Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information (SI):

Structure and Dynamics of an active polymer adsorbed on the surface of a cylinder

Chen Shen, Chao-ran Qin, Tian-liang Xu, Kang Chen*, Wen-de Tian*

1. Center for Soft Condensed Matter Physics & Interdisciplinary Research, School of Physical Science and Technology, Soochow University, Suzhou 215006, China

Email: tianwende@suda.edu.cn, kangchen@suda.edu.cn

1. Supplementary Fig.S1 and Fig.S2

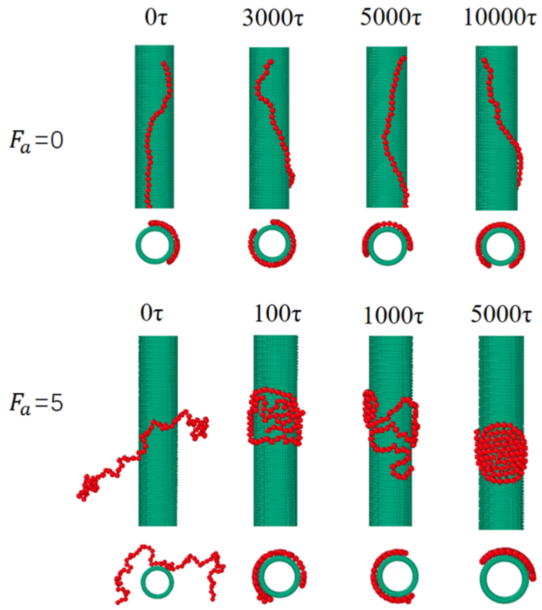

Fig.S1: Conformation evolution of a polymer adsorbed on the cylinder without active force ($f_a = 0.0$) and with active force ($f_a = 5.0$).

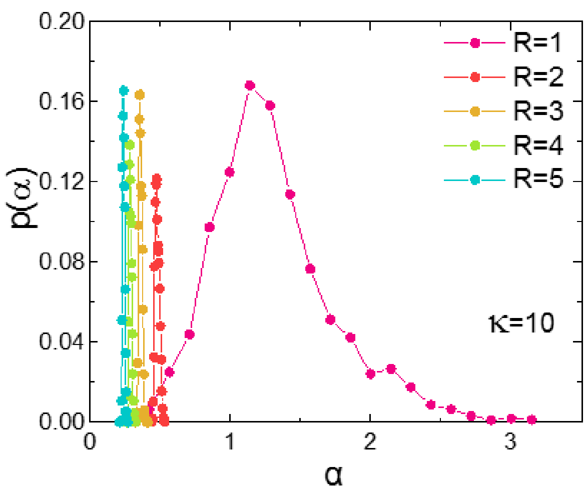

Fig.S2 Probability distribution functions of α for various Rs at $\kappa = 10$ and $f_a = 10.0$. The polymer is in the spiral state, the distribution of α is very narrow. The peaks of P(α) shift to the small α with the increase of R because the polymer is in the spiral state at R>=2, where the diameters of disk-like spirals are similar. For R=1, the distribution is broad, denoting a helix-like state of polymer.

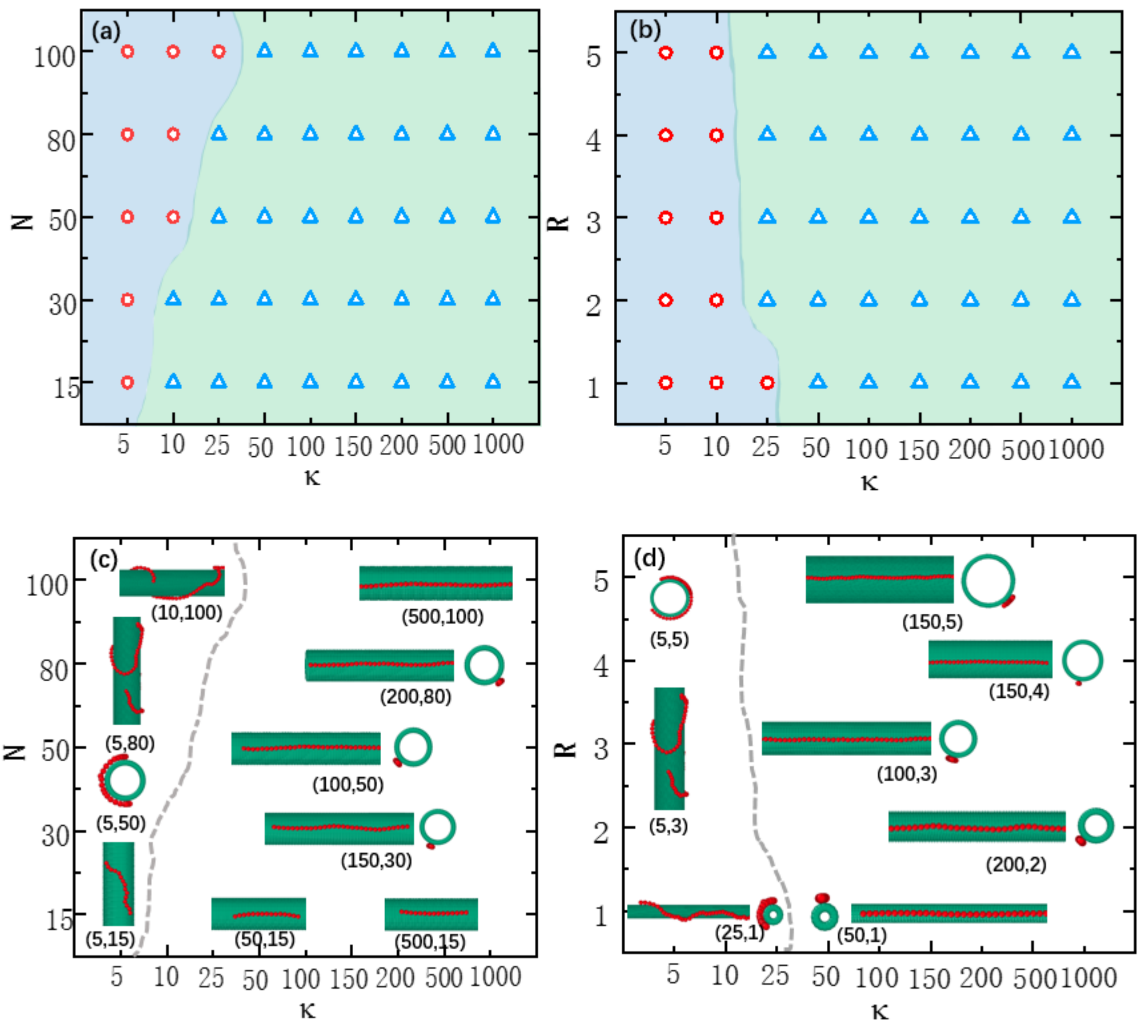

Fig. S3: Phase diagram in N-κ plane (a) and R-κ plane (b) characterizing the helix-like and straight state for polymer in an equilibrium state at N=80, $f_a = 0$. The red point (○) and blue triangle (Δ) represent the helix-like state and straight state, respectively. The typical snapshots are shown in (c) and (d). Typical snapshots are plotted corresponding to systems denoted by(κ,N) for (c) and (κ,R) for (d) . The gray-dash line is the eye-guided phase boundary.

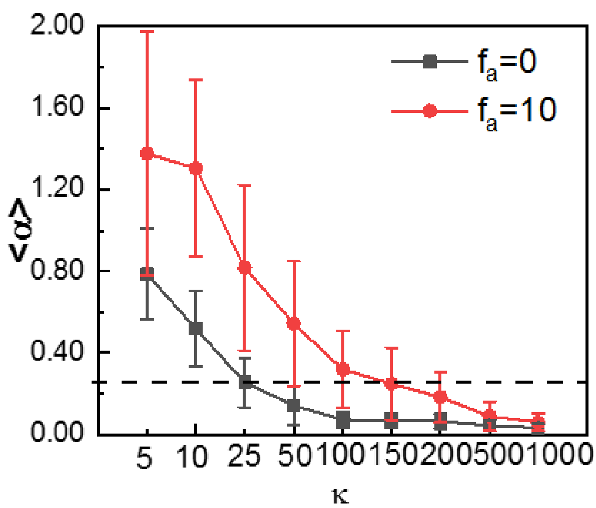

Fig.S4: The mean maximum wrapping number, $\langle\alpha\rangle$, as a function of bending rigidities κ (N=80 and R=1). The error bar is the standard deviation. The dashed line shows $\langle\alpha\rangle = \frac{1}{4}$, which is used as the criteria to distinguish the helix-like state and straight state. It can be found that, without active force, the value of $\langle\alpha\rangle$ is a little bit larger than 0.25. we assign the polymer configuration to the helix-like state based on our criteria. So, we do not pay attention to the transition of polymer configuration due to the decrease of R for the equilibrium system. Instead, we focus on the qualitative difference of phase boundary between active polymer and passive polymer in the main text.

2. The power-law relation of ω and *N* for the spiral at *R*=5.

We use Equation 4 and Fourier transform (FT) to verify the relation between the angular velocity ω and the chain length N for R=5σ. The result also shows the power-law relation $\omega \sim N^{-0.42}$(Fig.S3).

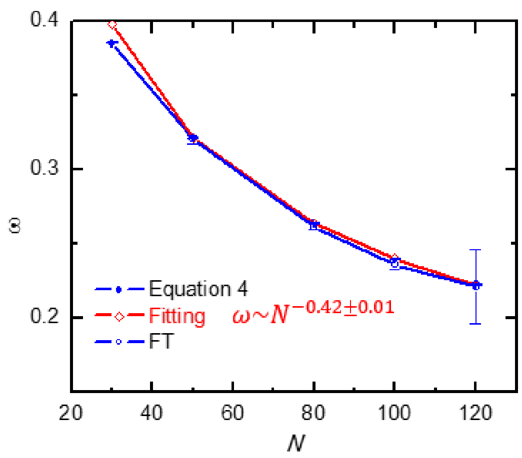

Fig.S5 Rotation speed ω as a function of chain length N at $\kappa = 5, R = 5\sigma$. The ω was calculated by Equation 4 in the main text and Fourier transform method. $\omega \sim N^{-0.42}$ is obtained.

3. Theory for a general Archimedean spiral in two dimensions.

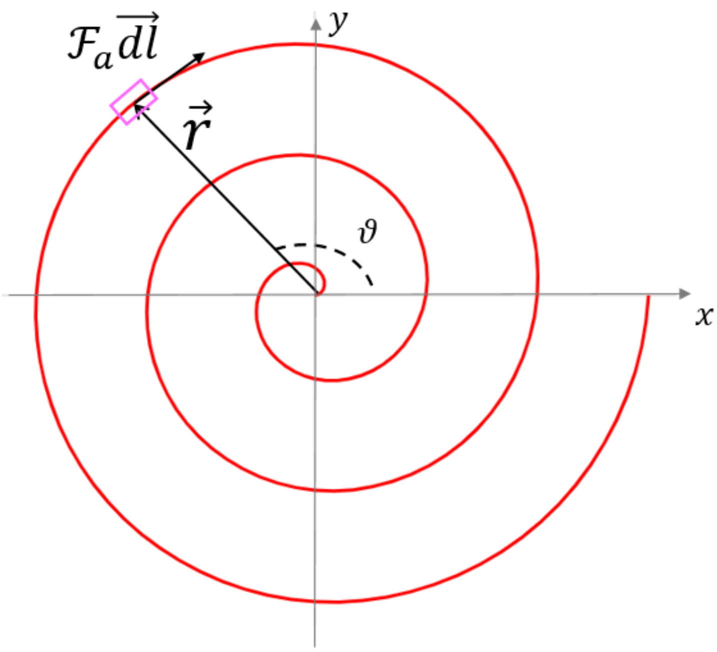

Fig.S6 Schematic diagram of a general Archimedean spiral. F_a is the linear density of active force, and $\vec{dl}$ is the infinitely small quantity of the contour at $\vec{r}$.

To understand why there exists a power-law relation between rotational angular velocity ω and chain length *N*, we assume that the chain morphology could be described by a general Archimedean spiral (Fig.S5), the polar equation of which is given as

$$\rho = c\vartheta^{\nu} \quad (1)$$

where c is a constant that controls the distance between loops, ν an exponent parameter. At $\nu = 1$, the equation is for the normal Archimedean spiral. For Fermat's spiral , $\nu = 0.5$. The coordinate vector along the contour as shown in Fig.S4:

$$\vec{r} = (x,y) = (\rho cos\vartheta,\rho sin\vartheta) \quad (2)$$

We assume the active force was exerted paralleling to the contour with linear density F_a. The viscosity coefficient of unit length is γ (Here we use the same symbol to the viscosity coefficient of a single monomer in the main text), rotational angular velocity ω. The contour length of the spiral is $L=N\sigma$ (σ=1, the length unit we used).

At the position, $\vec{r}$, the active force of unit length is

$$\vec{f}_a = F_a * \left(\frac{dx}{dl},\frac{dy}{dl}\right) = F_a \cdot \left(\frac{\nu\vartheta^{-1}cos\vartheta - sin\vartheta}{\sqrt{1+\nu^2\vartheta^{-2}}},\frac{\nu\vartheta^{-1}sin\vartheta + cos\vartheta}{\sqrt{1+\nu^2\vartheta^{-2}}}\right) \quad (3)$$

Thus the total active torque, Γ_1, is given by

$$\Gamma_1 = \int_0^L F_a * |\vec{r} \times \vec{dl}| = \int_0^{\vartheta} |\vec{r} \times \vec{f}_a| d\vartheta = \frac{c^2F_a}{2\nu+1}\vartheta^{2\nu+1} \quad (4)$$

Similarly, the drag torque, Γ_2, is

$$\Gamma_2 = \int_0^{\vartheta} |\vec{r}| * \omega|\vec{r}| * \gamma d\vartheta = \omega\gamma c^3 \int_0^{\vartheta} \sqrt{\vartheta^{6\nu} + \nu^2\vartheta^{6\nu-2}} d\vartheta$$

$$= \frac{\omega\gamma c^3\vartheta^{3\nu}}{3} * hypergeom\left(\left[-\frac{1}{2},\frac{3\nu}{2}\right],\left[\frac{3\nu}{2}+1\right],-\frac{\vartheta^2}{\nu^2}\right) \quad (5)$$

Where $hypergeom()$ is a Gaussian hypergeometric function with form:

$$hypergeom([a,b],[c],z) = \sum_{n=0}^{\infty} \frac{(a)^{(n)}(b)^{(n)}}{(c)^{(n)}} * \frac{(z)^n}{n!} \quad (6)$$

$(q)^{(n)}$ *is Pochhammer symbol*:

$$q^{(n)} = \begin{cases} 1 & if\ n = 0 \\ q(q+1)\cdots(q+n-1) & if\ n > 0 \end{cases}$$

In the stable state, $\Gamma_1 = \Gamma_2$, then we could get the angular velocity of rotation ω:

$$\omega = \frac{3F_a}{(2\nu+1)\gamma c\vartheta^{\nu-1} * hypergeom\left(\left[-\frac{1}{2},\frac{3\nu}{2}\right],\left[\frac{3\nu}{2}+1\right],-\frac{\vartheta^2}{\nu^2}\right)} \quad (7.1)$$

if we set $F_a = 10,\ \gamma = 10$ as the content, then we get

$$\omega = \frac{3}{c * (2\nu+1)\vartheta^{\nu-1} * hypergeom\left(\left[-\frac{1}{2},\frac{3\nu}{2}\right],\left[\frac{3\nu}{2}+1\right],-\frac{\vartheta^2}{\nu^2}\right)} \quad (7.2)$$

The contour length of the spiral is:

$$L = \int_0^{\vartheta} c * \sqrt{\vartheta^{2\nu} + \nu^2\vartheta^{2\nu-2}} d\vartheta = c\vartheta^{\nu} * hypergeom\left(\left[-\frac{1}{2},\frac{\nu}{2}\right],\left[\frac{\nu}{2}+1\right],-\frac{\vartheta^2}{\nu^2}\right) \quad (8)$$

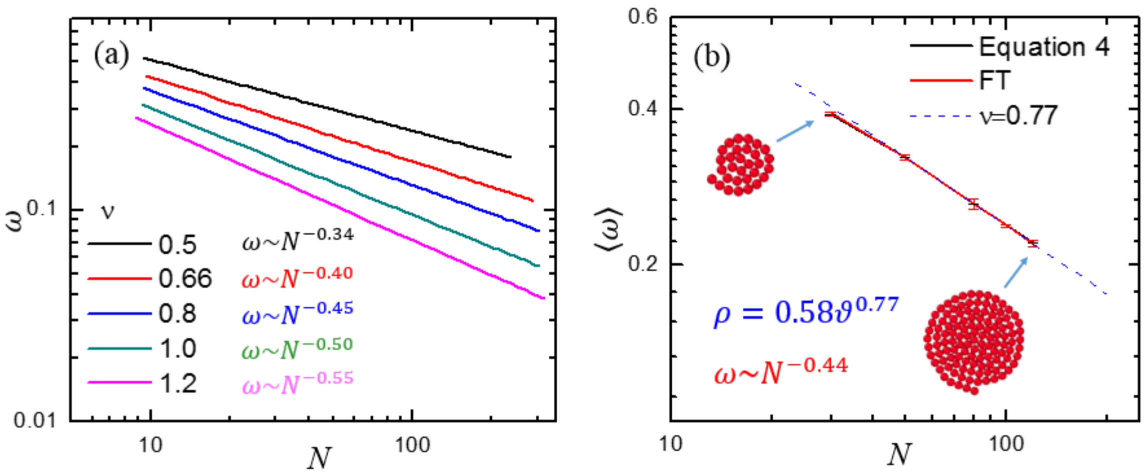

Fig.S6: (a) The power-law relation of ω and N fitted by numerical calculation of Equation 7.2 and Equation 8 at various νs with N from 10 to 300. (b) The rotation angular velocity calculated by simulations in two dimensions, $\omega \sim N^{-0.44}$, and the corresponding general Archimedean spiral, $\rho = 0.58\vartheta^{0.77}$.

It is hard to analytically calculate the hypergeometric function to get the $\omega \sim N$ power-law relation, so, we calculate the ω (Equation 7.2) and N (Equation 8) via choosing variable ϑ from 2.0 to 50.0 for various νs. Then, we obtain the power-law via linear fitting of log(N) and log(ω). The results are given in Fig.S6(a). It could be found that there indeed exists a power-law relation between N and ω at large N; the power exponent depends on the value of ν. We have tested the ν from 0.5 to 1.5, the power-law relation remains.

We perform additional simulations (namely, a polymer with various chain lengths are confined in two dimensions (2D)) to validate the theory. The simulation method is the same as that in the main content, except all simulations are in 2D. We found that $\omega \sim N^{-0.44}$ for 2D spiral and the corresponding equation is $\rho = 0.58\vartheta^{0.77}$.

4. Supplementary Movie.S1-S3

MovSI.avi shows the rotation of a polymer in the spiral state at N=80, f_d=10, κ= 1.
MovS2.avi displays the double layer of a polymer at N=80, f_d=15, κ= 1.
MovS3.avi displays the desorption of a polymer at N=80, f_d=30, κ=1 .
MovS4.avi shows the re-adsorption of a polymer at N=80, f_d=30, κ=1.
MovS5.avi gives the turning-back motion of a polymer at N=80, f_d=30, κ= 50.

5. The Simulation Method of polymer without active force

All simulations are performed by LAMMPS software. Similar to the active system. The simulation box is $80\sigma \times 80\sigma \times 100\sigma$ with periodic boundary conditions in all directions. Reduced units are used in the simulation by setting m=1, ε=1, and σ = 1. The friction coefficient, γ = 10. The difference is that we use the simulated annealing method to get the equilibrium conformation of the polymer. The temperature was decreased from $k_BT = 4.5$ to $k_BT = 1.2$ for the sufficient relaxation of the polymer. Then, each case was further run ($at\ k_BT = 1.2$) a long time of $3*10^4\tau$ with a time step, Δt = 0.001τ.