Polymer translocation into an attractive channel: Iso-flux tension propagation theory and Langevin dynamics simulations

Jalal Sarabadani,1,∗ Ralf Metzler,2 and Tapio Ala-Nissila3,4
1School of Nano Science, Institute for Research in Fundamental Sciences (IPM), 19395-5531, Tehran, Iran.
2Institute for Physics & Astronomy, University of Potsdam, 14476 Potsdam, Germany
3Department of Applied Physics and QTF Center of Excellence, Aalto University, P.O. Box 11000, FI-00076 Aalto, Espoo, Finland.
4Interdisciplinary Centre for Mathematical Modelling and Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire LE11 3TU, UK.

Iso-flux tension propagation (IFTP) theory and Langevin dynamics (LD) simulations are employed to study the dynamics of channel-driven polymer translocation in which a polymer translocates into a narrow channel and the monomers in the channel experience a driving force $f_c$. In the high driving force limit, regardless of the channel width, IFTP theory predicts $\tau \propto f_c^\beta$ for the translocation time, where $\beta = -1$ is the force scaling exponent. Moreover, LD data show that for a very narrow channel fitting only a single file of monomers, the entropic force due to the subchain inside the channel does not play a significant role in the translocation dynamics, and the force exponent $\beta = -1$ regardless of the force magnitude. As the channel width increases the number of possible spatial configurations of the subchain inside the channel becomes significant, and the resulting entropic force causes the force exponent to drop below unity.

I. INTRODUCTION

Starting with the seminal experimental works of Bezrukov et al. [1] and Kasianowicz et al. [2] as well as the theoretical study of Sung and Park [3], the understanding of the physical mechanisms behind the process of polymer translocation (PT) through a nanopore has attracted considerable interest both from experimental [4–12] and theoretical [3, 13–56] groups. The process of PT has a wide variety of applications in many different areas, ranging from gene transfer between bacteria [57], RNA transport through nuclear membrane pores [58], over DNA sequencing and drug delivery [59–61] to the filtration of polyelectrolytes by entropic ratchets [19].

The translocation of a polymer can be either driven [15, 25, 34] or unbiased [18, 24, 27, 33]. There exist several scenarios for the driven case, e.g., the external driving force can be localized in the nanopore [25, 34], be due to interaction of chaferones [21, 22] or active rods with the trans side subchain [56], or can be applied on the head monomer of the polymer (the end-pulled case [47]) by a magnetic or optical tweezers [7, 9, 12, 62, 63], or even by an atomic force microscope (AFM) [64]. In the localized case in which the driving acts on the monomer(s) inside the nanopore, the driving force may alternate [26, 65–67], and the process be influenced by flickering of the nanopore [35, 45]. The dynamics of the translocation process for all of the above scenarios has been theoretically described by the iso-flux tension propagation (IFTP) theory [15, 25, 34, 45, 56]. Particularly, in Ref. [45] the IFTP approach to pore driven polymer translocation through a flickering nanopore under an alternating external driving force was studied for three different regimes of weak, moderate, and strong driving.

In the weakly driven or unbiased cases the entropic force, arising from the fact that the polymer chain can assume different configurations in space, plays an important role [3] and has a significant contribution to the translocation dynamics. The spatial configurations of the chain can be controlled either by external fields and/or by the presence of a confining geometry [68, 69]. An interesting realization occurs when the nanopore is replaced by a long nanochannel, and the polymer is attracted into the channel by an external force acting on all monomers inside the channel (the “chain sucker”) [36]. As over time more monomers migrate into the channel, the net external driving force inside the channel naturally increases. In this case, due to the external channel driving force and the confinement by the channel the trans-side subchain possesses less spatial configurations with respect to the free space case. Consequently, the entropic force depends on both the channel driving force $f_c$ and the channel diameter $D$, as we will demonstrate below.

For polymer traversing a pore of finite length $L$, the total translocation time $\tau$ comprises three separate parts and can be written as $\tau = \tau_1 + \tau_2 + \tau_3$. Here $\tau_1$, $\tau_2$, and $\tau_3$ correspond to pore filling, traversing through the pore, and pore emptying, respectively [70, 71]. In the present work we focus on the case where the pore length $L$ is much longer than the polymer length $N_0$, i.e. $L \gg N_0$ and thus the pore filling time $\tau_1$ (see Fig. 1) is identified as the translocation time. Accordingly, the channel is considered to be the trans compartment in this process [36]. By using extensive Langevin dynamics (LD) simulations and the IFTP theory [25, 34, 42, 45] we show that in the strong channel driving force limit and in the absence of the entropic force (or when the entropic force is much weaker than the driving) the scaling form for the filling time is given by $\tau \propto f_c^\beta$, where $\tau$, $f_c$ and $\beta = -1$ are the average translocation time, the force acting on each indi-

∗Electronic address: jalal@ipm.ir
vivial monomer inside the channel, and the force scaling exponent, respectively. This dependence is the same as in the short-pore driven translocation in the high force limit [15]. We also verify this result with LD simulations for a narrow channel that allows single-file translocation only. Further, we demonstrate that when the channel diameter $D$ increases, the increased chain fluctuations inside the channel can cause deviations from the narrow-pore limit and the magnitude of the exponent $\beta$ decreases.

With experimental setups similar to the scenario considered here the genomic information has been visualized by studying DNA conformations inside long confining micro or nanochannels [72–76]. We expect that comparison of such experiments with the observations reported here may lead to a further quantitative testing of the predictions of translocation theory.

The outline of the paper is as follows. We present details on the simulation methods in Sec. II and introduce the IFTP approach in Sec. III. Section IV is devoted to the results, comparing IFTP predictions with the behavior observed in the LD simulations. Finally, summary and conclusions are in Sec. V.

II. LANGEVIN DYNAMICS SIMULATIONS

The 2D system under consideration is composed of a linear, flexible self-avoiding polymer modeled by a bead-spring model [77] and a rigid membrane including a long channel as depicted in Fig. 1. The interaction between any two bonded monomers is the sum of the Weeks-Chandler-Anderson (WCA) and finitely extensible nonlinear elastic (FENE) potentials. The WCA potential is the repulsive

$$U_{\text{WCA}}(r) = \begin{cases} U_{\text{LJ}}(r) - U_{\text{LJ}}(r_c), & \text{if } r \leq r_c; \\ 0, & \text{if } r > r_c, \end{cases}$$

with the depth $\varepsilon$ of the potential well, $\sigma$ is the radius of each monomer, and the monomer-monomer distance is $r$. Nearest neighbor monomers interact via the FENE potential

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

where $R_0$ and $k$ are the maximum distance allowed between the neighboring monomers and the effective spring constant, respectively. All non-bonded interactions are given by the WCA potential. The contour length of the polymer in LJ units is $N_0 = 100$ and the channel length $L = 200$ is larger than $N_0$.

The simulation box dimensions are $L_x = 400$ and $L_y = 300$ in the $x$ and $y$ directions, respectively, with periodic boundaries in the $y$ direction. The membrane walls inside and outside of the pore are made of spatially fixed (frozen) particles located at distance $\sigma$ from each other (small green circles in Fig. 1). The interactions between monomers and frozen particles (membrane and nanochannel particles) are governed by the repulsive WCA potential. In Fig. 1(a) $D$ denotes the channel width.
that varies as \( D = 2, 3, 4.5, \) and 6 in the LD simulations. The external driving force \( f_c \) (depicted in Fig. 1(a) in blue color), acts horizontally on each individual monomer inside the channel and assumes the values \( f_c = 0.2, 0.3, 0.5, \) and 1.2 (in LJ units). The resulting dynamical equation for the position vector \( r_i \) of monomer \( i \) then reads

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

where \( M \) is the monomer mass, \( \eta \) the solvent friction coefficient, and \( U_i \) is the sum of all interactions of the \( i \)th monomer. Here, \( \xi_i \) represents thermal white noise with zero mean \( \langle \xi_i(t) \rangle = 0 \) and correlation \( \langle \xi_i(t) \xi_j(t') \rangle = 2\eta k_B T \delta_{ij} \delta(t - t') \), to be understood component-wise, where \( k_B \) and \( T \) are the Boltzmann constant and temperature, respectively, \( \delta_{ij} \) is the Kronecker, and \( \delta(t - t') \) the Dirac delta function. Moreover, \( \sigma, M, \) and \( \varepsilon \) are used as the units of length, mass, and energy, respectively. The diameter of the monomers is \( \sigma = 1 \), and this also determines the size of each channel or membrane particle.

The mass of each monomer and other particles in the system is given by \( M = 1 \). We choose \( \varepsilon = 1, \eta = 0.7, \) and \( k_B T = 1.2 \). The time unit for the simulations is defined as \( \tau_0 = \sqrt{M \sigma^2 / \varepsilon} \). The maximum allowed distance between two bonded monomers is \( R_0 = 1.5, \) and \( k = 30 \) is the spring constant.

All LD simulations were performed by using the LAMMPS [78] package. In our model the size of each bead is about 1.5 nm in real units which corresponds approximately to the Kuhn length of a single-stranded DNA, the mass of each bead is about 936 amu, and the strength of interaction is \( 3.39 \times 10^{-21} \) J at \( T = 295 \) K (room temperature). Therefore, the force and time scales in LJ units are approximately 2.3 pN and 32.1 ps, respectively.

Within IFTP theory below we use dimensionless quantities, denoted by the tilde, as \( \tilde{Y} \equiv Y / Y_u \). Here the denominator indicates the units of time, length, monomer flux, velocity, force, and friction as \( t_u \equiv \eta \sigma^2 / (k_B T) \), \( s_u \equiv \sigma, \phi_u \equiv k_B T / (\eta \sigma^2), v_u \equiv \sigma / t_u \equiv k_B T / (\eta \sigma^2), f_u \equiv k_B T / \sigma, \) and \( \Gamma_u \equiv \eta \), respectively. The parameters without the tilde symbol are expressed in LJ units.

Before the actual translocation process, the head monomer of the polymer chain is fixed in the center of the entrance of the channel (pore) and the polymer is equilibrated. Then the fixed head monomer is released, and at the same time the external channel driving force \( f_c \) is switched on. To obtain sufficient statistics, averaging is performed over 1000 uncorrelated trajectories. Panel (a) in Fig. 1 shows a typical equilibrium state of the polymer chain (from LD simulations) just before starting the translocation process. Panels (b) and (c) correspond to the tension propagation (TP) and post propagation (PP) stages, respectively. Finally, panel (d) presents the configuration of the channel inside the nanopore at the termination of the translocation process which equals the filling time \( \tau_1 = \tau \) here. In the TP stage presented in panel (b) \( t < t_{TP} \), as the channel translocates into the channel by the external channel driving force \( f_c \) acting on each individual monomer inside the nanopore, tension propagates along the backbone of the subchain on the cis side. The snapshot, at time \( t \), in panel (b) shows that \( s \) monomers (in blue color) have translocated into the channel, while \( l \) monomers (in red color) on the cis side have been influenced by the tension force and are moving towards the channel, i.e., \( N = s + l \) is the number of all monomers that have been influenced by the tension force up to time \( t \). The remaining \( N_0 - N \) monomers are at equilibrium and have zero net velocity (monomers in black color). In the TP stage, as the tension force has not reached the chain end, we thus have \( N = s + l < N_0 \).

The picture above shows that the subchain on the cis side can be divided into two parts, a mobile part (in red color) and an equilibrium part (in black color). The location of the tension front, that is the border between the mobile and equilibrium parts, is specified by \( R \). The gray monomers represent the configuration of the polymer at time zero, for comparison of the polymer configurations at times \( t \) and zero. The snapshot of the system (from LD simulation) is shown in panel (c) for \( t > t_{TP} \). At time \( t_{TP} \), the tension propagation time, the tension reaches the chain end on the cis side, and by that time all monomers of the chain have already been influenced by the tension force, i.e. \( N = l + s = N_0 \). Finally, panel (d) illustrates the configuration of the chain just at the termination of the translocation process, when the entire polymer chain has been translocated inside the trans-side nanochannel.

III. ISO-FLUX TENSION PROPAGATION THEORY

The quantitatively accurate IFTP theory can be employed to describe the dynamics of the translocation process for the channel-driven case. To this end we generalize the IFTP theory by considering the effective force acting on the monomer(s) located just at the entrance of the channel. The dynamics of the translocation process can be unraveled by solving the equation of motion for the time evolution of the translocation coordinate \( \tilde{s} \) within the iso-flux (IF) approximation for the monomer flux \( \tilde{\phi} = d\tilde{s}/d\tilde{t} \). In the IF approximation the monomer flux in the mobile part of chain (cis side, red monomers in panels (b) and (c) in Fig. 1) is spatially constant but evolves in time.

To obtain the equation of motion for \( \tilde{s} \), the tension force \( \tilde{F}(\tilde{x}, \tilde{t}) \) at the distance \( \tilde{x} \) from the channel entrance on the cis side is needed. Integrating the local force-balance equation \( d\tilde{F}(\tilde{x}', \tilde{t}) = -\tilde{\phi}(\tilde{t})d\tilde{x}' \) over the distance from the channel entrance at \( \tilde{x}' = 0 \) to the distance \( \tilde{x}' = \tilde{x} \) from the channel entrance, the tension force at distance \( \tilde{x} \) on the cis side is written as \( \tilde{F}(\tilde{x}, \tilde{t}) = \tilde{F}_0 - \tilde{x}\tilde{\phi}(\tilde{t}) \), where \( \tilde{F}_0 = \int \tilde{f}(\tilde{t}) \).
the discussion below and the schematic in Fig. 2). Using the fact that the tension force vanishes at the tension front, i.e., \( \mathbf{F}(\hat{x} = \hat{R}, \hat{t}) = 0 \), the tension force just at the entrance of channel is related to \( \hat{R} \) via \( \mathbf{F}_0 = \hat{R}(\hat{t}) \hat{\phi}(\hat{t}) \).

Combining this with the definition of the monomer flux, the equation of motion for the translocation coordinates \( \hat{s} \) is obtained as

\[
\left[ \hat{R}(\hat{t}) + \tilde{\eta} \right] \frac{d\hat{s}}{d\hat{t}} = \hat{f}(\hat{t}). \tag{5}
\]

The expression in the brackets is the effective friction and is the sum of friction due to the cis-side mobile subchain \( \hat{R}(\hat{t}) \) and the channel friction \( \tilde{\eta} \). To solve the above equation, the time evolution of \( \hat{f}(\hat{t}) \) and \( \hat{R}(\hat{t}) \) must be known.

We first explain how \( \hat{f}(\hat{t}) \) can be obtained numerically and then the equation of motion for the time evolution of \( \hat{R}(\hat{t}) \) can be extracted within the IF approximation.

We performed extensive LD simulations to obtain the effective driving force \( f(\hat{t}) \), which is the force experienced by the monomer inside the channel entrance (i.e., the \( x \) component of its position is in the region \(-0.5 < x < 0.5\)). The channel driving force \( f_c \), the force \( f_{LJ} \) due to the other monomers inside the channel in the region of \( x > 0.5 \), and the interaction between the channel walls particles and the monomer(s) inside the entrance of the channel contribute to the total effective driving force \( f(\hat{t}) \). The contribution of \( f_{LJ} \) to the driving is the combination of the FENE-bond force and non-bonded repulsive Lennard-Jones (WCA).

Panel (a) in Fig. 2 presents the normalized effective force \( f(\hat{t})/f_c \) as a function of normalized time \( t/\tau \), for fixed channel driving force \( f_c = 1.2 \), evaluated for the channel widths \( D = 2.0 \) (orange filled triangles), 3.0 (green filled diamonds), 4.5 (red filled squares), and 6.0 (black filled circles). Turquoise solid and dashed lines are fitting curves to the normalized forces in the TP and PP stages, respectively (see text). Panels (b), (c), and (d) are the same as panel (a), but for \( f_c = 0.5, 0.3 \) and 0.2, respectively.

![FIG. 2](image-url)

**FIG. 2:** (a) Normalized effective force \( f(\hat{t})/f_c \) as function of normalized time \( t/\tau \), for fixed channel driving force \( f_c = 1.2 \), evaluated for the channel widths \( D = 2.0 \) (orange filled triangles), 3.0 (green filled diamonds), 4.5 (red filled squares), and 6.0 (black filled circles). Turquoise solid and dashed lines are fitting curves to the normalized forces in the TP and PP stages, respectively (see text). Panels (b), (c), and (d) are the same as panel (a), but for \( f_c = 0.5, 0.3 \) and 0.2, respectively.

The number of those monomers that at equilibrium (at time zero) are located between the entrance of the channel and the tension front (at time \( t \)) is, on average, the same as the number of monomers influenced by the tension force by the time \( t \), i.e., \( N = \tilde{s} + \hat{l} \), the sum of the monomers in blue color inside the channel and the mobile monomers in red color in the cis side at time \( t \). Then in equilibrium the size of the subchain that occupies the region between the entrance of the channel and the tension front is \( \hat{R} \).

Therefore, according to Flory theory one can write the end-to-end distance devoted to this portion of the polymer chain as \( \hat{R} = A_nN^\alpha \). Combining this end-to-end distance with the fact that \( N = \tilde{s} + \hat{l} \), and after taking

\[
\hat{f}(\hat{t})/f_c = a + b\hat{t}/\tau, \tag{6}
\]

\[
\hat{f}_{PP}(\hat{t})/f_c = c - d\hat{t}/\tau, \tag{6}
\]

respectively. For strong channel driving force \( f_c = 1.2 \) in panel (a), the values of the constants are \( a = 1.61, b = 29.46, c = 52.74 \) and \( d = 41.07 \), and for weaker channel driving forces the values of \( a, b, c \) and \( d \) can be found in the corresponding panels. At the tension propagation time \( t_{TP} \), the values of the effective forces in the TP and PP stages should be equal (continuity condition), i.e.

\[
\hat{f}(\hat{t})/f_c = a + b\hat{t}/\tau, \tag{6}
\]

\[
\hat{f}_{PP}(\hat{t})/f_c = c - d\hat{t}/\tau, \tag{6}
\]

By combining this equation with the equation (5), provided that the time evolution of the tension force \( f(\hat{t}) \) and \( \hat{R}(\hat{t}) \) must be known. We first explain how \( \hat{f}(\hat{t}) \) can be obtained numerically and then the equation of motion for the time evolution of \( \hat{R}(\hat{t}) \) can be extracted within the IF approximation.

The number of those monomers that at equilibrium (at time zero) are located between the entrance of the channel and the tension front (at time \( t \)) is, on average, the same as the number of monomers influenced by the tension force by the time \( t \), i.e., \( N = \tilde{s} + \hat{l} \), the sum of the monomers in blue color inside the channel and the mobile monomers in red color in the cis side at time \( t \). Then in equilibrium the size of the subchain that occupies the region between the entrance of the channel and the tension front is \( \hat{R} \).

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\hat{f}_{PP}(\hat{t})/f_c = c - d\hat{t}/\tau, \tag{6}
\]
FIG. 3: (a) Normalized waiting time $w/\tau$ as function of the translocation coordinate $s$, for fixed value $f_c=1.2$ of the channel driving force and the channel widths $D=2.0$ (orange triangles), 3.0 (green diamonds), 4.5 (red squares), and 6.0 (black circles). Solid orange, green dashed, red dashed-dotted, and black dashed-dotted-dotted lines represent the IFTP results in the strong stretching regime for channel widths $D=2.0$, 3.0, 4.5 and 6.0, respectively (not shown in the legend). Panels (b), (c), and (d) are the same as panel (a), but for $f_c=0.5$, 0.3, and 0.2, respectively. Panels (e), (f), (g) and (h) are the same as (a), (b), (c), and (d), respectively, but present the unnormalized waiting time distribution $w$ as a function of $s$. The values of the channel friction coefficients in the IFTP theory have been chosen as $\eta_c = 4.3, 3.0, 2.5$ and 2.3 corresponding to different channel widths $D = 2.3, 4.5$ and 6, respectively [39].

the time derivative of both sides of $\tilde{R} = A_c\phi(s + \tilde{l})^v$ in the strong stretching (SS) regime where the mobile subchain on the cis side is fully straightened ($\tilde{l} = \tilde{R}$), the equation of motion for the tension front location in the TP stage is obtained as

$$\dot{\tilde{R}}(\tilde{l}) = \frac{\nu A_c^{1/v} \tilde{R}(\tilde{l})^{(\nu-1)/v} \phi(\tilde{l})}{1 - \nu A_c^{1/v} \tilde{R}(\tilde{l})^{(\nu-1)/v}}$$

where the definition $\tilde{\phi} = d\tilde{s}/d\tilde{l}$ of the monomer flux has been used. Conversely, in the PP stage, in which the tension has reached the chain end on the cis side, the closure relation is $N = \tilde{s} + \tilde{l} = N_0$. Performing the time derivative on both sides of this closure relation in the SS regime, in which $\tilde{l} = \tilde{R}$, yields the equation of motion for the tension front,

$$\dot{\tilde{R}}(\tilde{l}) = -\tilde{\phi}(\tilde{l}).$$

To have a full solution, in the TP stage Eqs. (5) and (7) need to be solved self-consistently, while the PP stage is based on Eqs. (5) and (8).

A. Waiting time distribution

One of the most important quantities that reveals the dynamics of the translocation process at the monomer level is the distribution $w$ of waiting times (WT), the time that each bead spends at the entrance of the nanochannel (specifically when the $x$ component of the position vector of the corresponding bead is in the region $-0.5 \leq x \leq +0.5$) during the translocation process. Figure 3(a) shows the normalized WT distribution $w/\tau$ as function of the translocation coordinate $s$, for fixed value $f_c=1.2$ of the driving force and the channel widths $D=2.0$ (orange triangles), 3.0 (green diamonds), 4.5 (red squares), and 6.0 (black circles). Solid orange, green dashed, red dashed-dotted and black dashed-dotted-dotted lines represent the IFTP results in the SS regime for channel widths $D=2.0$, 3.0, 4.5 and 6.0, respectively (not shown in the legend). Panels (b), (c) and (d) are the same as panel (a), but for $f_c=0.5$, 0.3 and 0.2, respectively. The values of the channel friction coefficients that have been used in the IFTP theory are $\eta_c = 4.3, 3.0, 2.5$ and 2.3 corresponding to different channel widths $D = 2.3, 4.5$ and 6, respectively [39].

We can conclude from the data that the results of the IFTP theory increasingly deviate from the LD data as the value of the driving force decreases. This happens due to the fact that here we only consider the SS regime (the mobile subchain in the cis side is fully straightened) in IFTP theory in the absence of the entropic force. This discrepancy can be resolved in the weak and intermediate force regimes by taking the entropic force into account. There the spatial shape of the mobile subchain on the cis side assume the so-called trumpet (TR) and stem-flower (SF) shapes [34, 42], respectively. However, this

IV. RESULTS

This section is devoted to the presentation of the results from the IFTP theory and LD simulations for the translocation dynamics both at the monomer and global levels. To this end the waiting time distribution, translocation time, monomer mean-square displacement (MSD), and the monomer density are investigated.
is beyond the scope of the current study. However, the global dynamics of the translocation process is well explained by the IFTP theory in the high force limit (here, \( f_c = 1.2 \)) by the SS regime.

In panels (e), (f), (g) and (h) of Fig. 3, which correspond to panels (a), (b), (c) and (d), respectively, the unnormalized WT distribution \( w \) is shown as function of \( s \). As seen in panel (e), regardless of the channel width, for the highest value \( f_c = 1.2 \) of the driving force WT monotonically decreases as \( s \) increases. For smaller values of the driving force, \( f_c \leq 0.5 \) the WT curve is no longer monotonic, and a hump appears for small \( s \). This effect is more pronounced either by decreasing the value of the driving force, from panel (f) to panel (h), or at constant driving force, i.e. in each panel of (f), (g), and (h), by decreasing the channel width from \( D = 6 \) to \( D = 2 \).

The reason for the monotonicity of the WT curve in panel (e) is that for strong driving with \( f_c = 1.2 \), at the beginning of the translocation process the tension propagates very fast and the subchain in the vicinity of the channel entrance resists the driving force. This leads to the large value of the WT at the beginning of the process. At later moments, when more monomers traverse the channel entrance the total net force acting on the trans-side subchain increases, and the value of the WT decreases. Therefore, for strong driving the WT monotonically decreases. On the other hand for weaker driving force in panels (f) to (h), at the very beginning of the translocation process the entropic force due to spatial fluctuations of the cis-side chain configurations that resists translocation, is more pronounced for the wide channels, leading to the larger WT for the channel with \( D = 6 \) and smaller values for \( D = 2 \) (star symbols in panel (h)). Then with time more monomers experience the friction due to the mobile part of the cis-side subchain, while the driving is not strong and \( s \) does not increase fast enough. Consequently, the WT increases at the starting moments of the translocation process. At the later time as enough monomers have already traversed the channel entrance, the net effective driving force becomes large enough to accelerate the translocation process and therefore the WT decreases. At constant driving force, the non-monotonicity in the WT curves is more pronounced with decreasing channel width. This is due to the fact that decreasing channel width increases the effective channel friction making the translocation dynamics slower and thus the hump in the WT curve is more pronounced.

### B. Scaling of translocation time

The fundamental quantity that reveals the global dynamics of the translocation process is the translocation time \( \tau \), which is the average time for the whole chain to enter the channel and fully translocate to the trans-side channel of the system. In Fig. 4 we show the translocation times \( \tau \) from LD simulations. In panel (a) \( \tau \) is shown as a function of the driving force \( f_c \) for the channel diameters \( D = 2 \) (orange triangles), 3 (green diamonds), 4.5 (red squares) and 6 (black circles). The orange dashed and black dashed-dotted lines are fits to the data with \( D = 2 \) and 6, respectively, but shifted for better visibility. The inset shows the scaling exponent \( \beta \) of the scaling form \( \tau \propto f_c^\beta \) as function of the channel width \( D \). Panel (b) shows \( \tau \) as a function of \( D \), for \( f_c = 0.2 \) (orange triangles), 0.3 (green diamonds), 0.5 (red squares) and 1.2 (black circles). The inset shows the normalized translocation time \( \tau / \tau(D = 2) \) as function of \( D \).

![FIG. 4: (a) Translocation time \( \tau \) as function of the channel driving force \( f_c \), for channel widths \( D = 2 \) (orange triangles), 3 (green diamonds), 4.5 (red squares) and 6 (black circles). The orange dashed and black dashed-dotted lines are fits to the data with \( D = 2 \) and 6, respectively, but shifted for better visibility. The inset shows the force exponent \( \beta \) of the scaling form \( \tau \propto f_c^\beta \) as function of the channel width \( D \). Panel (b) shows \( \tau \) as a function of \( D \), for \( f_c = 0.2 \) (orange triangles), 0.3 (green diamonds), 0.5 (red squares) and 1.2 (black circles). The inset shows the normalized translocation time \( \tau / \tau(D = 2) \) as function of \( D \).](image)
Combining Eqs. (9) and (6) and using the closure relation $\bar{R} = A_{\nu} N^\nu$, where $A_{\nu} = 1.1$ (from LD data) for the end-to-end distance in the TP stage and $\nu = 3/4$ is the Flory exponent in 2D, the translocation time is given by [56]

$$\bar{\tau} = \left[ \frac{A_{\nu} N_{1+\nu}}{1+\nu} + N_1 \bar{\eta}_c \right] / (G \bar{f}_c),$$

(10)

where $G = -0.5(c-\alpha)^2/(b+d) + c-d/2 \approx 13.7$ for panel (a) in Fig. 2. Equation (10) shows that the translocation time scales with the channel driving force as $\bar{\tau} \propto \bar{f}_c^{-1}$, i.e., for the SS regime the force exponent is $\beta = -1$. Moreover, the translocation exponent $\alpha$ is bounded between 1 and $1+\nu$, i.e., $1 < \alpha < 1+\nu$, due to the competition between the two terms in the brackets of Eq. (10), in which the first and the second terms originate from the cis-side and channel frictions, respectively. The lower and the upper bounds are assumed in the very short and very long chain limits, respectively [42].

To compare the scaling result of Eq. (10) with the LD simulation data, the inset of Fig. 4(a) shows the force exponent $\beta$ from LD as a function of the channel width $D$. As the channel width decreases $\beta$ moves closer to $-1$. The reason for this is that as an increasing channel diameter allows more pronounced spatial fluctuations of the trans-side subchain, leading to an increased entropic force. Consequently, the force exponent $\beta$ changes as a function of the channel diameter. For the minimum channel width $D = 2$ the force exponent assumes its ideal value $\beta = -1$, due to negligible configurational fluctuations of the subchain on the trans side (see Fig. 4(a)). This is the value in Eq. (10) from IFTP theory. Moreover, as shown in the inset of Fig. 4(a), increasing the channel width changes the value of the force exponent toward its asymptotic value $\beta \sim -0.9$ for a very wide channel, corresponding to a half-space with infinite $D$ [39]. It should be mentioned that at high channel driving forces the force exponent approaches $\beta = -1$ regardless of the channel width, as in this limit the value of the driving force by far exceeds the entropic one.

To investigate the effect of the entropic force on the translocation time the inset of Fig. 4(b) shows the normalized translocation time $\tau/\tau(D=2)$ as function $D$ for various values of $f_c$. As can be seen, the deviation of $\tau$ from the value for $D = 2$ (when the entropic force is negligible due to the small configurational fluctuations of the trans side subchain) grows with increasing $D$. This is more pronounced at weaker driving forces, again due to the fact that by increasing $D$ the entropic force plays a more important role.
C. Distribution of translocation times

We next study the effect of the channel driving force $f_c$ as well as the channel diameter $D$ on the distribution $P(\tau)$ of translocation times $\tau$. Figure 5(a) shows $P(\tau)$ as function of $\tau$ for fixed contour length $N_0 = 100$ and channel width $D = 6$, for the channel driving force values $f_c = 1.2$ (black bars), 0.5 (red bars), 0.3 (green bars), and 0.2 (blue bars). Panels (b), (c), and (d) are the same as panel (a), but for channel widths $D = 4.5, 3$, and 2, respectively. As can be seen in each panel, decreasing channel driving force increases the mean translocation time, and $P(\tau)$ becomes wider (note the log scale on the horizontal axis). This is again due to the fact that decreasing $f_c$ allows more substantial spatial fluctuations of the mobile subchain in the cis and on the trans sides. Consequently, the fluctuations of translocation times increase as well. In panel (e) $P(\tau)$ is shown as function of $\tau$, for fixed value of $f_c = 1.2$ and for channel widths $D = 6.0$ (black bars), 4.5 (red bars), 3.0 (green bars), and 2.0 (blue bars). Panels (f), (g) and (h) are the same as panel (e) but for channel driving forces $f_c = 0.5, 0.3$, and 0.2, respectively. As can be seen from panel (e) to panel (h) decreasing $f_c$ leads to increasing separation of the distributions in each panel.

To quantify the distinctions, in panel (i) the normalized standard deviation $\sigma/\tau$ is shown as function of $f_c$ for the channel widths $D = 2.0$ (orange triangles), 3.0 (green diamonds), 4.5 (red squares), and 6.0 (black circles). Moreover, panel (j) shows $\sigma/\tau$ as function of $D$ for the driving forces $f_c = 0.2$ (orange triangles), 0.3 (green diamonds), 0.5 (red squares), and 1.2 (black circles). As can be clearly seen, in panel (i) at constant $D$ the change in $\sigma/\tau$ is more pronounced by increasing $f_c$ as compared to its change at constant $f_c$ when increasing $D$ in panel (j).

D. Mean-square displacement

Next we consider the dynamics of the translocation process in more detail by monitoring different parts of the chain motion as function of time. To this end the $x$ component of the positions of the head monomer (the first monomer of the chain in terms of the chemical distance along the chain), the front monomer (leading edge of the chain in physical space, i.e., the monomer with the largest $x$ coordinate), the center of mass of the whole chain (CM), and the center of mass for the trans-side subchain (CM$_{\text{chl}}$), as well as the corresponding mean-square displacements (MSDs) are studied. Panel (a) in Fig. 6 shows the $x$ component of the head monomer (black squares), front monomer (red circles), CM (green diamonds), and CM$_{\text{chl}}$ (blue triangles) as function of normalized time $t/\tau$ and for fixed $f_c = 1.2$ and $D = 6.0$. Panel (b) is the same as panel (a) but for fixed value of $f_c = 0.2$. Panels (c) and (d) are the same as panels (a) and (b), respectively, but for fixed $D = 2.0$. Panels (a)–(d) show that the $x$ component for the head monomer (black squares) and front monomer (red circles) coincide with each other. Moreover, at short times the values of CM$_{\text{chl}}$ (blue triangles) are the same as of the data for the head and front monomers, however, at long times its behavior is similar to that of CM.

In Fig. 6(c) the MSD $\langle (x(t) - x(0))^2 \rangle$ is shown as function of the normalized time $t/\tau$ with fixed values $f_c = 1.2$ and $D = 6.0$, for the head monomer (black solid line), front monomer (red solid line), CM (green solid line), and CM$_{\text{chl}}$ (blue solid line). Panel (f) is the same as panel (e) but for fixed $f_c = 0.2$. Panels (g) and (h) are the same as panels (e) and (f), respectively, but for fixed $D = 2.0$. As seen in panels (e)–(h) the behavior of the MSD for the head, front and CM$_{\text{chl}}$ are similar to each other in almost all time regimes. At the very short times their local slope is 4, followed by 0.75 in the short time regime, then 2 and 1.5 at intermediate times, and finally the slope is 2.5 at long times. In contrast, the MSD for CM is different from the other MSDs in different time regimes. Indeed, the MSD slopes for CM are 2, 1, and 4 at very short, intermediate, and long time regimes, respectively.

Panel (i) shows the variance of the $x$ component $\langle (\delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$ as function of normalized time $t/\tau$, with fixed $f_c = 1.2$ and $D = 6.0$, for the head monomer (black solid line), front monomer (red solid line), CM (green solid line) and CM$_{\text{chl}}$ (blue solid line). Panel (j) is the same as panel (i) but for fixed $f_c = 0.2$. Panels (k) and (l) are the same as panels (i) and (j), respectively, but for fixed $D = 2.0$. The behavior of the variance for the head, front, and CM$_{\text{chl}}$ in panels (e)–(h) are again similar to each other. The slopes of the variance are 3, 4, 0.75, 2, and 1.5 at very short, short, intermediate, and long times, respectively. Conversely, for CM (green line) the slope is zero and becomes 3 at long times.

Finally, we consider the time-averaged MSD MSD$_{\text{t-ave}}$ computed as a running average over single trajectories $[79, 80]$. Sampling positions as the time series $x(0), x(\Delta t), x(2\Delta t), x(3\Delta t), \ldots, x((n-1)\Delta t)$ with time step $\Delta t$, MSD$_{\text{t-ave}}$ at ("lag"$t$) time $j\Delta t$ is defined as

$$\text{MSD}_{\text{t-ave}}(j\Delta t) = \frac{1}{(n-j)} \sum_{i=0}^{n-1-j} [x((i+j)\Delta t) - x(i\Delta t)]^2,$$

where $j = 1, 2, 3, \ldots, n - 1$. In equilibrium systems$^1$ and systems with stationary increments MSD$_{\text{t-ave}}$ converges to the ensemble-averaged MSD, $\text{MSD} = \langle [x(t) - x(0)]^2 \rangle$. Given small numbers of independent trajectories, the statistics of MSD$_{\text{t-ave}}$ for sufficiently long time series is often better than the ensemble-averaged MSD. For finite trajectories the time-averaged

$^1$ Up to a factor of 2 occurring naturally due to the definition of MSD$_{\text{t-ave}}$ [83].
FIG. 6: (a) Horizontal position ($x$) of the head (black squares), front (red circles), center of mass of the whole chain (CM, green diamonds) and center of mass for the trans-side subchain (CM_{chl} blue triangles), as function of the normalized time $t/\tau$ for fixed values of the channel force $f_c = 1.2$ and channel diameter $D = 6.0$. Panel (b) is the same as panel (a) but for $f_c = 0.2$. Panels (c) and (d) are the same as panels (a) and (b), respectively, but for $D = 2.0$. (e) ensemble-averaged MSD as a function of normalized time $t/\tau$ for head (black line), front (red line), CM (green line), and CM_{chl} (blue line) as function of $t/\tau$ for $f_c = 1.2$ and $D = 6.0$. Panel (f) is the same as panel (e) but for $f_c = 0.2$. Panels (g) and (h) are the same as panels (e) and (f), respectively, but for $D = 2.0$. The dashed lines and the slopes serve as guide to the eye. Panels (i), (j), (k), and (l) present the variance ($\langle (\delta x)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$) as function of $t/\tau$. Panels (m), (n), (o), and (p) show the time-averaged MSD, MSD_{t-ave}, as function of $t/\tau$. 
MSD fluctuates from one trajectory to the next, as often measured in terms of the ergodicity breaking parameter \[ [82] \]. In "weakly non-ergodic" systems \[ [80–82] \] the time-averaged MSD may differ from the ensemble-averaged MSD even in the limit of long measurement times.

To check the above argument, in panel (n) MSD\(_{t\text{-ave}}\) is shown as function of normalized time \( t/\tau \) with fixed \( f_c = 1.2 \) and \( D = 6.0 \), for the head monomer (black solid line), front monomer (red solid line), CM (green solid line), and CM\(_{\text{chl}}\) (blue solid line). Panel (n) is the same as panel (m) but for fixed value \( f_c = 0.2 \). Panels (o) and (p) are the same as panels (m) and (n), respectively, but for fixed value of \( D = 2.0 \).

As panels (m)–(p) clearly show in the long time limit the data on all curves scale like \( t^2 \). At very short times for CM\(_{\text{chl}}\) the time-averaged MSD scales as MSD\(_{t\text{-ave}} \sim t^2 \), while it scales as \( t^2 \) for the head, front, and CM. Moreover, in panels (n) and (p) in the weak force limit \( (f_c = 0.2) \) another intermediate scaling regime appears in which the time-averaged MSD for CM\(_{\text{chl}}\) scales as \( t^{0.75} \). The time-averaged MSD analysis may thus provide additional information on the details of translocation processes, however, a more detailed study of the relation between ensemble and time-averaged MSDs will be the topic of future work.

E. Monomer density

Finally, we study the time evolution of the monomer density. It reveals the average spatial configuration of the polymer during the translocation process. In Fig. 7(a) the monomer density is shown for the maximum channel width \( D_{\text{max}} = 6 \) and channel driving force \( f_c = 1.2 \) at the times \( t = 0, 0.2\tau, 0.4\tau, 0.6\tau, 0.8\tau \) during the translocation process, and for the final configuration. Averaging has been performed over 1000 independent trajectories. For the sake of better visibility a blow-up of the channel is added underneath the actual narrow channel. Inside the channel the size of the cells in the \( y \) and \( x \) directions is normalized by \( D_{\text{max}} \) and \( N_0 \), respectively. At time zero the whole chain is on the cis side, and as the first bead is fixed at the entrance of the channel the polymer possesses an average pear-like shape. Over time more monomers traverse the channel entrance. At all moments of the translocation process the density of monomers around the corners of the channel entrance is higher than that along the channel axis due to the high driving force. At constant channel with \( D_{\text{max}} = 6 \) when the channel driving force decreases to \( f_c = 0.2 \) (panel (b)), the monomer density is more pronounced along the channel axis.

Panels (c) and (d) are the same as panels (a) and (b), respectively, but for channel width \( D = 2 \). Comparing panels (c) and (d) reveals that by decreasing the channel width to \( D = 2 \), the narrowest one in the current
study, as the monomers inside the channel do not have enough space in the y direction to perform significant spatial fluctuations, one finds them sharply around the channel axis, regardless of the value of the channel driving force. Moreover, it should be noted that the value of the monomer density in panels (c) and (d) is twice that in panels (a) and (b) (see the color bar).

V. SUMMARY AND CONCLUSIONS

In this work we have combined IFTP theory with extensive LD simulations to unravel the dynamics of polymer translocation into a long channel. The axial driving force \( f_c \) in this ”chain sucker” scenario [36] acts on all monomers inside the channel, away from the pore (entry point of the channel), and the monomers inside the channel thus pull the other monomers on the \( \textit{cis} \) side along. When the channel width \( D \) is wide enough to allow the polymer to fluctuate in the channel, an entropic force due to the spatial fluctuations of the \( \textit{trans} \)-side subchain starts to play a role in the translocation dynamics when its magnitude becomes comparable to that of the driving force. Our analysis demonstrates how the \( \textit{trans} \)-side entropic force depends on the values of both \( D \) and \( f_c \), as the spatial configuration of the \( \textit{trans} \)-side subchain is determined by both.

To further verify this, in Fig. 8(a) the horizontal size of the last configuration of the chain inside the channel \( R_{\|} \) is shown as function of \( D \) for the channel driving force \( f_c = 1.2 \) (turquoise open circles), 0.5 (orange open squares), 0.3 (green open diamonds), and 0.2 (pink open triangles). The black solid curve is shown as a guide to the eye and depicts the scaling exponent for the equilibrium configuration of the chain inside a channel width \( D \). From blob theory the equilibrium axial chain size exponent is \(-1/3\) in the absence of any channel driving force \( R_{\|} \propto D^{-1/3} \) [69]. As the driving force increases the axial chain-size exponent deviates from its equilibrium value of \(-1/3\). Moreover panel (b) shows that at constant \( D \), the value of \( R_{\|} \) also depends on \( f_c \). Therefore, panels (a) and (b) clearly confirm that \( R_{\|} \) depends on both \( f_c \) and \( D \), and it is hard to separate the effect of their individual contributions to \( R_{\|} \). In particular, the contributions of \( f_c \) and \( D \) to the entropic force are coupled to each other.

The only case in the current study, wherein the \( \textit{trans} \)-side entropy does not play any significant role in the translocation dynamics is for the narrow channel width \( D = 2 \), and the corresponding LD result for the force exponent is \( \beta = -1 \) (orange dashed line in Fig. 4(a)), as predicted by IFTP theory wherein the contribution of the entropic force is not taken into account, see Eq. (10). As the value of \( D \) increases, the \( \textit{trans} \)-side subchain possesses more spatial configurations, and entropic force effects on the dynamics of translocation process are more pronounced, and consequently \( \beta \) deviates from \(-1\) (see inset of Fig. 4(a)).

Our study has unveiled a rich behavior of the observed translocation dynamics as function of the system parameters of channel driven translocation. Such scenarios are important for experimental systems such as long micro- or nano-channels that confine the DNA and apply flows along the channel [72–76].

Appendix A: Bond length distribution

One of the quantities that shows the dynamics of the translocation process at the monomer level is the bond length distribution. In Fig. 9 the normalized bond length \( l_b/l_{b,\text{equil}} \) is shown as function of the bond index \( b \), for constant channel driving force \( f_c = 1.2 \) and different channel widths \( D = 6.0 \) (solid filled symbols), 4.5 (vertical hashed filled), 3.0 (horizontal hashed filled), and 2.0 (cross hashed filled), at the times \( t/\tau = 0.2 \) (black circles), 0.4 (red squares), 0.6 (green diamonds), 0.7 (blue triangles), and 0.8 (orange upside triangles). Here \( l_{b,\text{equil}} \approx 0.96 \) is the average value of the bond length at equilibrium, and \( \tau \) is the average translocation time for the corresponding set of parameters. Panels (b), (c) and (d) are the same as panel (a) but for channel driving forces \( f_c = 0.5, 0.3, \) and 0.2, respectively. As can be seen, at the beginning of the translocation process fewer bonds are affected by the tension force as compared to later

![FIG. 8: (a) Horizontal size \( R_{\|} \) of the final chain configuration at the end of the translocation process, as function of the channel width \( D \), for the channel driving forces \( f_c = 1.2 \) (turquoise open circles), 0.5 (Orange open squares), 0.3 (green open diamonds), and 0.2 (pink open triangles). As can be seen, all fitted slopes are far from the equilibrium behavior (for \( f_c = 0 \) with size exponent \(-1/3\) (black solid curve as guide to the eye). (b) \( R_{\|} \) as function of \( f_c \) for channel widths \( D = 6 \) (turquoise open circles), 4.5 (Orange open squares), 3 (green open diamonds) and 2 (pink open triangles), with the corresponding values of the exponents 0.034, 0.067, 0.86 and 0.093, respectively.](image-url)
times. At the TP time of about $t_\text{TP} = 0.7\tau$, all bonds in the polymer on average are stretched by the tension force. This is clearly shown by the blue curves in all panels of Fig. 9. As the channel driving force gets weaker (from panel (a) to panel (d)) the bonds are less stretched by the tension force. This is another confirmation for the existence of TP along the backbone of the chain. Each empty circle approximately shows the bond index inside the entrance of the channel at the corresponding moment.

Appendix B: Velocity length distribution

We consider the monomer velocity distribution here. Its $x$ component is obtained from averaging over 1000 uncorrelated trajectories for each set of parameters. In Fig. 10(a) the normalized $x$ component of the monomer velocity $v_x/f_c$ is shown as function of the monomer index $m$, for fixed value of the channel driving force $f_c = 1.2$ and channel widths $D = 6.0$ (solid filled symbols), 4.5 (vertical hashed filled), 3.0 (horizontal hashed filled), and 2.0 (cross hashed filled), at the different times $t/\tau = 0.2$ (black circles), 0.4 (red squares), 0.6 (green diamonds), 0.7 (blue triangles), and 0.8 (orange upside triangles). Panels (b), (c) and (d) are the same as panel (a) but for channel driving forces $f_c = 0.5$, 0.3, and 0.2, respectively. To assess how the driving force affects the monomer velocity distribution, the normalized velocity has been plotted in all panels. As can be seen the behavior of the curves at any given moment is similar for different values of the driving force. As the value of $f_c$ decreases (from panel (a) to panel (d)) the fluctuations in the curves increase originating from two facts. The first one is that by decreasing the force the value of the normalized velocity increases (note that $f_c$ is in the denominator of $v_x/f_c$) and this increases the fluctuations of the normalized velocity. The second reason is that by decreasing the driving force, the tension force along the backbone of the chain becomes weaker, giving rise to more pronounced spatial fluctuations of the chain and consequently higher fluctuations of the monomer velocity. To have the same amount of monomer velocity fluctuations the average must be taken over more trajectories as the channel driving force decreases.

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[1] S. M. Bezrukov, I. Vodyanoy and A. V. Parsegian, Nature 370, 279 (1994).
[2] J. J. Kasianowicz, E. Brandin, D. Branton and D. W. Deamer, Proc. Natl. Acad. Sci. U.S.A. 93, 13770 (1996).
[3] W. Sung and P.J. Park, Phys. Rev. Lett. 77, 783 (1996).
[4] A. Meller, L. Nivon and D. Branton, Phys. Rev. Lett. 86, 3435 (2001).
[5] A.F. Sauer-Budge, J.A. Nyanwanda, D.K. Lubensky and D. Branton, Phys. Rev. Lett. 90, 238101 (2003).
[6] A.J. Storm, J.H. Chen, X.S. Ling, H.W. Zandbergen and C. Dekker, Nature Materials 2, 537 (2003).
[7] U.F. Keyser et al., Nat. Phys. 2, 473 (2006).
[8] E. H. Trepagnier, A. Radenovic, D. Sivak, P. Geissler and J. Liphardt, Nano Lett. 7, 2824 (2007).
[9] U.F. Keyser, N.H. Dekker, C. Dekker, and S.G. Lemay, Nat. Phys. 5, 347 (2009).
[10] C. Raillon, P. Granjon, M. Graf, L. J. Steinbock and A. Radenovic, Nanoscale 4, 4912 (2012).
[11] F. Traversi, C. Raillon, S. M. Benameur, K. Liu, S. Khlybov, M. Tousn, D. Krasnozhon, A. Kis and A. Radenovic, Nature Nanotech. 8, 939 (2013).
[12] R.D. Bulushev, S. Marion, and A. Radenovic, Nano Lett. 15, 7118 (2015).
[13] M. Muthukumar, Polymer Translocation (Taylor and Francis, 2011).
[14] V.V. Polyulin, T. Ala-Nissila and R. Metzler, Soft Matter 10, 9016 (2014).
[15] J. Sarabadani and T. Ala-Nissila, J. Phys.: Condens. Matter 30, 274002 (2018).
[16] A. Milchev, J. Phys.: Condens. Matter 23, 103101 (2011).
[17] M. Muthukumar, J. Chem. Phys. 111, 10371 (1999).
[18] J. Chuang, Y. Kantor and M. Kardar, Phys. Rev. E 65, 011802 (2001).
[19] F. Tessier and G. W. Slater, Appl. Phys. A 75, 285 (2002).
[20] Y. Kantor and M. Kardar, Phys. Rev. E 69, 021806 (2004).
[21] T. Ambjörnsson and R. Metzler, Phys. Biol. 1, 77 (2004).
[22] R. Zandi, D. Reguerra, J. Rudnick, and W. M. Gelbart, Proc. Natl. Acad. Sci. U.S.A. 100, 8649 (2003).
[23] A.Y. Grosberg, S. Nechaev, M. Tamm and O. Vasilyev, Phys. Rev. Lett. 96 228105 (2006).
[24] K. Luo, T. Ala-Nissila and S.-C. Ying, J. Chem. Phys. 124, 034714 (2006).
[25] T. Sakae, Phys. Rev. E 76, 021803 (2007).
[26] G. Sigalov, J. Comer, G. Timp and A. Aksimentiev, Nano Lett. 8, 56 (2008).
[27] M.G. Gauthier and G.W. Slater, Phys. Rev. E 80, 021907 (2009).
[28] K. Luo, R. Metzler, T. Ala-Nissila, and S.-Ch. Ying, Phys. Rev. E 80, 021907 (2009).
[29] K. Luo, T. Ala-Nissila, S.-Ch. Ying, and R. Metzler, Europhys. Lett. 88, 68006 (2009).
[30] K. Luo and R. Metzler, J. Chem. Phys. 133, 075101 (2010).
FIG. 9: (a) Normalized bond length $l_b/l_{b,equil}$ as function of the bond index $b$ for fixed channel driving force $f_c = 1.2$ and channel widths $D = 6.0$ (solid filled symbols), 4.5 (vertical hashed filled), 3.0 (horizontal hashed filled), and 2.0 (cross hashed filled), at times $t/\tau = 0.2$ (black circles), 0.4 (red squares), 0.6 (green diamonds), 0.7 (blue triangles) and 0.8 (orange upside triangles). Panels (b), (c) and (d) are the same as panel (a), but for $f_c = 0.5, 0.3, 0.2$, respectively. Empty circles approximately show the bond index inside the entrance of the channel at the corresponding moments. $l_{b,equil} \approx 0.96$ is the equilibrium average value of the bond length.

FIG. 10: (a) Normalized $x$-component of the monomer velocity $v_x/f_c$ as function of the monomer index $m$, for fixed channel driving force $f_c = 1.2$ and channel widths $D = 6.0$ (solid filled symbols), 4.5 (vertical hashed filled), 3.0 (horizontal hashed filled), and 2.0 (cross hashed filled), during the translocation process at times $t/\tau = 0.2$ (black circles), 0.4 (red squares), 0.6 (green diamonds), 0.7 (blue triangles) and 0.8 (orange upside triangles). The empty circles approximately specify the monomer index inside the entrance of the channel at the corresponding moments. Panels (b), (c) and (d) are the same as panel (a) but for channel driving forces $f_c = 0.5, 0.3, 0.2$, respectively.

[31] K. Luo and R. Metzler, Phys. Rev. E 82, 021922 (2010).

[32] T. Sakaue, Phys. Rev. E 81, 041808 (2010).

[33] H.W. de Haan and G.W. Slater, Phys. Rev. E 81, 051802 (2010).

[34] P. Rowghanian and A.Y. Grosberg, J. Phys. Chem. B 115, 14127 (2011).

[35] J.A. Cohen, A. Chaudhuri and R. Golestanian, J. Chem. Phys. 107, 238102 (2011).

[36] K. Luo and R. Metzler, J. Chem. Phys. 134, 135102 (2011).

[37] T. Saito and T. Sakaue, Phys. Rev. E 85, 061803 (2012).

[38] T. Ikonen, A. Bhattacharya, T. Ala-Nissila and W. Sung, Phys. Rev. E 85, 051803 (2012).

[39] T. Ikonen, A. Bhattacharya, T. Ala-Nissila and W. Sung, J. Chem. Phys. 137, 085101 (2012).

[40] H.W. de Haan and G.W. Slater, J. Chem. Phys. 136, 204902 (2012).

[41] N. Nikoofard, H. Khalilian and H. Fazli, J. Chem. Phys. 139, 074901 (2013).

[42] J. Sarabadani, T. Ikonen and T. Ala-Nissila, J. Chem. Phys. 141, 214907 (2014).

[43] A. Suma, A. Rosa and C. Micheletti, Asp Macro Lett. 4, 1420 (2015).

[44] R. Adhikari and A. Bhattacharya, Phys. Rev. E 92, 032711 (2015).

[45] J. Sarabadani, T. Ikonen and T. Ala-Nissila, J. Chem. Phys. 143, 074905 (2015).

[46] T. Menais, S. Mossa and A. Buhot, Sci. Rep. 6, 38558 (2017).

[47] J. Sarabadani, B. Ghosh, S. Chaudhury and T. Ala-Nissila, Europhys. Lett. 120, 38004 (2017).

[48] A. Suma and C. Micheletti, Proc. Natl. Acad. Sci. U.S.A. 114 (15), E2991-E2997 (2017).

[49] J. Sarabadani, T. Ikonen, H. Mikkonen, T. Ala-Nissila, S. Carson, M. Wanunu, Sci. Rep. 7, 7423 (2017).

[50] T. Menais, Phys. Rev. E 97, 022501 (2018).

[51] S. Buyukdagli, J. Sarabadani and T. Ala-Nissila, Polyhedra 10, 1242 (2018).

[52] S. Buyukdagli, J. Sarabadani and T. Ala-Nissila, Polyhedra 11, 118 (2019).

[53] A. Bhattacharya and S. Seth, Phys. Rev. E 101, 052407 (2020).

[54] J. Sarabadani, S. Buyukdagli and T. Ala-Nissila, J. Phys.: Condens. Matter 32, 385101 (2020).

[55] B. Ghosh, J. Sarabadani, S. Chaudhury and T. Ala-Nissila, J. Phys.: Condens. Matter 33, 015101 (2020).

[56] H. Khalilian, J. Sarabadani and T. Ala-Nissila, Phys. Rev. Research 3, 013080 (2021).

[57] H. Ochman, J. G. Lawrence, and E. A. Groisman, Nature 405, 299 (2000).
[58] S. Nakielny and G. Dreyfuss, Cell 99, 677 (1999).
[59] D. Branton et al., Nature BioTechnology 26, 1146 (2008).
[60] D. Deamer, M. Akeson and D. Branton, Nature Biotechnology 34, 518 (2016).
[61] L. Messager et al., Angew. Chem. Int. Ed. 55, 11106 (2016).
[62] R.D. Bulushev et al., Nano Lett. 146006 (2014).
[63] R.D. Bulushev et al., Nano Lett. 16 7882 (2016).
[64] F. Ritort, J. Phys.: Condens. Matter 18, R531 (2006).
[65] A. Fiasconaro, J.J. Mazo, and F. Falo, Phys. Rev. E 91, 022113 (2015).
[66] R.I. Stefureac, A. Kachayev, and J.S. Lee, Chem. Commun. 48, 1928 (2012).
[67] M. Bates, M. Burns, and A. Meller, Biophys. J. 84, 2366 (2003).
[68] G.J. Fleer, M.A. Cohen Stuart, J.M.H.M. Scheutjens, T. Cosgrove and B. Vincent, Polymers at Interfaces (Chapman & Hall, 1998).
[69] P.-G. De Gennes, Scaling Concepts in Polymer Physics (Cornell University Press, 1979).
[70] K. Luo, T. Ala-Nissila, S.-C. Ying, and A. Bhattacharya Phys. Rev. Lett. 99, 148102 (2007).
[71] H. Yong, Y. Wang, S. Yuan, B. Xu and K. Luo, Soft Matter 8, 2769 (2012).
[72] J.O. Tegenfeldt et al., Anal. Bioanal. Chem. 378, 1678 (2004).
[73] J.O. Tegenfeldt et al., Proc. Natl. Acad. Sci. U.S.A. 101, 10979 (2004).
[74] Y.M. Wang et al., Proc. Natl. Acad. Sci. U.S.A. 102, 9797 (2005).
[75] R.H. Liu and A.P. Lee, Integrated Biochips for DNA Analysis, chapter 12 (Springer 2007).
[76] F. Persson and J.O. Tegenfeldt, Chem. Soc. Rev. 39, 985 (2010).
[77] G.S. Grest and K. Kremer, Phys. Rev. A 33, 3628 (1986).
[78] S. Plimpton, J. Comp. Phys. 117, 1 (1995); http://lammps.sandia.gov.
[79] E. Barkai, Y. Garini, and R. Metzler, Phys. Today 65(8), 29 (2012).
[80] R. Metzler, J.-H. Jeon, A. G. Cherstvy, and E. Barkai, Phys. Chem. Chem. Phys. 16, 24128 (2014).
[81] J.-P. Bouchaud, J. Phys. (Paris) I 2, 1705 (1992).
[82] Y. He, S. Burov, R. Metzler, and E. Barkai, Phys. Rev. Lett. 101, 058101 (2008).
[83] J.-H. Jeon and R. Metzler, Phys. Rev. E 85, 021147 (2012).