\sqrt{n}$ .

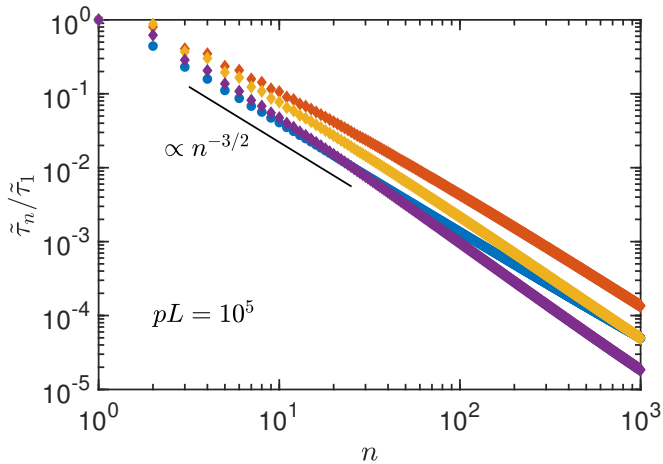


FIG. S.3: Mode-number dependence of the relaxation times  $\tilde{\tau}_n$  for a flexible polymer with  $pL = 10^5$  and the Péclet numbers  $Pe = 10^{-2}$  (blue),  $2 \times 10^1$  (orange),  $1.5 \times 10^2$  (yellow), and  $10^3$  (purple).  $\tilde{\tau}_1$  is the longest relaxation time. The black line indicates the power law  $\tilde{\tau}_n \sim n^{-3/2}$ .

### S-III. RELAXATION TIMES

Figure S.3 presents the mode-number dependence of the relaxation times  $\tilde{\tau}_n$  (36). The passive polymer exhibits the Zimm behavior  $\tilde{\tau}_n \sim n^{-3/2}$ . A similar power law is obtained for higher Péclet numbers over a more or less wide range of mode numbers. However, at higher  $Pe$ , a faster drop is obtained due to the slower decay of  $\Omega_{nn}$  with increasing mode number.

### S-IV. SOLUTION OF THE EQUATION OF MOTION FOR THE ORIENTATION VECTOR

To determine a stochastic orientation vectors  $\mathbf{e}_i$ , the following procedure is applied. An unnormalized estimation,  $\mathbf{e}'_i(t + \Delta t)$ , of the vector  $\mathbf{e}_i(t + \Delta t)$  is obtained via

$$\mathbf{e}'_i(t + \Delta t) = \mathbf{e}_i(t) + \mathbf{e}_{\theta,i}(t)\Delta\eta_{\theta,i} + \mathbf{e}_{\phi,i}(t)\Delta\eta_{\phi,i}, \quad (1)$$

where  $\mathbf{e}_i = (\cos\phi_i \sin\theta_i, \sin\phi_i \sin\theta_i, \cos\theta_i)^T$  is the propulsion direction in spherical coordinates, and  $\Delta t$  denotes the time step [4]. The unit vectors  $\mathbf{e}_{\xi,i}$  ( $\xi \in \{\phi, \theta\}$ ) follow by differentiation of  $\mathbf{e}_i$ , i.e.,  $\mathbf{e}_{\xi,i} = \partial\mathbf{e}_i/\partial\xi_i/|\partial\mathbf{e}_i/\partial\xi_i|$ . The  $\Delta\eta_{\xi,i}$  are again Gaussian and Markovian stochastic processes with the first two moments

$$\langle \Delta\eta_{\xi,i} \rangle = 0, \quad (2)$$

$$\langle \Delta\eta_{\xi,i} \Delta\eta_{\xi',j} \rangle = 2D_R \delta_{\xi\xi'} \delta_{ij} \Delta t. \quad (3)$$

Normalization of  $\mathbf{e}'_i(t + \Delta t)$  yields  $\mathbf{e}_i(t + \Delta t) = \mathbf{e}'_i(t + \Delta t)/|\mathbf{e}'_i(t + \Delta t)|$  as the new orientation vector at time  $(t + \Delta t)$ .

### S-V. MOVIE

The movie illustrates the dynamics of an active polymer in the presence of hydrodynamic interactions. The polymer length is  $N_m = 200$  and the Péclet number  $Pe = 200$ .

- [1] B. H. Zimm, J. Chem. Phys. **24**, 269 (1956).  
 [2] M. Doi and S. F. Edwards, *The Theory of Polymer Dynamics* (Clarendon Press, Oxford, 1986).  
 [3] L. Harnau, R. G. Winkler, and P. Reineker, J. Chem.

- Phys. **104**, 6355 (1996).  
 [4] R. G. Winkler, A. Wysocki, and G. Gompper, Soft Matter **11**, 6680 (2015).