

Translocation of a Self-propelled Polymer through a Narrow Pore

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Abstract Recent studies indicate that active polymers often show curious conformational and dynamical properties. Specially, rigid polymers with self-propelled tangential forces can move directionally and even push a cargo. Motivated by this, the translocation of an active bead-spring polymer through a narrow pore is studied simulationly in this work. Each bead of the polymer is propelled by a tangential active force (f_a) along the contour of the polymer. Simulation results show that the active polymer translocates through the pore in a railway-motion manner. The translocation velocity v of the polymer is determined only by f_a , resulting that the translocation time (τ) as a function of the polymer length (N) and the active force f_a can be expressed as $\tau \propto Nf_a^{-1}$, which is independent of the rigidity of the polymer. Our results indicate that the translocation dynamics of active polymers is quite different from that of passive polymers.

Keywords Active polymer; Translocation; Dynamics; Simulation

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INTRODUCTION

The translocation of polymer chains through small pores has been a hot topic in the biology and the chemistry communities for a long time. It is not only universal in biological processes, such as transportation of biological polymers (proteins, RNA, DNA) through protein pores in biological membranes,^[1–3] but also related to many potential technological applications, such as DNA packaging, nanopore-based DNA or protein sequencing and separation,^[4–14] genome mapping,^[15] etc. Moreover, the translocation dynamics is affected by many factors, such as the temperature,^[16,17] solvent condition,^[18,19] polymer-pore interaction,^[20–24] the topology of polymer,^[25–28] etc., and then the corresponding physical mechanism is complex and has been one challenging problem in the physics community in the last two decades.

In real systems, the size of the polymer (DNA chain or protein) is much larger than that of the pore, so the translocation can only occur under the help of an external driving force (specially the electrical field force). In many studies, the dependence of the translocation time (τ) on the polymer length (N) and the strength of the driving force (f) is often concerned, because it is related to the physical nature of the translocation process. It was found that τ as a function of N and f can be described by a scaling relation, $\tau \propto N^\alpha f^\beta$. The value of β is well known to be about 1. Specifically, $\beta \sim 0.8$ for large driving force, and $\beta \sim 1$ for small driving force.^[29–31] However,

there are many arguments about the value of α . Based on the equilibrium assumption, Sung and Park^[32] and Muthukumar^[33] have theoretically predicted that $\alpha=2$ for very small driving force and $\alpha=1$ for strong driving force. Though $\alpha=1$ is in consistence with the experiment result,^[11] the translocation process is non-equilibrium in nature. Chuang *et al.* argued that the translocation time should be shorter than the Rouse equilibration time of a self-avoiding polymer.^[34] It was predicted that $\alpha = 1 + 2\nu$ for unforced translocation and $\alpha = 1 + \nu$ for forced translocation,^[34,35] with ν the Flory exponent ($\nu=0.588$ in three dimensions (3D) and $\nu=0.75$ in 2D), which have been verified by several simulation works, respectively.^[29,30,36–41] However, there is no final conclusion about α until now, because α is found to be dependent on many parameters, such as the temperature,^[17] intrapolymer interaction,^[42] the polymer-pore interaction,^[43] the rigidity of the polymer,^[44] and so on.

Recently, the driven motion of microtubules or filaments in a quasi-2D motility assay has attracted lots of attention. In that *in vitro* setup, the protein motors are fixed on the surface of the substrate and exert forces on the microtubules with which they come into contact. The microtubules then gain activity with the interaction with the protein motors.^[45,46] Theoretically and simulationly, a rigid bead-spring chain with each bead subjected to a tangential force is often adopted as an active polymer model to study the conformational and dynamical properties of microtubules or filaments driven by protein motors. In 2D space, the active polymers can spontaneously form stable spirals at strong active force and small rigidity of the polymer, and there are several distinct regimes of polymer behavior.^[47,48] In the presence of steady laminar

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flows and external force, active polymers show rich movement patterns and even move in the direction opposite to the external force.^[49] In 3D space, linear active polymers undergo a coil-globule transition with increasing the active force, and the diffusion coefficient of the polymer is independent of the polymer length for long polymers or large active force.^[50] The conformation is also dependent on the topology of the polymer. It was found that ring polymers show an inflation-collapse transition with increasing the polymer length at large active force.^[51]

In the free space, a linear active polymer with large rigidity often moves in a straight line under the driving of the self-propelled force. However, this motion is easily disturbed by spatially restricting the polymer. Several works have been done and found that the polymer shows spiral form and rotational motion when the head is fixed by a frictionless pivot, and exhibits flapping motion when the head is pinned by a clamp.^[52–56] Recent studies indicate that the rigid active polymer can even push a load or cargo attached to the head of the polymer. Depending on the strength of the tangential force, the size and the hydrodynamic friction of the load, the active polymer shows versatile buckling instabilities and different motion types, including elongated, rotating, beating and beat-and-circle motion.^[53,57,58] For active polymers adsorbed on the surface of a cylinder, three typical (spiral, helix-like, and rod-like) conformations are observed, and polymer at different conformation states shows specific (rotational, snake-like, and straight translational) motion types.^[59] For active polymers with chirality confined in a transversal asymmetric channel, the transport direction of the polymer can be rectified and even show current reversals due to the competition of the chirality of the chain and the properties of the channel.^[60]

Motivated by the interesting dynamics of the active polymer in 2D and 3D free space, we here study simulation of a bead-spring polymer through a narrow pore in 2D space. Each bead of the polymer is subjected to a tangential active force. We find that the active polymer translocates through the pore in a railway-motion manner with a constant velocity, which is quite different from the translocation of passive polymers driven by a transmembrane force.

SIMULATION MODELS AND METHODS

Simulation system is embedded in the two-dimensional (2D) space. Fig. 1 shows a sketch of the model system. The whole space is divided into two parts, the *cis* side and the *trans* side, by an infinite flat wall with thick L_p at $x=0$. The *cis* side and the *trans* side are connected by a narrow pore with height w_p in the middle of the wall. The center of the pore entrance is located at (0, 0). The active polymer chain is initially generated in the *cis* side. The wall is impenetrable for the polymer chain. So, the polymer can only translocate from the *cis* side to the *trans* side through the pore.

In our simulation, a coarse-grained bead-spring chain is adopted to model the polymer. The polymer with length N is composed of N sequentially connected monomers numbered from 1 to N . The interaction between any two monomers is described by the purely repulsive Weeks-Chandler-Andersen (WCA) potential,

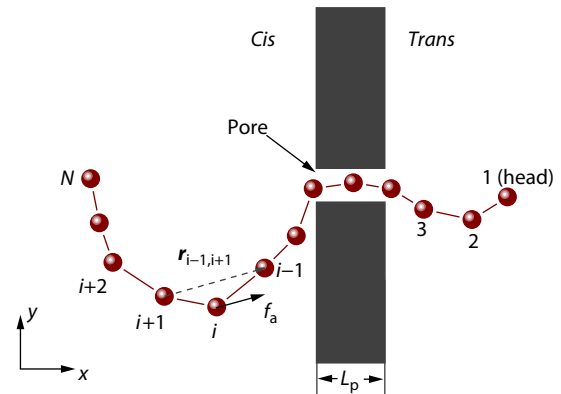


Fig. 1 A sketch of the simulation model system. The *cis* side and the *trans* side are connected by a narrow pore with length L_p and height w_p in the middle of an infinite flat wall. The active polymer is composed of N identical beads. The i^{th} monomer ($1 < i < N$) of the polymer experiences a tangential force f_a along the vector $r_{i-1,i+1}$ between the position of the monomers $i-1$ and $i+1$. The polymer chain can translocate from the *cis* side to the *trans* side through the pore under the tangential force.

$$U_L(r) = \begin{cases} 4\epsilon_0 \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] + \epsilon_0, & r \leq r_{\text{cutoff}} \\ 0, & r > r_{\text{cutoff}} \end{cases} \quad (1)$$

where r is the distance between two monomers, ϵ_0 is the interaction strength, σ is the diameter of monomers, and $r_{\text{cutoff}} = 2^{1/6}\sigma$ is the cut-off distance. Moreover, there are additional interactions between bonded monomers, which are described by the finitely extensible nonlinear elastic (FENE) potential:

$$U_{\text{FENE}}(r) = -\frac{k}{2} R_0^2 \ln \left[1 - \left(\frac{r}{R_0} \right)^2 \right] \quad (2)$$

where k is the spring constant, r and R_0 represent the bond length and the maximum bond length, respectively.

To model the rigidity of the polymer chain, the bending energy between two adjacent bonds are also considered, which is described by

$$U_{\text{bend}} = k_b (\theta - \theta_0)^2 \quad (3)$$

where θ is the angle between two neighboring bond vectors, k_b is the bending rigidity, and θ_0 is a specific angle at which $U_{\text{bend}} = 0$. In our simulation we choose $\theta_0 = 0$, i.e., U_{bend} reaches its minimum value when the two neighboring bonds are in a straight line. The rigidity of the polymer chain is determined by k_b , i.e., the polymer is more and more rigid with increasing k_b . The polymer is completely flexible at $k_b = 0$, and tends to be rod-like at infinite k_b . When k_b is finite, the polymer is semi-flexible.

To model the activity of the polymer chain, we assume the i^{th} monomer ($1 < i < N$) experiences a self-propelled tangential force,^[53,57]

$$\mathbf{F}_a^{(i)} = f_a \frac{\mathbf{r}_{i-1,i+1}}{|\mathbf{r}_{i-1,i+1}|} \quad (4)$$

where, $f_a \geq 0$ represents the strength of the active force, and $\mathbf{r}_{i-1,i+1} = \mathbf{r}_{i+1} - \mathbf{r}_{i-1}$ is the vector between the position of the monomers $i-1$ and $i+1$. The activity of the polymer is dependent on f_a , i.e., the polymer is more and more active with increasing f_a . Specially, the polymer is passive at $f_a = 0$. For the two end monomers ($i = 1$ and N), we assume $\mathbf{F}_a^{(i)} = 0$.

In our model, the surface of the wall and the pore are continuous and frictionless. Between the polymer and the boundary of the wall and the pore. There are only volume exclusive interactions, which are also described by the WCA potential (Eq. 1) with r the nearest distance between the monomer and the boundary of the wall and the pore.

The motion of each monomer is described by the Langevin equation:

$$m \frac{d\mathbf{v}}{dt} = -\nabla(U_L J + U_{\text{FENE}} + U_{\text{bend}}) + \mathbf{F}_a - \eta \mathbf{v} + \mathbf{F}^T \quad (5)$$

where m is the mass of the monomer, η is the friction coefficient, and $\mathbf{F}^T$ is the random force with $\mathbf{F}^T(t) = 0$ and $\mathbf{F}^T(t) \cdot \mathbf{F}^T(t') = 4\eta k_B T \delta(t - t')$, where k_B is the Boltzmann constant and T is the temperature. For the numerical integration of Eq. (5), the velocity Verlet algorithm is adopted with a time step $\Delta t = 0.005$.

At the beginning of the simulation, the polymer is generated in the *cis* side with the head monomer ($i=1$) being fixed in the middle of the pore at $(L_p/2, 0)$. We at first run a long time ($=10^6$) of Brownian motion with $f_a=0$ to equilibrate the polymer, and then turn on the active force and run a long steadying time t_s to let the active polymer reach the final steady-state, under the constraint that the head monomer is fixed. We finally release the head monomer and set this moment as time $t=0$, and monitor the translocation of the polymer chain under the driving of the tangential force on each monomer (except for the two end monomers). During the translocation process, the whole polymer may go back to the *cis* side under the random thermal fluctuation. In that case, we stop the simulation and begin a new run until a successful translocation occurs eventually. In this work, the time interval from the last enter of the first (the head) monomer into the *trans* side to the first enter of the last (N^{th}) monomer into the *trans* side is defined as the translocation time τ .

In this work, σ , m , and $k_B T$ are chosen as the units of length, mass, and energy, respectively. So, the time scale and the force scale are defined by $t_{LJ} = (m\sigma^2/k_B T)^{1/2}$ and $f_0 = k_B T/\sigma$, respectively. In the simulation, we fix $\varepsilon_0=1$, $k=15$, $R_0=2$, $\eta=1$, $L_p=2$. To ensure the monomer move across one by one, we choose a narrow pore with height $w_p=2.4$. Moreover, in the most case, we adopt a large steadying time $t_s=10^6$ to ensure the polymer is in the steady state before the start of the translocation. We mainly study the influence of f_a , k_b , and N on the translocation dynamics of the active polymer through the narrow pore.

RESULTS AND DISCUSSION

Effect of the Bending Rigidity on the Polymer Conformation

In our model, the polymer is semi-flexible, and the conformation of the polymer is dependent on the bending rigidity k_b . To study the effect of k_b on the polymer conformation, we have calculated the persistence length (l_p), the radius of gyration (R_g), and the bond vector correlation function $C(i)$ for polymer chain in 2D free space. The persistence length l_p is an important mechanical parameter describing the stiffness of the polymer chain, which is defined as the projection length of the end-to-end vector $\mathbf{r}_{1,N} = \mathbf{r}_N - \mathbf{r}_1$ on the first bond vector $\mathbf{r}_{1,2} = \mathbf{r}_2 - \mathbf{r}_1$,

i.e.,

$$l_p = \frac{\mathbf{r}_{1,N} \cdot \mathbf{r}_{1,2}}{|\mathbf{r}_{1,2}|} \quad (6)$$

for infinite long polymer chain.^[61] For any given k_b , l_p is independent of the polymer length N , and it is calculated based on $N=200$ in our work. The bond vector correlation function $C(i)$ is defined as:

$$C(i) = \frac{\mathbf{r}_{1,2} \cdot \mathbf{r}_{i,i+1}}{|\mathbf{r}_{1,2}| \cdot |\mathbf{r}_{i,i+1}|} \quad (1 \leq i < N) \quad (7)$$

where $\mathbf{r}_{i,i+1} = \mathbf{r}_{i+1} - \mathbf{r}_i$ represents the bond vector between monomers $i-1$ and $i+1$.

Fig. 2(a) shows the dependence of l_p and R_g on k_b for $N=200$ and $f_a=0$. We can see that l_p increases monotonously with k_b . This means that the polymer chain is stiffer and stiffer with k_b increasing, leading to the monotonous increase of R_g with k_b , as shown in Fig. 2(a). Moreover, l_p increases roughly linearly with k_b , which is the same as that of 3D model.^[44,62] Fig. 2(b) presents the dependence of the bond vector correlation function $C(i)$ on i for different k_b , where $N=200$ and $f_a=0$. When k_b is small, the polymer chain is flexible, and then $C(i)$ decreases and approaches zero quickly with i increasing, indicating that the correlation between the bond vectors is weak. While when k_b is large, the polymer chain is stiff, and $C(i)$ decreases slowly with i increasing and approaches zero at

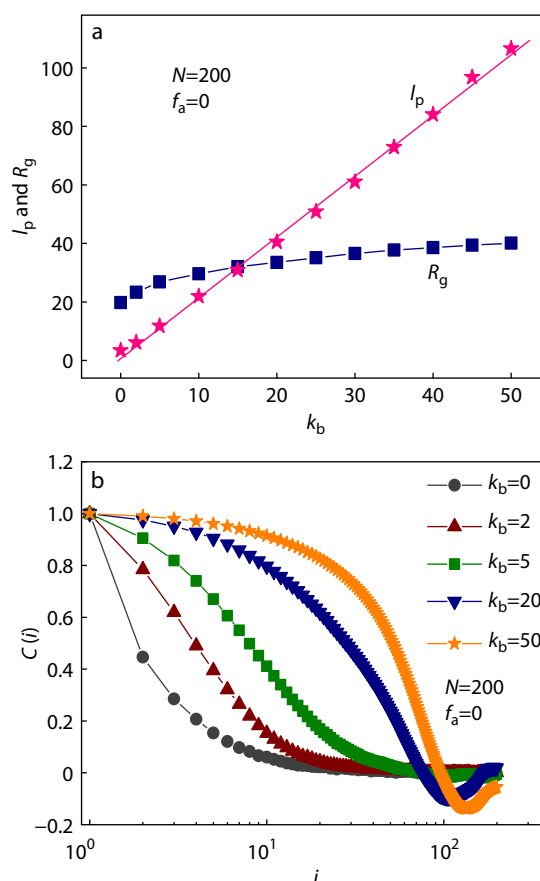


Fig. 2 (a) The dependence of the persistence length (l_p) and the radius of gyration (R_g) on the bending rigidity (k_b), where $N = 200$ and $f_a=0$. (b) The dependence of the bond vector correlation function $C(i)$ on i for different k_b , where $N=200$ and $f_a=0$.

large i , meaning that the correlation between the bond vectors is strong. Our results indicate that the conformation of the polymer chain is significantly dependent on the bending rigidity k_b .

The Flapping Motion Before the Start of the Translocation

In our simulation, the head monomer is fixed in the middle of the pore before the start of the translocation process. Correspondingly, the first bond vector connecting the head monomer and the second monomer is confined in the narrow pore and nearly keeps its direction along the axis (the x axis) of the pore, i.e., the head of the active polymer chain seems like to be clamped. It is well known that the rigid polymer with self-propelled tangential force often buckles into a periodically beating state when the head of the polymer is pinned by a clamp.^[52–55]

To check our model, we have specially studied the motion of the active polymer with the head monomer being fixed in the middle of the pore after the polymer reaches the final steady-state. Fig. 3(a) shows a typical snapshot of the polymer, where $N=120$, $k_b=40$ and $f_a=0.5$. Under the compression of the tangential active force, the polymer chain often adopts instantaneous waveform-like conformation and undergoes flapping motion, leading to the periodical oscillation of the angle (θ) between the end-to-end vector r_{ee} and the direction

of the x axis (shown in Fig. 3a). We define that $\theta>0$ when $y_N>0$ and $\theta<0$ when $y_N<0$, where y_N represents the y component of the position of the end (N^{th}) monomer. As an example, Fig. 3(b) shows the evolution of $\sin\theta$ for $N=120$, $k_b=40$ and $f_a=0.5$, where $t=0$ corresponds to the time when the head monomer is released. Clearly, the curve of $\sin\theta$ oscillates periodically with time t , from which we can obtain the period T_p and then the frequency $\omega = 1/T_p$ of the oscillation. Fig. 3(c) shows the dependence of the oscillation frequency ω on the active force f_a for different k_b , where $N=120$. We can see that ω increases monotonously with f_a increasing for any given k_b . Specifically, ω as a function of f_a and k_b can be described by a scaling relation $\omega \propto f_a^{4/3} k_b^{-1/3}$, which is in good agreement with the theoretical and the simulation results.^[52,55]

Translocation Process

We then study the translocation of polymer through the pore after the head monomer is released. Figs. 4(a) and 4(b) show the dependence of the translocation time τ on the polymer length N and the active force f_a , respectively. We can see that τ increases monotonously with N increasing or f_a decreasing. Specially, τ as a function of N and f_a can be expressed by a scaling relation $\tau \propto N^a f_a^b$ with $a=1$ and $b=1$. The value of a is much smaller than $1+\nu$ ($=1.75$ for 2D) for the forced translocation and $1+2\nu$ ($=2.5$ for 2D) for the unforced translocation of passive flexible

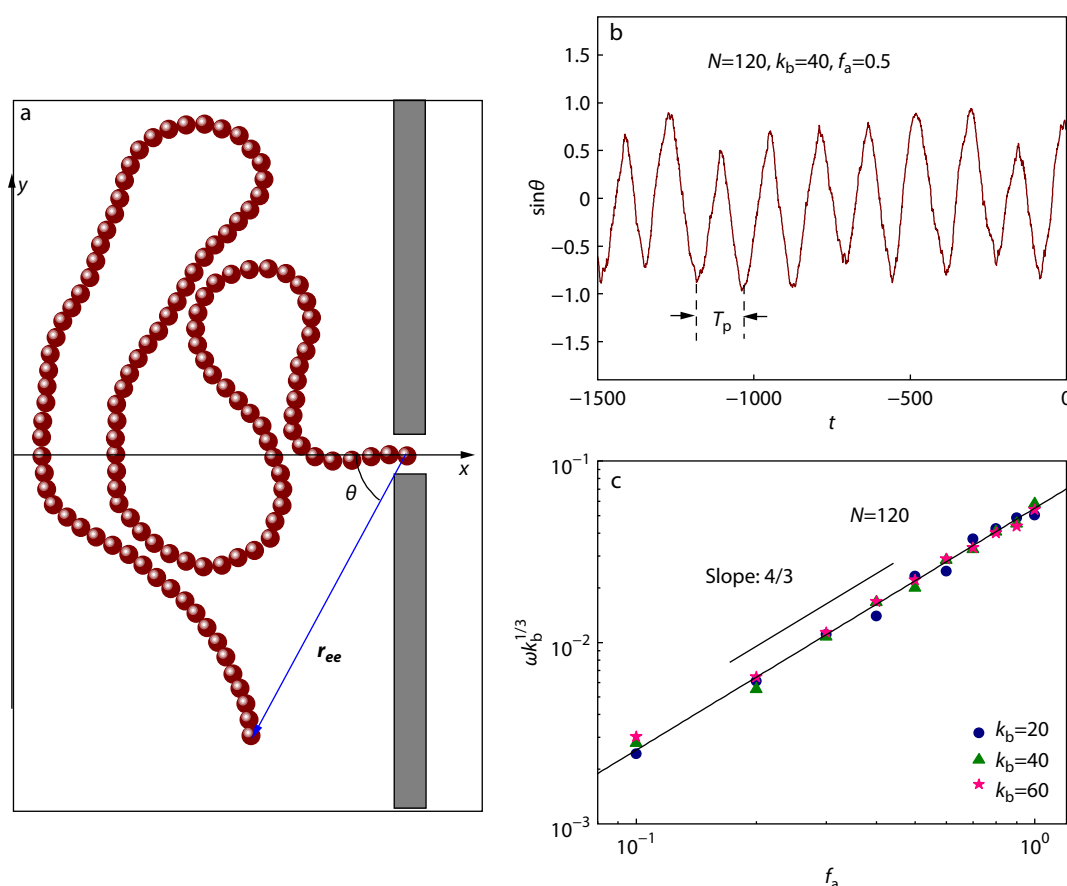


Fig. 3 (a) A snapshot of the active polymer before the start of the translocation, where $N=120$, $k_b=40$ and $f_a=0.5$. (b) The evolution of $\sin\theta$. Here θ represents the angle between the end-to-end vector r_{ee} and the direction of the x axis, as shown in (a). (c) The dependence of the oscillation frequency $\omega=1/T_p$ on f_a for different k_b , where $N=120$. Here T_p represents the oscillation period of $\sin\theta$, as shown in (b).

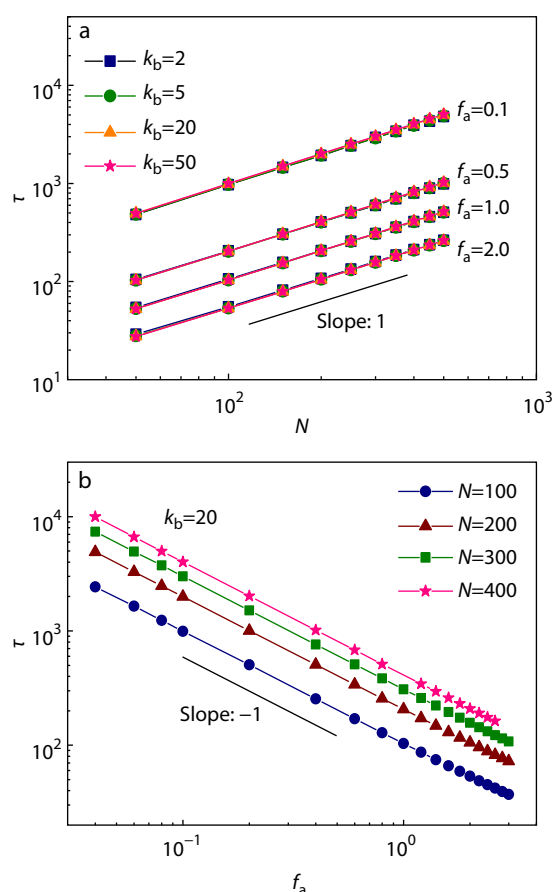


Fig. 4 (a) The dependence of the translocation time τ on N for different f_a and k_b ; (b) The dependence of the translocation time τ on f_a for different N , where $k_b = 20$.

polymers through small pores.^[34,35] Interestingly, we can also see from Fig. 4(a) that the translocation time τ is nearly independent of the rigidity of the polymer (k_b) for any given N and f_a . Wu *et al.* studied the influence of the polymer stiffness on the translocation of passive polymers through a small pore under a transmembrane force f .^[44] Their results showed that τ increases monotonously with k_b increasing. Moreover, the values of the scaling exponents α and β of τ with N and f are also dependent on k_b . Our simulation results indicate that the translocation process of rigid active polymers under self-propelled force is quite different from that of passive polymers under transmembrane force.

To understand the dependence of τ on N , f_a , and k_b , we studied the details of the translocation process. Fig. 5 shows a series of snapshots of an active polymer at different times of a successful translocation sample, where $N = 120$, $k_b = 20$, and $f_a = 0.5$. Although the overlapping section of any two sequential snapshots exhibits small deviations from each other due to the thermal noise, the whole polymer nearly moves along its counter under the driving of the tangential active force, and seems like a train moving slowly on a railway across the narrow pore, *i.e.*, the polymer shows a railway motion during the translocation process, which is quite similar to the railway motion of the active polymer in 2D free space.^[47]

The railway motion of the active polymer during the trans-

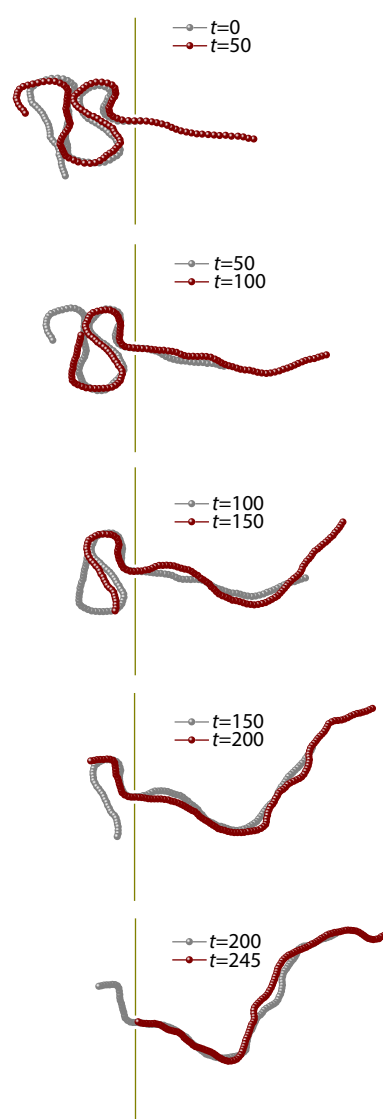


Fig. 5 A series of snapshots of an active polymer at different time of a successful translocation sample, where $N = 120$, $k_b = 20$, and $f_a = 0.5$.

location process can be verified further by the evolution of the mean square displacement (MSD) Δr^2 of monomer $j+i$ relative to the position of monomer j at $t = 0$, (x_{j0}, y_{j0}) ,^[47] as shown in Fig. 6, where $N = 120$, $k_b = 20$, $f_a = 0.5$, and $j = 24$. When t is very small, monomer $j+i$ has no enough time to move, and then Δr^2 nearly keeps a constant value determined by the average distance between monomers $j+i$ and j at $t = 0$. With t increasing, monomer $j+i$ moves along the contour of the polymer and approaches (x_{j0}, y_{j0}) , resulting that Δr^2 decreases gradually and reaches the minimum value $\Delta r_{\min}^2$ when monomer $j+i$ is the closest to (x_{j0}, y_{j0}) . With t increasing further, monomer $j+i$ leaves (x_{j0}, y_{j0}) and moves towards the pore in the wall, leading to the increase of Δr^2 . We can see from Fig. 6 that $\Delta r_{\min}^2$ is small but is not equal to zero, meaning that monomer $j+i$ does not pass through (x_{j0}, y_{j0}) perfectly during the railway motion, because of the thermal noise.^[47] $\Delta r_{\min}^2$ is dependent on i . For large i , the time for monomer $j+i$ reaching (x_{j0}, y_{j0}) is large, and then the thermal diffusion of the posi-

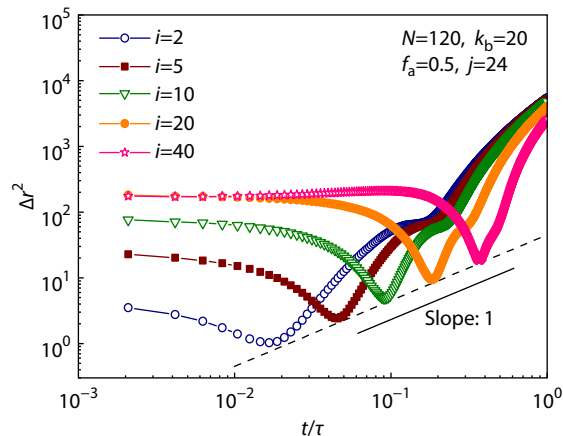


Fig. 6 The evolution of the mean square displacement (MSD) Δr^2 of bead $j+i$ relative to the position of bead j at $t=0$, where $N=120$, $k_b=20$, $f_a=0.5$, and $j=24$.

tion of monomer $j+i$ from (x_{j0}, y_{j0}) is large too when Δr^2 reaches its minimum, leading to the monotonous increase of $\Delta r_{\min}^2$ with i or t . Specifically, the dependence of $\Delta r_{\min}^2$ on t can be described by a scaling relation $\Delta r_{\min}^2 \propto t$, shown as the dashed line in Fig. 6, which is the same as that of the MSD of the thermal diffusion of a passive polymer or particle in free space.^[47]

Since the active polymer undergoes railway motion during the translocation process, the translocation dynamics will be independent of the initial configuration of the polymer before the start of the translocation. We have studied the influence of the steadying time t_s on the translocation, and found that the translocation time τ is nearly independent of t_s (results not shown). However, for the passive polymer translocation, the initial polymer configuration plays an important role in the translocation dynamics.^[17,18,44] For example, Luo *et al.* found that there is a coil-globule transition of the polymer configuration with decreasing the temperature, which results that the translocation time varies non-monotonously and reaches its minimum value near the coil-globule transition temperature.^[17]

Based on the railway motion of the active polymer, the dependence of τ on N , f_a , and k_b can be explained by the following simple dynamical model. In the over-damped limit, all the energy supplied by the tangential active force is eventually dissipated viscously by the railway motion. Assuming the translocation velocity of the polymer is v , the active energy input into the system in a small time interval dt is the product of the total active force ($\sim Nf_a$) and the small displacement (vdt), and the energy dissipated viscously is the product of the total viscous force ($N\eta v$) and the displacement (vdt). So, we have $Nf_a v dt = N\eta v v dt$, i.e.,

$$v = f_a / \eta \quad (8)$$

The translocation time can then be obtained as

$$\tau = Nb_0 / v \propto Nf_a^{-1} \quad (9)$$

where b_0 is the average bond length. This is in good agreement with our simulation results shown in Fig. 4.

For the forced translocation of passive semiflexible polymers through a small pore, it was found that the translocation

time τ increases monotonously with the polymer rigidity k_b .^[44] The underlying physics is that stiffer polymer can cause more monomers to move in step, and then lead to larger viscous drag force on the polymer. In our work, the active polymer undergoes railway motion, so all the monomers of the polymer move in step during the translocation process. Therefore, the viscous drag force exerting on the active polymer is independent of the polymer rigidity k_b , leading to the independence of τ on k_b , as shown in Fig. 4.

Intuitively, the monomer slows down when it enters the narrow pore, and then the part of polymer in the *cis* side will be compressed under the tangential active force and undergo translocation accompanied by the flapping motion. However, the pore in our model is frictionless, so it can only restrict the direction of the translocation but not affect the velocity of the monomer in it. We have calculated the total passive force f_{ti} (including the monomer-monomer interaction (Eq. 1), the bond interaction (Eq. 2), bond bend interaction (Eq. 3), and the monomer-pore interaction (Eq. 1)) exerting on the i th monomer when it is in the pore during the translocation. As an example, Fig. 7 shows the dependence of f_{ti} on i for different k_b , where $N=120$ and $f_a=0.5$. We can see that $f_{ti} \sim 0$ for all i and k_b . Moreover, we can see from the inset of Fig. 7 that $|f_{ti}/f_a| < 0.2$ for the most of i . This means that f_{ti} is much smaller than f_a , and the motion of the monomers in the pore is mainly determined by the active force. At the steady state, the active force f_a is balanced by the viscous force (ηv), and then the velocity of the monomer in pore is $v = f_a / \eta$, which is the same as that of monomer in free space. Therefore, the translocation of the whole polymer through the pore is determined by the active force and shows railway-motion manner similar to that of active polymer in 2D free space.^[47]

To get more detail information of the railway motion, we counted the number of monomers (n) in the *trans* space during the translocation process. Fig. 8 shows the dependence of n on time t for different f_a , where $N=120$ and $k_b=40$. We can see that n nearly increases linearly with t , i.e., $n = \gamma t$ with γ the slope, indicating that the polymer moves across the pore with a constant velocity. The velocity of the polymer can be

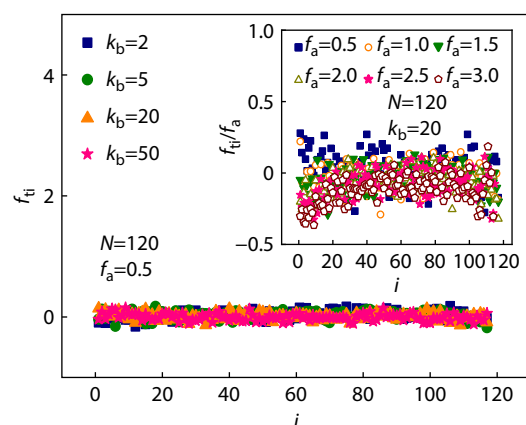


Fig. 7 The dependence of the total passive force f_{ti} (exerting on the i th monomer when it is in the pore) on i during the translocation for different k_b , where $N=120$ and $f_a=0.5$. The inset shows the dependence of the ratio f_{ti}/f_a on i for different f_a , where $N=120$ and $k_b=20$.

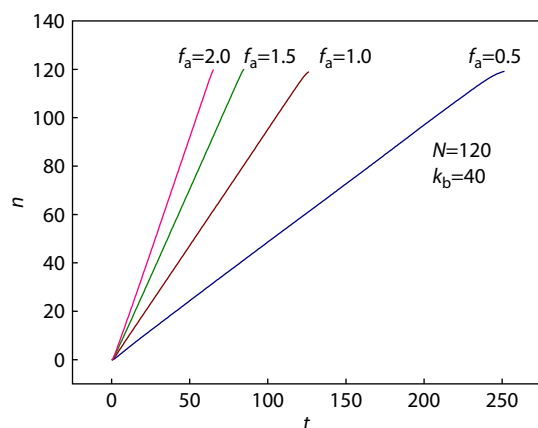


Fig. 8 The evolution of the number of monomers (n) in the *trans* space for different f_a , where $N=120$ and $k_b=40$.

defined as $v = \gamma b_0$, with b_0 (~ 1.03) the average bond length in our model. Fig. 9 presents the dependence of v on f_a for different N and k_b . Clearly, v increases monotonously with f_a increasing, but is nearly independent of N and k_b . Moreover, v as a function of f_a can be described by a simple scaling relation $v = 0.98 f_a^{0.98}$, which is in good agreement with the theoretical result Eq. (8).

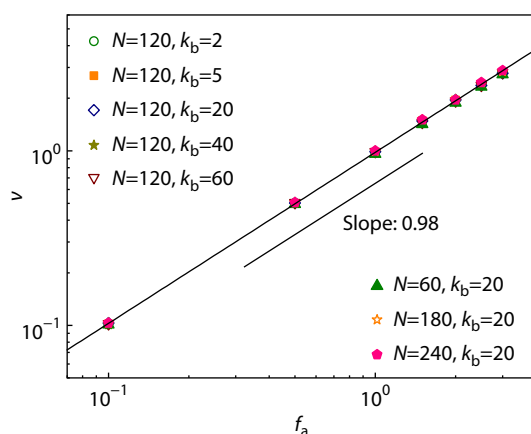


Fig. 9 The dependence of the translocation velocity v on f_a for different N and k_b .

CONCLUSIONS

The translocation of an active polymer through a narrow pore is studied by using Langevin dynamics simulation. A self-avoiding bead-spring chain is adopted to model the polymer. Each bead of the polymer is propelled by a tangential active force (f_a) along the contour of the polymer. The head monomer of the polymer is initially fixed in the middle of the pore. Before the head monomer is released, the polymer buckles into a periodically beating motion, which is the same as that of the active polymer with one end being clamped. After the head monomer is released, the polymer can translocate continuously through the pore under the driving of the self-propelled tangential force. Simulation results indicate that the translocation time (τ)

increases monotonously with the polymer length (N) increasing or the active force (f_a) decreasing, and τ as a function of N and f_a can be expressed as $\tau \propto N f_a^{-1}$, which is independent of the rigidity (k_b) of the polymer. From the evolution of the position and the configuration of the polymer, we find that the active polymer undergoes a railway motion with constant velocity during the translocation process. Based on the railway motion, the dependence of τ on N , f_a , and k_b can be understood by a simple dynamical model. Our results indicate that the translocation dynamics of active polymers are quite different from that of passive polymers.

NOTES

The authors declare no competing financial interest.

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