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Translocation of Polymer Chains Through a Channel with Complex Geometries

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The elastic behavior of a single chain transporting through complex channel which can be seen as the combination of three different channels (left channel, middle channel, and right channel, respectively) is investigated using the new pruned-enriched Rosenbluth method with importance sampling. The elastic force during the translocation process is calculated. At the entrance into the middle channel, there is the first plateau in the curve of the elastic force f ($f>0$) versus x, here x represents the position of the first monomer along the x-axis direction. When the first monomer moves to a certain position, a second plateau is observed with the elastic force $f<0$, which represents spontaneous translocation. The free energy difference between the subchain in the right channel and the subchain in the left channel may drive the translocation. The influence of chain length and width of the left and right channels on the translocation process are also investigated. From the simulation results, more detailed explanations for the reason why the component translocation time is not the same for different channels can be presented.

Key words: Elastic behavior, nPERMis, Polymer translocation

I. INTRODUCTION

The process of translocation, in which a polymer chain worms its way through a narrow pore, is very important in many biological systems and industrial processes. It is ubiquitous in biological systems, such as DNA and RNA translocations across nuclear pores; protein transportation through membrane channels and virus injection [1,2]. Moreover, there are various technological applications such as gene therapy [3], delivery of drug molecules to their activation sites, and DNA migration through microfabricated channels and devices [4]. In view of its biological and technological significance, polymer translocation has attracted a considerable number of experimental [5-7], simulation-based [8-10], numerical [11-13], and theoretical [14-16] studies.

The translocation time of a single polymer was also studied [6-9,13-24]. Numerous groups have done deep research into translocation time via experimental, simulation-based and theoretical methods. In the experimental aspect, Meller and Branton has found the translocation time increases with the chain length [6]. The results of Kasianowicz *et al.* have shown that translocation takes place more readily when the chain is introduced through the side of the asymmetric α-hemolysin membrane channel that has the larger vestibule [7]. In the simulation approach, Clementi *et al.* have shown the time of translocation through nanopores grows with chain length via molecular dynamics [8]. Luo *et al.* studied the polymer chain translocation from the donor to the receptor infinite sphere through a middle narrow channel using Langevin dynamics simulations and divided translocation time into three components, i.e., the time τ_1 of finding the entrance of pore, the time τ_2 of filling the pore, and the time τ_3 of transporting the polymer chain into the right part completely [9]. With very weak attractive nanopore-polymer interactions, τ_2 dominates the total contribution to the translocation time, while τ_3 is the shortest. In the theoretical approach, Muthukumar has studied polymer chain translocation through a cylindrical channel between two spherical compartments and found the translocation time grows with the chain length [14]. Pasquali did more detailed research and found channel structure plays a significant role in controlling translocation through membrane channels in biological systems [15]. He investigated the time of a single chain translocation in asymmetric α-hemolysin membrane channel. Results show that the pore length and diameter have great influence on the translocation time, and the process of transportion into large pore from small pore requires less time than the contrary process. However, few studies show detailed research on the component time difference, so it remains worthwhile to perform more detailed studies on the great influence of the free energy barrier on component translocation time.

In this work, we construct a model and outline the simulation technique in detail, study the effect of the chain length, the left and right channel width on the elastic force during the translocation, and analyze the difference for translocation time at different channels. Some comparisons are also made.

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II. MODEL

In this work, we use the model of a self-avoiding chain of length N on a two-dimensional lattice. The total energy of the chain is assumed to contain contact energy only:

$$E = \sum_{|i-j|\geq 3} \varepsilon_c \delta\left(r_{ij} - a\right) \tag{1}$$

where r_{ij} is the distance between monomers i and j, ε_c is the contact energy, and ε_c=−1 (in the unit of $k_{\mathrm{B}}T$, here k_{B}=1 and T=0.3). a is the length of one lattice, and it is also set to 1. $\delta(x)$=1 for x=0 and $\delta(x)$=0 for $x\neq 0$. Monomers i and j can form a contact if two monomers are in two adjacent lattice sites while not adjacent along the chain.

An effective simulation method at low temperature is used here, which is called the new pruned-enriched Rosenbluth method with important sampling (nPERMis) method [25]. nPERMis is a bias chain growth algorithm with population control. At first, it calculates the upper threshold and lower threshold defined by $W_n^{>}=CZ_n/Z_0\left(C_n/C_0\right)^2$ and $W_n^{<}=0.2W_n^{>}$ respectively. Here, C_n is the total number of configurations of chain length n already created during the run, Z_n is the partition sum estimated from these configurations, and C is some positive number. Then it estimates a predicted weight W_n^{pred} for the (n-1)th step and counts the number k_{free} of free sites where the nth monomer can be placed. If $W_n^{\mathrm{pred}}>W_n^{>}$ and $k_{\mathrm{free}}>1$, k $\left(k=\min\left\{k_{\mathrm{free}},\left|W_n^{\mathrm{pred}}/W_n^{>}\right|\right\}\right)$ different configurations are created; If $W_n^{\mathrm{pred}}<W_n^{<}$, the configuration is pruned at random; If $W_n^{<}\leq W_n^{\mathrm{pred}}\leq W_n^{>}$, it chooses a free site randomly for the next growth. It can avoid choosing the same configurations, so it is very effective.

In Fig.1, we present the schematics of a polymer chain through a channel along the x-axis direction. The channel can be seen as the combination of three different channels with different widths. The width of the left channel is W_{l} and its length is infinite. The width of the middle channel is W_{m} and we set W_{m}=1, and its length is L=9. The width of the right channel is W_{r} and its length is also infinite. The channel walls are impenetrable and there are no interactions between the polymer chains and the channel. We only consider the interactions of monomers. In our model, one end of the polymer chain is placed at the entrance of the middle channel, and then the end monomer is pulled slowly along the direction of x-axis through the channel. Figure 1 represent the process of the polymer chain moving from the left to the right channel through the middle narrow channel.

The partition function of the system is

$$Z(x) = \sum_i \exp\left(\frac{-E_i}{kT}\right) \tag{2}$$

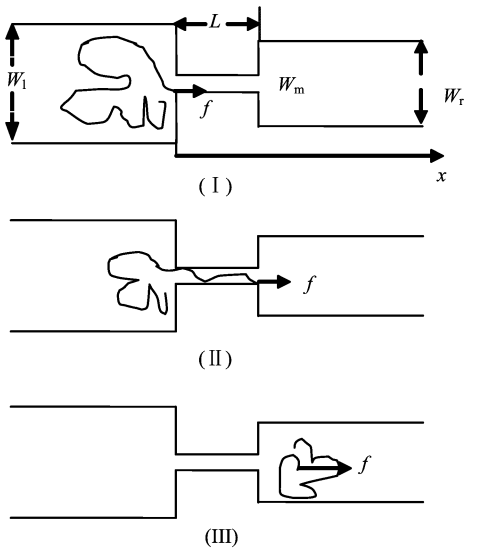

FIG. 1 Schematics of polymer chain during the translocation from the donor to the receptor infinite channel through a middle narrow channel along the x-axis direction.

where $\sum_i$ is the sum of all configurations whose end monomer is at position x.

The Helmholtz free energy of the polymer chains can be derived from the partition function:

$$A(x) = -kT \ln Z(x) \tag{3}$$

At the same time, the elastic force can be obtained from the dependence of A on the elongated distance along the force direction [26,27]:

$$f = \frac{\partial A(x)}{\partial x} \tag{4}$$

III. RESULTS AND DISCUSSION

A. Effect of channel width when N=60

Figure 2 shows the elastic force f as a function of x (the position of the first monomer along the x-axis direction) with different values of W_{l} with W_{r}=3. In Fig.2, there are three force plateaus for all values of W_{l}. The first plateau at x=2-15 should represent the translocation of the chain from the left channel to the middle small channel. The values of f are larger than 0. Thus, polymer chains should be pulled by external force when they escape from wide channels to small channels. The second plateau from x=20 to 24 indicates the escaping process of the chain from the middle channel to the right channel. As the values of f are less than 0, the chain can escape from narrow space to wide space by itself. The third plateau is formed when x>25, which suggests that all monomers of the chain have reached

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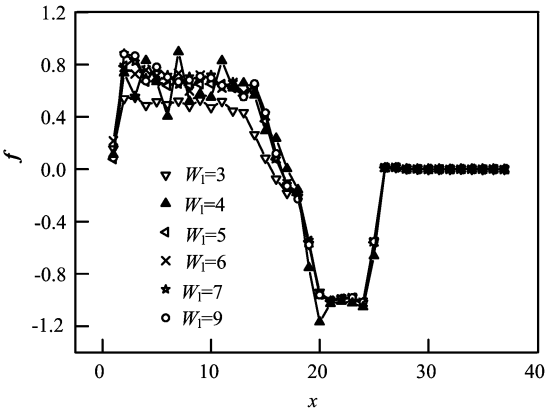

FIG. 2 Elastic force f as a function of x with different values of $W_{\rm l}$. N=60, L=9, $W_{\rm m}$=1, and $W_{\rm r}$=3.

the right channel. For $W_{\rm l}$=3, the elastic force f is about 0.52 and −1.0 for the first and second plateaus, respectively. The values of f for $W_{\rm l}$=4 at the first plateau fluctuate between 0.4 and 0.91. For $W_{\rm l}\geq$5, the values of f are larger than those for $W_{\rm l}$=3. Similar values of f are observed at the second plateau for all of $W_{\rm l}$. When all of the chain monomers move from the left and middle channel to the right channel, no external force is needed to pull the chain. Hence, f=0 for all of $W_{\rm l}$ is observed at the third plateaus. We have also noted that force value of the first plateau is more dependent on the values of $W_{\rm l}$ than that of the second plateau.

From these numerical results, we can conclude it is not favorable to translocate through the narrow channel from the large channel. The reason may be that the free energy barrier is very high in the translocation process. In order to overcome this barrier, an external force acting on the chain is needed. We have also found that when the width of the left channel is very small, the shape of the polymer chain looks like a long strip. Thus, the chain needs to deform only a little to squeeze itself into the middle channel, which leads to small values of f for $W_{\rm l}$=3 at the first plateau. When $W_{\rm l}$ increases, the chain's shape changes from strip to compact globule, hence the chain needs larger values of f to be pulled through the middle channel. We think that there should be some critical values of $W_{\rm l}$, for which the chain's shape is between the strip and compact globule. This may be the reason why the values of f are fluctuating at the first plateau for $W_{\rm l}$=4. When $W_{\rm l}\geq$5, the chain begins to form a compact structure. The walls of the left channel have little effect on the chain, hence, the values of f stay unchanged. Therefore, the process of translocation from the left channel to the middle channel requires a very long time. Lou *et al.* indicate that with very weak attractive nanopore-polymer interactions the process of entrance into a narrow channel from a large space requires the longest time compared to other component times [9]. Our results are in agreement with them. This component time increases with the left channel width increasing. The left channel width has effect on the translocation time. The second and third plateaus stay almost unchanged for all values of $W_{\rm l}$. The reason may be that the monomer density in the left channel is low in the process of escaping from the middle channel, thus the walls of left channel have few effects on this translocation process.

To investigate the influence of the right channel, we change the values of $W_{\rm r}$ and fix $W_{\rm l}$=3 . The elastic force is plotted as a function of x with various values of $W_{\rm r}$ in Fig.3. For small values of $W_{\rm r}$, three plateaus can be also observed as a whole, and similar explanation as above could be used here. In fact, this translocation process can be seen as the opposite of the process above, since the first plateau does not change for different values of $W_{\rm r}$, but the values of the second plateau changes obviously as $W_{\rm r}$ changes. The values of the second plateau are about f=−0.98, −1.88, −2.13, −3.64, and −4.54 for $W_{\rm r}$=3, 4, 5, 7, and 9, respectively. The wider the right channel is, the larger the spontaneous force is. The wider the right channel is, the more compact the polymer chain structure is, and the larger the entropic difference between the middle channel and right channel is. Therefore, we do not need any force to pull the chain to enter into the right channel, and the polymer chain can move spontaneously. The values of the third plateau are zero, which indicates that the polymer chain has entered the right channel completely. The polymer chain is favorable to enter the large channel from the narrow channel, since it is subjected to an entropic bias toward the right channel. The wider the right channel is, the more easily the chain enters the right channel, and the driving force f is produced by itself. The experimental results have shown that translocation occurs more easily from narrow channel to large channel [7], It takes longer time to enter into narrow pore [9]. Our results are in agreement with those results, and this process of translocation from middle to right channel requires a much shorter time, and this component time is cut down further with the right channel width increasing.

B. Effects of chain length

Here we study the elastic behavior of polymer translocation further with different chain length and different values of $W_{\rm l}$ and $W_{\rm r}$. First, we fix $W_{\rm r}$=3 and change $W_{\rm l}$. The elastic force is plotted as a function of x with different values of $W_{\rm l}$ and chain lengths in Fig.4. As seen in Fig.4, similar results as Fig.2 can be observed, i.e., there are also three plateaus for each curve. For each chain length, the two curves for $W_{\rm l}$=5 and 9 almost overlap. Mainly, we focus on the influence of the chain length. It is obvious that as the chain length increases the length of the transition region from the first plateau to the second plateau, but the values of f for the first plateaus are comparable. The second plateau

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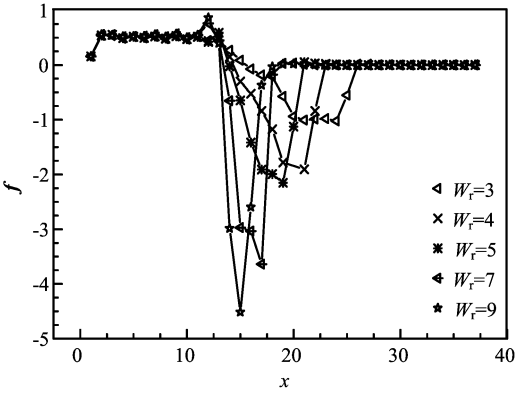

FIG. 3 Elastic force f as a function of x with different values of W_r. N=60, W_l=3, L=9, and W_m=1.

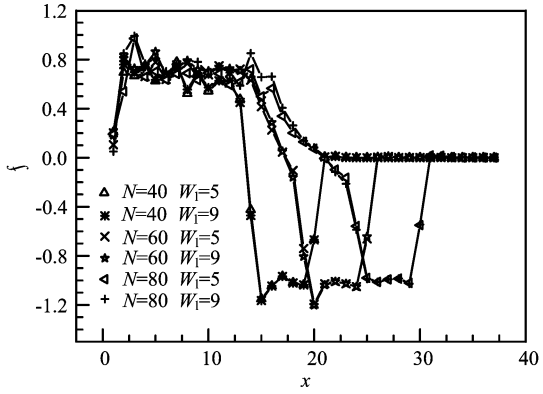

FIG. 4 Elastic force f as a function of x with different values of N and W_l. L=9, W_m=1, and W_r=3.

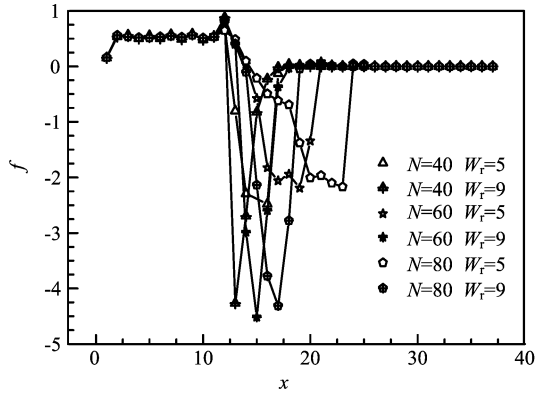

FIG. 5 Elastic force f as a function of x with different values of N and W_r. W_l=3, L=9, and W_m=1.

shifts to right as the chain length is increased, and the values of f stay unchanged for different chain lengths. The second plateaus are at x=15-19, 20-24, and 25-29 for N=40, 60, and 80, respectively. The results should indicate that as the chain length increases, it becomes more difficult for the polymer chain to get through the narrow channel. The curves of these chains have the same tendency. It indicates further that the time of translocation from the left channel to the middle channel is very long.

Second, we fix W_l=3 and change W_r. The elastic force is plotted as a function of x for different W_l and chain lengths in Fig.5. Similar behaviors as Fig.3 are observed. The right channel width has almost no influence on the first plateau, while it has great effect on the second plateau. For N=40, the second plateau is at x=14-16 with the f value of -2.40 for W_r=5, while it is an indentation instead of a plateau for W_r=9. The second plateau disappears and becomes an indentation, and the largest value is -4.27. For N=60, the second plateau is at x=16-19 with f=-2.06 for W_r=5, and it is also an indentation for W_r=9 with the largest f value of -4.51. For N=80, the second plateau is at x=20-23 with f=-2.03 for W_r=5, and an indentation for W_r=9 with the largest f value of -4.31. Hence, for a given value of W_r, the plateau or indentation will move to right when the chain length increases.

The chain length has few effects on the process of the chain moving from the left to the middle channel, but it is very influential on the translocation from the middle channel to the right channel. For a given W_r and W_l, the second force plateau may move to right as the chain length increases. The transition region from the first plateau to the second plateau will become broad with the chain length increasing. Thus it should be more difficult for longer chains to get through the middle narrow channel to the right channel. Therefore, the longer the translocation time is, the longer the chain length is. The results in Refs.[6,8] indicate that the translocation time grows with chain length. Our results are in agreement with these findings. From Fig.4, we can find that all the curves have the same tendency. This indicates further the time of translocation from the middle to the right channel is very much shorter than that of translocation from the left to the middle channel.

IV. CONCLUSION

In this work, the translocation of polymer chains through a specified channel is investigated by nPER-Mis. We study the translocation from the donor to the receptor infinite passage through a middle narrow channel. Results show that chronologically there are three plateaus in the force spectrums, whose values are larger than zero, less than zero and equal to zero, respectively. For a given W_r and chain length, the values of the first plateau increase a little as W_l is increased, i.e., the chain needs larger external force to pull it into the middle narrow channel. Therefore, the wider the right channel is, the harder it is for the chain to enter into the middle channel. This indicates the time of translocation through the middle channel is very long and the translocation time increases with the left chan-

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nel width increasing. W_l is not influential to the second and the third plateau. Thus the width of left channel should only influence the entrance of chains to the narrow middle channel, and may not influence the entrance to the right channel. The wider the left channel is, the higher the free energy barrier of entrance into the middle channel is. In order to enter the middle channel, the chain needs a larger external force. When the monomers of the chain enter the right channel, the monomer density is low in the left channel. Therefore, the walls of the left channel have few effects on the translocation. For a given chain length and W_l, the first plateau changes very little as W_r changes. The transition region from the first plateau to the second plateau becomes narrow, and the second plateau becomes short, even disappearing, with W_r increasing. However, the driving force becomes large, which is produced by itself, with the right channel width increasing. Thus, it is easy for the chain to move from the middle narrow channel to the right channel for large value of W_r. This indicates that the translocation time of entrance into the right channel is much shorter, and the time required for that is cut down further with the right channel width increasing. The entropic barrier lowers as the right channel width increases in this process, and it becomes easier for the chain to enter the right channel. The chain length is also very influential to the translocation process of polymer chains. We have found that for a given W_l and W_r, the width of the transition region will be increased and the second plateau shifts to right as the chain length increases. Thus a longer time is required for longer chains to get through the middle narrow channel. Every chain has the same transition tendency in translocation process. The data indicates further that the time of entrance into middle channel from the left channel is longer than the time of entrance into the right channel. These simulation results are in agreement with the previous results. [6-9,14,18].

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