Polymer translocation in an environment of active rods

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We consider the dynamics of a translocation process of a flexible linear polymer through a nanopore into an environment of active rods in the trans side. Using Langevin dynamics simulations we find that the rods facilitate translocation to the trans side even when there are initially more monomers on the cis than on the trans side. Structural analysis of the translocating polymer reveals that active rods induce a folded structure to the trans-side subchain in the case of successful translocation events. By keeping the initial number of monomers on the cis-side subchain fixed, we map out a state diagram for successful events as a function of the rod number density for a variety of system parameters. This reveals competition between facilitation by the rods at low densities and crowding that hinders translocation at higher densities.

I. INTRODUCTION

Polymer translocation through a synthetic or biological nanopore has become an active field of research since the seminal experimental works by Bezrukov et al. in 1994 [1] and two years later by Kasianowicz et al. [2], and by Sung and Park [3] in 1996 on the theoretical side [4–46]. The translocation process has many applications in different areas, such as transport of mRNA through nuclear membrane pores [47], drug delivery and DNA sequencing [48–50] and gene transfer between bacteria [51]. Biological polymers often translocate through a nanopore embedded in a membrane into an environment composed of other biological organisms [52], such as diffusive or fixed spherical obstacles [53–56], chaperones [57–59] and other biomolecules or even micro-organisms.

The nature of the dynamics of polymer translocation depends on the details of the setup. There are multiple different scenarios including the pore-driven case [19, 20, 24, 26], wherein the external driving force only acts on those monomers inside the nanopore, the end-pulled case [23, 29], in which the external driving force acts on the head monomer of the polymer either by atomic force microscope [60] or by optical or magnetic tweezers [13, 61–63], and the unbiased case with no external drive [32–34]. In biological systems chaperons and other active agents can strongly influence translocation processes. To this end, pore-driven polymer translocation into an environment of active spherical particles has been studied and it has been shown numerically that the crowding effect in two dimensions increases the translocation speed provided that the particles activity is high enough [64]. Also, using the same model, the translocation time has been obtained as a function of the size of spherical active particles, and the most favorable case occurs when the size of the active particles is comparable to the segment (monomer) size of the polymer [65].

In the externally unbiased translocation process there must be an effective driving force on the chain to overcome the repulsive entropic force. Without an external drive, an imbalance may come from a net attractive entropic force due to unequal fluctuations of the spatial configurations of the polymer between the cis and the trans sides [32–34]. For example, the presence of chaperons [57], attractive binding particles [44] or active particles [66] in the trans side may lead to a directed motion of

![FIG. 1: Configuration of the system after equilibration and before the actual translocation process. N_{01} and N_{02} are the initial contour lengths of the cis- and trans-side polymer subchains, respectively. After equilibration the self-propelling (SP) force F_{sp} is switched on and acts on the head of each rod (filled red circles in the trans side) from its tail to its head. In all simulations, the initial cis-side subchain contour length is fixed at N_{01} = 100. There is one monomer at the pore and thus the total contour length of the polymer is N_0 = N_{01} + N_{02} + 1. The directions perpendicular and parallel to the membrane (green vertical line) are denoted by x and y, respectively.](image-url)
the polymer either to the cis or to the trans side depending on the values of the system parameters [44, 64, 66]. In particular, we have recently shown in Ref. [66] that active rodlike particles in the trans side can induce an effective driving force which facilitates translocation when part of the chain is initially in the trans side. Using extensive computer simulations and the iso-flux tension propagation (IFTP) theory we obtained the scaling form of the mean translocation time as a function of the initial polymer contour length in the cis side, the rod activity, and the rod length [66].

In Ref. [66] the initial contour length of the chain in the trans side was fixed to a constant value of \( N_{02} = 100 \) monomers while the other relevant parameters were varied such that translocation events were successful. An interesting question then remains concerning the role of \( N_{02} \) in determining successful translocation events. To this end, in the present work we use extensive Langevin dynamics simulations to investigate this issue. While the initial contour length of the cis-side subchain is fixed at \( N_{01} = 100 \), the contour length of the polymer subchain in the trans side \( N_{02} \) is varied together with other system parameters. This allows us to map out a “state diagram” with a boundary separating successful and failed translocation events.

A particularly interesting finding in our work is that due to their shape anisotropy the rods may align with the membrane and induce folds on the trans-side polymer subchain. This facilitates directed translocation towards the trans side for cases where \( N_{02} < N_{01} \), which would not be possible without the active rods. The state diagram also reveals that for fixed \( N_{01} \), the boundary between successful and unsuccessful events has non-monotonic dependence on the number density of the rods due to rod crowding, which will eventually hinder translocation for higher densities.

The paper is structured as follows. The Langevin dynamics (LD) simulation model is explained in detail in Sec. II. Section III is devoted to the numerical results. Finally, our summary and conclusions can be found in Sec. IV.

II. SIMULATION MODEL

We consider a two-dimensional simulation box of size \( L_x = 400\sigma \) and \( L_y = L_x/2 \) in the \( x \) and \( y \) directions, respectively (see Fig. 1). A one-dimensional dimensional composed of particles with size \( \sigma \) separated by \( \sigma \) from each other divides the simulation box in the \( y \) direction. A nanopore of radius 1.5\( \sigma \) is located at \( x = y = 0 \) in the membrane. A flexible linear polymer with a total number of monomers \( N_0 \) modeled by the bead-spring model [67] is set in the simulation box such that one of its monomers is inside the nanopore. The cis- and trans-side subchains contain \( N_{01} \) and \( N_{02} \) monomers, respectively, and \( N_0 = N_{01} + N_{02} + 1 \). In the trans side, there are \( N_r \) rigid rods, each composed of \( L_r \) beads with diameter \( \sigma \). Two walls (constructed similar to the membrane) parallel to the \( y \) direction are located at \( x = -200\sigma \) and \( x = 200\sigma \) and periodic boundary conditions are applied in the \( y \) direction.

The bonded interaction between consecutive monomers in the polymer is a combination of a finitely extensible nonlinear elastic (FENE) potential

\[
U_{\text{FENE}}(r) = -\frac{1}{2}kr_0^2 \ln(1 - r^2/R_0^2),
\]

where \( k, R_0 \), and \( r \) are the spring constant, the maximum allowed distance, and the distance between the consecutive monomers, respectively, and the Weeks-Chandler-Anderson (WCA) potential

\[
U_{\text{WCA}}(r) = \begin{cases} U_{\text{LJ}}(r) - U_{\text{LJ}}(r_c), & r < r_c; \\ 0, & r \geq r_c, \end{cases}
\]

with \( r_c = 2^{1/6}\sigma \) is the cut-off radius. The term \( U_{\text{LJ}}(r) \) is the Lennard-Jones (LJ) potential

\[
U_{\text{LJ}}(r) = 4\varepsilon \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right),
\]

with \( \varepsilon \) and \( r \) as the potential well depth and the distance between two given particles, respectively. The non-bonded monomers as well as the monomers and the wall particles, and also membrane particles and the rod beads, interact each other via the WCA excluded volume interaction.

The LD equation is employed to describe the dynamics of the position of the \( i \)th monomer of the polymer as

\[
M\ddot{r}_i = -\eta\dot{r}_i - \nabla U_{\text{mi}} + \xi_i(t),
\]

where \( \eta \) and \( U_{\text{mi}} \) are the solvent friction coefficient and the sum of all interactions for the \( i \)th monomer, respectively. \( \xi_i \) is the white noise with \( \langle \xi_i(t) \rangle = 0 \) and \( \langle \xi_i(t)\xi_j(t') \rangle = 4\eta k_BT\delta_{ij}\delta(t-t') \), where \( k_B, T, \delta_{ij} \) and \( \delta(t-t') \) are the Boltzmann constant, the temperature, the Kronecker and Dirac delta functions, respectively.

The time evolution of the \( i \)th bead of each rod is governed by the following Langevin equation:

\[
M\ddot{r}_i = -\eta\dot{r}_i + F_{\text{SP}}\delta_{ih}\hat{e} - \nabla U_{ri} + \xi_i(t),
\]

where \( F_{\text{SP}} \) and \( h \) stand for the self-propelling (SP) force and the head bead of the rod, respectively, \( \hat{e} \) is the unit vector parallel to the rod’s main axis from the tail to the head bead, and \( U_{ri} \) is the sum of all interactions on the \( i \)th bead of the rod.

\( M, \sigma \) and \( \varepsilon \) are employed as the units for mass, length, and energy, respectively. In our simulations, we use \( M = 1 \) as mass of each monomer in the polymer and bead in the rod, and set \( \sigma = 1 \) and \( \varepsilon = 1 \). The temperature is kept at \( k_BT = 1.2 \) and the solvent friction coefficient is \( \eta = 0.7 \). The integration time step is \( dt = 0.001\tau_0 \) where \( \tau_0 = \sqrt{M\sigma^2/\varepsilon} \) is the simulation time unit. The spring
constant is set to $k = 30$, and $R_0 = 1.5$. LAMMPS package [68] has been used to perform the simulations and the results have been averaged over 2000 uncorrelated trajectories.

In our model each bead size corresponds to the single-stranded DNA Kuhn length which is about 1.5 nm, and the interaction strength at room temperature $T = 295 K$ is $3.39 \times 10^{-21} J$. Thus, the timescales and force in LJ units are approximately 32.1 ps and 2.3 pN, respectively.

Before starting the actual translocation process, when the monomer inside the pore is fixed such that there are $N_{01}$ and $N_{02}$ monomers in the cis and trans sides of the simulation box, respectively, and in the absent of the SP constant is set to $N$. The trajectories.

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FIG. 2: (a) The probability of polymer translocation through a nanopore back to the cis side (open red circles) and into the trans side (open black squares) as a function of the initial value of the polymer subchain contour length in the trans side, $N_{02}$, for fixed values of $L_r = 16$, $F_{sp} = 4$ and $\rho_r = 0.04$ ($N_r = 100$). The filled green square at $N_{02,m} = 14$ represents the boundary between the to-cis and to-trans states. The horizontal blue-dashed line is plotted at 1/2. (b) A diagram showing the regions of to-cis and to-trans states in the $N_{02,m} - \rho_r$ plane for fixed values of $L_r = 16$ and $F_{sp} = 4$. The open black circles connected by the solid line denote the boundary between the two regions. The top and the bottom insets show snapshots of final configurations of the system in the vicinity of the nanopore for a fixed value of $N_{02,m} = 14$. (c) Additional diagrams in the $N_{02,m} - \rho_r$ plane separating the to-trans (above the curves) from the to-cis (below the curves) events for $L_r = 16$ and various values of $F_{sp} = 4$ (black line - circles), 8 (red line - squares), 16 (blue line - diamonds) and 32 (green line - triangles). (d) The same as in panel (c) but for fixed $F_{sp} = 32$ and different values of $L_r = 4$ (black line - circles), 8 (red line - squares), 16 (green line - triangles) and 20 (blue line - diamonds).

towards the trans side increases due to the interactions between the ARs and the trans-side polymer subchain. This increases the probability of successful events [66] leading to smaller values of $N_{02,m}$. On the other hand, for large values of the rod length $L_r$ and increasing the rod density $\rho_r$, the crowding effect due to the presence of ARs in the vicinity of nanopore in the trans side can block translocation to-trans, which leads to larger values of $N_{02,m}$. Moreover, for small values of the rod length, $N_{02,m}$ becomes a monotonically decreasing function for increasing $\rho_r$ due to negligible crowding.

B. Mean translocation time

The central quantity that reveals the dynamics of the translocation process at the global level is the mean translocation time which is the time it takes for the whole polymer to enter the trans side (translocation time for the to-trans state). On the other hand, the time it takes for the polymer to completely retract and enter the cis side will be defined as the translocation time for the to-cis state.

In the main panel of Fig. 3(a) the mean translocation time ($\tau$) for the to-trans state is plotted as a function of the rod density in the trans side $\rho_r$, for fixed $L_r = 16$ and various values of the SP force $F_{sp} = 4$ (black line - circles), 8 (red line - squares), 16 (blue line - diamonds) and 32 (green line - triangles) [cf. Fig. 2(c)]. The inset shows the same quantity as in the main panel but for the to-cis state. Panel (b) of Fig. 3 is the same as panel (a) but for fixed values of the SP force $F_{sp} = 32$ and for different values of the rod length $L_r = 4$ (black line - circles), 8 (red line - squares), 16 (green line - triangles) and 20 (blue line - diamonds). Some typical translocation time distributions are shown in the SI.

As mentioned before, the top snapshot in the inset of Fig. 2(b) clearly shows that the polymer is sucked into the active environment in the trans side if a folded structure is induced on the trans-side polymer subchain by the ARs. The main panels in Figs. 3(a) and (b), which are for the to-trans state, show interesting non-monotonic behavior of the translocation time. For small densities the effective force first increases and the mean translocation time decreases together with $N_{02}$. The fastest translocation occurs around $\rho_r \approx 0.04$ where also $N_{02,m}$ has a minimum, after which the translocation time starts to increase as crowding of the rods becomes relevant. It is interesting to note that the position of the minimum is almost independent of the activity force and the rod length in the range of parameters studied here. In the insets of panels (a) and (b) in Fig. 3 we show data for the to-cis state and the behavior of the translocation time is very similar to that of the to-trans state.

C. Waiting time distribution

An important quantity which shows the translocation dynamics at the monomer level is the waiting time (WT) distribution, that is the time that each bead spends at the nanopore during the course of translocation process. In order to present the difference between the to-cis and to-trans states, in panels (c), (d) and (e) in Fig. 3 the WT distribution $w$ has been plotted as a function of $(s - N_{02})/N_{01}$, where $s$ is the monomer index minus one, for...
FIG. 3: (a) Mean translocation time $\langle \tau \rangle$ as a function of the rod density $\rho_r$ for fixed rod length $L_r = 16$ and various values of the SP force $F_{sp}$ in the to-trans state for the values of the trans-side polymer subchain contour length on the boundaries depicted in the Fig. 2(c). Inset shows the same quantity as in the main panel for the to-cis state. (b) same as the panel (a) but for fixed value of the SP force $F_{sp} = 32$ and various values of the rod length $L_r$. Inset presents the same quantity as the main panel for the to-cis state. (c) Waiting time distribution $w$ as a function of normalized and rescaled translocation coordinate $(s - N_{02})/N_{01}$ with $N_{02} = 4$ (blue line - circles) and 14 (red line - squares) for the to-cis state. (d) The same quantity as panel (c) but for the to-trans state with $N_{02} = 4$ (blue line - circles), 14 (red line - squares) and 30 (green line - diamonds). (e) The same quantity as in panels (c) and (d) for fixed value of $N_{02} = 14$ and for the to-cis (blue line - circles) and to-trans (red line - squares) states. In panels (c), (d) and (e) the values of the rod length, SP force and number of rods in the trans side are fixed at $L_r = 16, F_{sp} = 4$ and $\rho_r = 0.04$ ($N_t = 100$), respectively, and the vertical black dashed line denotes the pore position.

FIG. 4: (a) Top and bottom panels show the monomer number density of the polymer chain for the to-trans and to-cis states, respectively, as a function of the distance from the nanopore $x$ (pore is at $x = 0$) at times $t = 0$ (top: open pink circles, bottom: open blue squares), $t = 0.5\langle \tau \rangle$ (top: open turquoise squares, bottom: open red squares) and $t = 1.0\langle \tau \rangle$ (top: open black diamonds, bottom: open green diamonds), with fixed values of $L_r = 16, \rho_r = 0.04$ ($N_t = 100$), $F_{sp} = 4$ and $N_{02} = N_{02m} = 14$ for all panels. (b) Top: Bond-orientation order parameter $\phi(x)$ for the to-trans state as a function of the distance to the pore $x$ at $t = 0$ (open pink circles), $t = 0.5\langle \tau \rangle$ (open turquoise squares) and $t = 1.0\langle \tau \rangle$ (open black diamonds). Bottom: The same as top panel but for the to-cis state. (c) Top: Bond-orientation order parameter in the trans side $\phi_t(x)$ as a function of normalized time $t/\langle \tau \rangle$, for the to-trans state with initial values of the polymer subchain contour length in the trans side $N_{02} = 4$ (open pink circles), 14 (open turquoise squares) and 30 (open black diamonds). Bottom: Order parameter on the cis side $\phi_c(x)$ as a function of normalized time $t/\langle \tau \rangle$, for the to-trans state with initial values of the polymer subchain contour length in the trans side $N_{02} = 4$ (filled pink circles), 14 (filled turquoise squares) and 30 (filled black diamonds). (d) The same as panel (c) but for the to-cis state.

fixed values of the rod length, SP force and rod density $L_r = 16, F_{sp} = 4$ and $\rho_r = 0.04$ (corresponding to $N_t = 100$), respectively.

Panel (c) in Fig. 3 shows the WT distribution ($w$) of the to-cis state for the initial trans-side polymer subchain contour lengths $N_{02} = 4$ (blue line - circles) and 14 (red line - squares). Obviously, increasing $N_{02}$ slows down the dynamics. Panel (d) is the same as (c) but for the to-trans state for $N_{02} = 4$ (blue line - circles), 14 (red line - squares) and 30 (green line - diamonds). Here, the waiting time decreases as it becomes more probable to form a larger fold for increasing $N_{02}$. Finally, panel (e) compares the WT distributions for the to-cis (blue line - circles) and to-trans (red line - squares) states when the
value of the initial trans-side polymer subchain contour length lies on the border curve in the phase diagram in Fig. 2(b) with $N_{02} = N_{02,m} = 14$ for $\rho_t = 0.04$.

D. The polymer structure

To further clarify the role of the folds in the trans side that assist translocation to-trans, we have performed a more detailed analysis of the polymer configurations during translocation. In the top panel of Fig. 4(a) we plot the monomer number density profile of the polymer chain $\rho_p$ as a function of the distance from the nanopore $x$ at different times $t = 0$ (pink circles), $0.5(\tau)$ (turquoise squares) and $1.0(\tau)$ (black diamonds) for the to-trans state. The cis and the trans sides are at $x < 0$ and $x > 0$, respectively, and the nanopore at $x = 0$. The bottom panel of (a) shows the same data for the to-cis state. The crowding of the monomers close to the pore in the trans side indicates that the polymer has folds for the to-trans state. To quantify this, we define the bond-orientation order parameter with respect to the membrane as

$$\phi(x_i) = \left\langle \frac{1}{n_i(t)} \sum_{k=1}^{n_i(t)} \left[ 1 - 2(\hat{e}_{i,k} \cdot \hat{u}_y)^2 \right] \right\rangle,$$  \hspace{1cm} (6)

where $x_i$ is the horizontal coordinate of a bin (a thin slab parallel to the wall with thickness of unity), $n_i(t)$ is the number of polymer bonds located in the $i^{th}$ bin at time $t$, $\hat{e}_{i,k}$ is the unit vector of the $k^{th}$ bond in the $i^{th}$ bin, $\hat{u}_y$ is a unit vector parallel to the membrane (y axis), and $\langle \cdots \rangle$ denotes an ensemble average. This quantity measures the average orientation of the bond vectors with respect to the wall. The value of $\phi$ varies between $[-1, +1]$ and its value is 1, -1, or 0 if the bond orientations are perpendicular, parallel, or randomly distributed with respect to the membrane, respectively.

In the top panel of Fig. 4(b) we plot the order parameter $\phi(x)$ for the to-trans state as a function of $x = x_i$, at different moments $t = 0$ (pink circles), $t = 0.5(\tau)$ (turquoise squares) and $t = 1.0(\tau)$ (black diamonds). With the passage of the time a spatially oscillating profile forms on the trans side, indicating a folded structure. In the bottom panel of (b) for the to-cis state the profile remains mostly flat.

Another useful way to quantify the configurations is to divide the order parameter into two spatially averaged components that evolve in time. They are defined as

$$\phi_t(t) = \left\langle \frac{1}{n_t(t)} \sum_{k=1}^{n_t(t)} \left[ 1 - 2(\hat{e}_k \cdot \hat{u}_y)^2 \right] \right\rangle,$$

$$\phi_c(t) = \left\langle \frac{1}{n_c(t)} \sum_{k=1}^{n_c(t)} \left[ 1 - 2(\hat{e}_k \cdot \hat{u}_y)^2 \right] \right\rangle,$$  \hspace{1cm} (7)

respectively, where $\hat{e}_k$ is the unit bond vector for the $k^{th}$ bond either in the trans side in $\phi_t(t)$, or in the cis side in $\phi_c(t)$, and $n_t(t)$ and $n_c(t)$ are the total number of bonds in the trans and in the cis sides, respectively, at time $t$.

These trans- and cis-side components are plotted in Figs. 4(c) and (d) for to-trans and to-cis states, respectively, as a function of the normalized time $t/\tau$. The negative values of $\phi_t(t)$ as time progresses indicate folds in the trans side for the to-trans state. At the same time tension propagates in the cis side as shown in more detail in the SI, making $\phi_c(t)$ positive because the bonds tend to align perpendicular to the wall. On the other hand, for the to-cis state, in the top panel of (d), the trans-side polymer subchain retracts to the cis side and $\phi_t(t)$ remains positive. Moreover, as can be seen in the bottom panel of (d), for this case the process is very slow and the cis-side subchain remains in a state close to equilibrium with $\phi_c(t) \approx 0$.

IV. SUMMARY AND CONCLUSIONS

In the present work we have quantified the role of different physical parameters for active-rod-assisted polymer translocation through a nanopore. In this setup the polymer has a fixed number of $N_{01}$ monomers on the cis side of the membrane and a varying number density of active rods (ARs) $\rho_t$ in the trans compartment. The interaction between ARs and the polymer in the trans side of the subchain with $N_{02}$ initial monomers facilitates successful to-trans events even for $N_{02} < N_{01}$, which is not possible for non-driven translocation. We map out state diagram of successful events in the $N_{02,m} - \rho_t$ plane revealing competition between facilitation and crowding by the ARs, which results in an optimal value of $\rho_t$ for a minimum value of $N_{02,m}$ and correspondingly to fastest translocation. We have further done detailed analysis of the configurations of the translocating polymers which shows that successful translocation to the to-trans state is accompanied by formation of folds in the trans side and crowding of the rods near the membrane wall. These results may shed light on better understanding polymer translocation process into or out of the living cells which typically contain various kinds of active particles.

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