Electronic Supplementary Material (ESI) for Soft Matter.

Configuration and dynamics of a self-propelled diblock copolymer chain

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I. Calculation of the angular speed

Angular speed is an important quantity characterizing the chiral motion of the ACP chain. The distributions of the angular speed (Fig. 4) and the mean values (Fig. 5 and used in eqn (4) and (5)) are obtained by simulation data. In the final Spiral(+) and Tadpole(+) states, the packed structure of the A block is *stable*. Therefore, we choose three monomer pairs with indexes (1, 5), (6, 10) and (11, 15) and they give three vectors. Every 1τ, we calculate the changes of the angles of the three vectors (they are almost the same) and obtain the "instantaneous" angular speed—a mean value over 1τ.

II. Estimation of F_{drag}

We can estimate F_{drag} by the torques on the spiral-like B block and its rotational motion. The end monomer of index 40 acts as the center of the spiral-like B block. Six monomers (index from 39 to 34) form the first layer of the spiral and twelve monomers (index from 33 to 22) form the second layer (Fig. 1(e)). The monomer of index 21 is left as the start one of the third layer. Hence, the driving torque on the spiral-like B block is roughly $\sim 6|F_a| \cdot \sigma + 12|F_a| \cdot 2\sigma + |F_a| \cdot 3\sigma = 33|F_a|\sigma$. The frictional torque due to rotation with angular speed ω is roughly $\sim 6\frac{\omega \cdot \sigma}{v_a}|F_a| \cdot \sigma + 12\frac{\omega \cdot 2\sigma}{v_a}|F_a| \cdot 2\sigma + \frac{\omega \cdot 3\sigma}{v_a}|F_a| \cdot 3\sigma = 63\frac{\omega\sigma}{v_a}|F_a|\sigma$ (the end monomer of index 40 is *approximate* as the rotational center). Here $v_a = |F_a|/\zeta$ is the drift speed of a monomer and $\omega\sigma/v_a$ is the dimensionless angular speed. Then, we have the balance relation $F_{drag} \cdot 3\sigma = \left(33 - 63\frac{\omega\sigma}{v_a}\right)|F_a|\sigma$, i.e. $F_{drag} = \left(11 - 21\frac{\omega\sigma}{v_a}\right)|F_a|$.

III. Estimation of the correlations

For the Spiral(+) state, the chirality $\bar{h}_A$ is high and the tail B block wraps tightly around the head A block as the third layer. Therefore, $\bar{\rho}_B/\sigma \approx 3$ (see the solid line in Fig. 5(a)). The spiral rotates locally. The magnitude of the mean driving torque contributed by the head A block due to propulsion is $F_a \cdot \bar{h}_A$ and that contributed by the tail B block is $\sim 17F_a \cdot 3\sigma + 2F_a \cdot 4\sigma = 59F_a\sigma$ (the last three monomers of indexes 38, 39 and 40 enter the fourth layer and there is no propulsion on the end monomer $i = 40$; see Fig. 1(a)). The magnitude of the mean frictional torque due to rotation is $\sim\zeta\bar{\omega}\overline{\sum_{i=2}^{40}\rho_i^2} \approx \zeta\bar{\omega}(6 + 12 \times 2^2 + 18 \times 3^2 + 3 \times 4^2)\sigma^2 = 264\zeta\bar{\omega}\sigma^2$. The balance requires $F_a\bar{h}_A + 59F_a\sigma = 264\zeta\bar{\omega}\sigma^2$, i.e. $\bar{\omega}\sigma/v_a \approx (\bar{h}_A/\sigma + 59)/264$ (see the solid line in Fig. 5(b)).

For the Tadpole(+) state that the chirality is *medium or high*, the whole chain rotates locally (circular trajectory with small radius) as in the Spiral(+) state (see Movie S2, ESI). But, the tail B block leaves from the very vicinity of the head A block. Due to softness of the tail and hence randomness of its configuration, the mean effect of the push on the head A block by the tail B block could be assumed negligible. The magnitude of the propelling torque on the head is $\sim F_a\bar{h}_A$, while the magnitude of the frictional torque is $\sim\zeta\bar{\omega}\overline{\sum_{i=2}^{20}\rho_i^2}$ (the monomer of index 1 is assumed close to the rotational center). The summation could be approximated by a perfect spiral packing, i.e. $\overline{\sum_{i=2}^{20}\rho_i^2} \approx (6 + 12 \times 2^2 + 1 \times 3^2)\sigma^2 = 63\sigma^2$. Torque balance gives $\bar{\omega}\sigma/v_a \approx \bar{h}_A/63\sigma$ (see dashed line in Fig. 5(b)). The tail B block sustains its motion mostly by itself as well. The magnitude of the frictional torque on the B block is $\sim\zeta\bar{\omega}\overline{\sum_{i=21}^{40}\rho_i^2} \approx 20\zeta\bar{\omega}\bar{\rho}_B^2$, while the magnitude of the propelling torque is $\sim\left|F_a\sum_{i=21}^{39}\vec{\rho}_i \times \hat{t}_i\right| \approx 19F_a\bar{\rho}_B$. Hence, the torque balance leads to $\bar{\rho}_B/\sigma = 19\,v_a/(20\bar{\omega}\sigma) \approx 60\,\sigma/\bar{h}_A$ (see dashed line in Fig. 5(a)).

IV. Supplemental figures

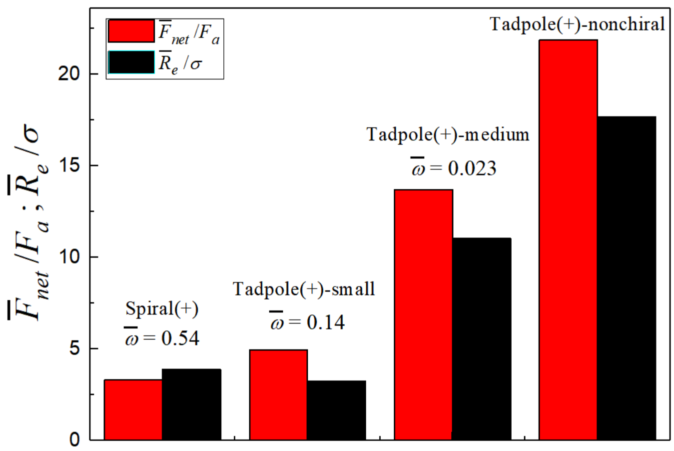

Fig. S1: Mean net propelling forces and mean angular speeds of the four example trajectories obtained by simulation data. One is in the Spiral(+) state ($F_a = 15$ and $\varepsilon = 1$) corresponding to Movie S1, ESI. The other three are in the Tadpole(+) state (under the same condition of $F_a = 5$ and $\varepsilon = 15$). They are denoted as Tadpole(+)-small (Movie S2, ESI with small trajectory radius), Tadpole(+)-medium (Movie S3, ESI with medium trajectory radius) and Tadpole(+)-nonchiral (Movie S4, ESI without chiral motion). It's clear that $\overline{F}_{net} \propto \overline{R}_e$ ($\overline{R}_e$ is the mean end-to-end distance) is not valid.

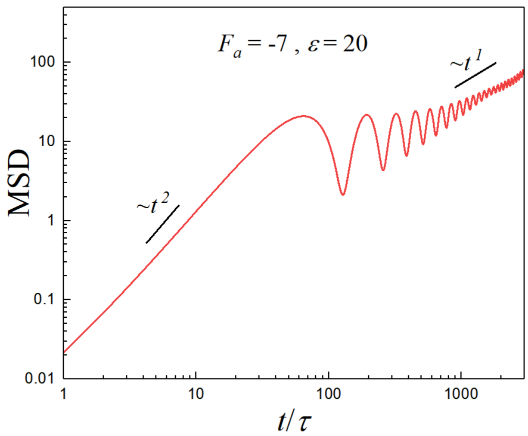

Fig. S2: Mean square displacement of an example trajectory in the Bean state ($F_a = -7$ and $\varepsilon = 20$).

V. Supplemental movies

Movie S1: Spiral(+) ($F_a = 15$ and $\varepsilon = 1$)

Movie S2: Tadpole(+)-small (small trajectory radius; $F_a = 5$ and $\varepsilon = 15$)

Movie S3: Tadpole(+)-medium (medium trajectory radius; $F_a = 5$ and $\varepsilon = 15$)

Movie S4: Tadpole(+)-nonchiral (without chiral motion; $F_a = 5$ and $\varepsilon = 15$)

Movie S5: Bean ($F_a = -5$ and $\varepsilon = 20$)

Movie S6: Tadpole(-) ($F_a = -1$ and $\varepsilon = 20$)

Movie S7: The unwrapping process showing the transition from a Bean configuration to a Spiral(-) configuration.