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Translocation of compact polymer chains through a nanopore

Zhiyong Yang [a], Zhengquan Pan [a], Linxi Zhang [b,*], Haojun Liang [c]

[a] Department of Physics, Zhejiang University, Hangzhou 310027, PR China
[b] Department of Physics, Wenzhou University, Wenzhou 325027, PR China
[c] Department of Polymer Science and Engineering, University of Science and Technology of China, Hefei, Anhui 230026, PR China

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ABSTRACT

We perform dynamical Monte Carlo simulation to study the forced translocation of compact polymer chains in three-dimensional lattices. The chains are driven through a nanopore connecting two infinite channels by an external field. The scaling properties of average translocation time τ and translocation time distribution (TTD) are studied. The effects of contact energy (ε_C), electric field strength (E), and nanopore width (L) on the scaling exponent (α) of average translocation time $\tau \sim N^{\alpha}$ and the TTD are investigated. For the scaling behavior of $\tau \sim N^{\alpha}$, we have found that there is no crossover behavior with weak field strength when the nanopore width is one lattice spacing, which is less than average bond length, while crossover behaviors are observed for larger nanopore widths. The scaling exponent α also depends on contact energy ε_C and electric field strength E. For the TTD, it shifts from the Gaussian to a right-skew distribution with the electric field E increasing for short chains; while for long chains, multi-peak distributions are observed. As a primary and simple model, compact polymer chains are extensively used to capture the structure and thermodynamic properties of proteins, therefore we can investigate the protein translocation by simulating compact chain translocation, and this study will be useful for exploring the complex translocation behaviors of proteins.

1. Introduction

The translocation of biopolymers, such as RNAs, DNAs and proteins through channels or nanopores, is very important in many biological processes [1]. Examples include DNA and RNA translocation across nuclear pores, protein translocation through membrane channels [2,3], the translocation of nascent proteins inside the ribosomal tunnel or across the endoplasmic reticulum [4–7], and the incorporation of membrane proteins into lipid bilayers [8]. Meanwhile, protein translocation in the cell is also inspired by much interest such as protein degradation by ATP-dependent proteases, mitochondrial protein import, and protein synthesis [9,10]. They involve the threading of proteins through narrow constrictions whose dimensions are too small to accommodate folded proteins [11]. With the development of biotechnologies, this simple translocation behavior is also applied in the gene therapy [12,13], the protein translocation in mitochondria [12–16], and the delivery of drug molecules to their activation sites [17–19]. In view of its biological and technological significance, in recent years there has been much interest in the study of the biopolymer translocation through channels or nanopores. Understanding this process enables us to deepen our comprehension of many fundamental problems in cell biology, and maybe also contribute to the development of promising biotechnologies.

Although the translocation process is influenced by many biological factors, many scientists are trying to make use of a simple model to study the translocation process. A large amount of theory and simulation studies of biopolymer translocation have been performed [20–26]. In theory, Sung and Park [20] described the process by the Fokker–Planck equation of probability distribution function of translocation monomers where the chain diffusivity is assumed to be a constant. Their results show that average translocation time τ as a function of chain length N scales like N^2/D or N/D when the external bias is small or large (where D is the effective diffusion coefficient of chain), respectively. Muthukumar [21] treated the translocation of polymer chains with classical nucleation theory where the nucleation rate k_0 is assumed to be a constant for each monomer. For the translocation along the chemical potential gradient $\Delta\mu$, τ is proportional to $N(T/k_0\Delta\mu)$ and N^2/k_0 for large and small external bias, respectively. Dubbeldam et al. [22] found that $\tau \sim N^{1.50}$ based on a rigorous mathematical treatment of the fractional Fokker–Planck equation. Both Lubensky et al. [23] and Chuang et al. [24] have found that the translocation time distribution of Gaussian chains has a long tail without the external force.

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* Corresponding author. Tel.: +86 571 88483790; fax: +86 571 87951328.
E-mail address: Lxzhang@zju.edu.cn (L. Zhang).

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In recent simulations [25–43], extensive results have been obtained for various models, methods or conditions. Luo et al. [27] used the bond fluctuating polymer model and Monte Carlo method to simulate the translocation of self-avoiding walk chain in two-dimensional lattices. The self-avoiding walk chains are driven to translocate through a nanopore under an external field which only exists in the nanopore [27]. Their results indicate that the average translocation time versus polymer chain length satisfies $\tau \sim N^{2\upsilon}$ for short chains and it crosses over to $\tau \sim N^{1+\upsilon}$ for long chains, where the value of υ is 0.588 in three-dimensional space (3D) and 0.75 in two-dimensional space (2D) [28]. Kantor et al. [29] simulated the forced translocation using dynamic Monte Carlo method and two-dimensional self-avoiding model. They found a power-law scaling of the average translocation time with chain length and the scaling exponent is 1.53 in 2D, which is less than $1+\upsilon$. Loebl et al. [30] performed Monte Carlo simulation in 3D and showed the average translocation time of self-avoiding short chain scales as N. Milchev et al. [31] investigated polymer translocation through a nanopore induced by adsorption in 3D by dynamic MC simulation method, and they found that there is crossover exponent whose value is 1.65. Dubbeldam et al. [22] used extensive MC simulation means to study the translocation dynamics of polymer chains threaded through a nanopore under a chemical potential. Their results indicate that the average translocation time scales as $\sim N^{1.50}$ in 3D. Vocks et al. [32] used extensive MC simulations and a three-dimensional self-avoiding lattice polymer model to study the driving translocation, and they found that the scaling exponent of average translocation time with chain length is 1.37 for moderate electric field. Luo et al. [33] used molecule dynamics (MD) and Langevin dynamics methods to simulate the polymer translocation process in 3D, and the values of scaling exponents are 1.42 and 1.41, respectively. Fyta et al. [34] got the value of scaling exponent 1.36 using a multiscale approach. Gauthier et al. [36] found a systematic variation of these exponents as a function of the pore width. In a very recent study, Luo et al. [37] indicates that the translocation time distribution (TTD) is influenced by polymer-pore interactions. Some studies [38,39] also demonstrate that multi-peak of translocation time distribution are invoked by many factors, such as temperature, the nanopore size, the nanopore geometry, and so on. The main reason for crossover behavior is that there is obvious hinder effect at the pore exit for long chains while there is no hinder effect for short chains.

In previous studies, more attention is paid to investigating the general polymer translocation. Although the phenomenon of protein translocation is very universal in many biological processes, there have been few studies about it at present [32,38–42]. Proteins are considered as compact polymers [44–46]. The compact structures of compact polymers are the principal configurations of the native states of globular protein. “Compact” refers to those configurations of single-chain molecules which are tightly packed, i.e., fully contained within a volume of space (a box) with the minimal (or near minimal) surface/volume ratio, and compact chains can represent protein chains [46]. Therefore, the translocation of compact polymer chain can be considered simply as the protein translocation. Moreover, lattice model may capture some key features of polymer chains, for instance, chain connectivity, excluded-volume effect, atom–atom contact, etc, and lattice model is easier to embody the hydrogen bond interaction energy than off-lattice model. This is the reason why we use the lattice model to simulate compact chains translocation through a nanopore. In this paper, we concentrate on investigating the scaling properties and translocation time distributions of single compact polymer chain through a nanopore. The results will be useful for understanding the complex translocation behaviors of proteins.

2. Model

In this paper, we use the 3D lattice fluctuating bond model [47] and dynamic Monte Carlo method to simulate the chain translocation through a nanopore. In our model, the bond length b is allowed to vary in the range of $1 \le b \le \sqrt{2}$. Therefore, each monomer can have six nearest and twelve next nearest neighbor sites to walk on a cubic lattice. Fig. 1 shows the schematics of a compact chain translocation in an infinite channel. The channel can be considered as the combination of three parts. The left and right parts are cylindrical with the infinite length, and both radii are $R_\mathrm{l} = R_\mathrm{r} = 4$. The middle part is also a cylindrical pore with finite width of L and radius of $R_\mathrm{m} = 1$. One should note that the basic unit of length is one lattice spacing through the whole paper if not specify, and $R_\mathrm{m} = 1$ means that the radius is one lattice spacing.

The external driving force in this paper is modeled as a potential difference described by an electric field E. The potential [30,47] is expressed as

$$U_\mathrm{e} = \begin{cases} -E\frac{L}{2}, & x > \frac{L}{2} \quad \text{and} \quad z^2 + y^2 \le R_\mathrm{m}^2 \\ -Ex, & \frac{L}{2} \ge x \ge -\frac{L}{2} \quad \text{and} \quad z^2 + y^2 \le R_\mathrm{m}^2 \\ E\frac{L}{2}, & x < -\frac{L}{2} \quad \text{and} \quad z^2 + y^2 \le R_\mathrm{m}^2 \\ \infty, & \text{otherwise}, \end{cases} \tag{1}$$

The channel walls are neutral and can't be penetrated. All monomers interact with each other via contacts [45,46]

$$U = \sum_{|i-j| \ge 3} \varepsilon_\mathrm{C} \delta(r_{ij} - a), \tag{2}$$

where r_{ij} is the distance between monomers i and j. ε_C is the contact energy. $\delta(x) = 1$ for $x = 0$ and $\delta(x) = 0$ for $x \ne 0$. Monomers i and j can form a contact if they are in two adjacent lattice sites while not adjacent along the chain. All the contact energy and electric field strength in our simulation are taken in units of $k_\mathrm{B}T$.

Trial movements with a probability of acceptance $\min[\mathrm{e}^{-\Delta U/k_\mathrm{B}T}, 1]$ are used here [48,49], where ΔU is the energy difference between the new and old configurations. Firstly, a monomer is chosen randomly and attempted to move to one position of eighteen adjacent lattice sites. If the new position does not violate the excluded-volume interaction, or bond-length restriction and no bond crossover, the move is accepted according to acceptance probability. If the new position only leads to one bond breakup, the reputation is introduced and it is continued until a valid polymer conformation is obtained. The move will be rejected else. In this study, the translocation time t is measured in units of Monte Carlo step (MCS). One MCS means the average moves of every monomer at once.

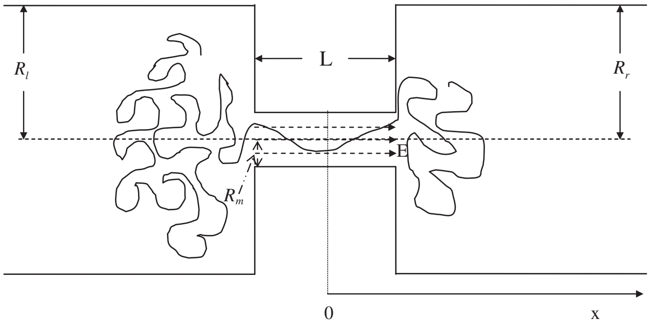

Fig. 1. Schematics of a compact polymer chain translocation through a nanopore. Here $R_\mathrm{l} = 4$, $R_\mathrm{m} = 1$, $R_\mathrm{r} = 4$, and the nanopore width is L.

3. Results and discussion

Following the method of previous studies [22,25,27,30,33,39,50,51], we fix the first monomer of chain at the entrance of nanopore at the beginning of simulation, while other monomers are in the left channel. The chain is then allowed to relax in the left part of nanopore. Once the energy of chain has only a little fluctuation, the first monomer is released, and this moment is designated as $t = 0$. To avoid the situation in which the chain withdraws from the hole and drifts away to infinity, we impose a limitation on the translocation that the first monomer is never allowed to cross back out of the pore [22,24,25,29,52]. Duration time, which takes for the chain to just move through the pore, is defined as the translocation time t. Typically, we average our data over 5000 independent runs.

3.1. *Effects of contact energy and external field on the average translocation time*

We first study the effects of contact energy ε_C on the average translocation time τ. Here τ is acquired by averaging translocation time of over 5000 independent runs. Contact energy has great effects on the average translocation time τ, as shown in Fig. 2a. Here $L = 4$, and $E = 1.0$. There is crossover behavior for all chains, and the values of scaling exponent α increase with contact energy decreases for both short and long chains. For short SAW chains (self-avoiding walk chains), $\tau \sim N^{1.04}$ is observed, while the slope becomes 1.32 ± 0.01 for long SAW chains. MC simulation results of Chern et al. [53] and Langevin dynamics simulation results of Forrey et al. [54] indicate that there should be a linear scaling behavior for short SAW chains. The simulation results of Izmitli et al. [55] show that the scaling exponent of average translocation time with chain length N is 1.31 ± 0.3 without hydrodynamic interaction for long SAW chains. Therefore, their results have confirmed the validity of our simulation method and lattice model.

Fig. 2a shows that the values of α for short and long chains increase from 1.04 to 1.31 and 1.32 to 1.92, respectively, with ε_C decreasing from 0 to -1.0. In addition, the crossover behavior becomes more remarkable as ε_C is decreased. In fact, for a given chain length, the average translocation time should be increased as ε_C decreases, since longer time is needed to unfold more compact structures. For long chains, because of their flexibility, their configuration is more compact than that of short chains, resulting in slower translocation velocities. Moreover, there are hinder effects for long chains: when most of monomers have entered the right channel, it is difficult for them to diffuse away without the help of external field, leading to the deposition of monomers at the pore exit. Also, the density profiles of monomers near the pore exit should be increased as the contact energy decreases. These may be the main reason for the crossover behaviors.

In order to understand the translocation in more detail and to confirm the phase states of chains with different contact interactions, we also investigate the coil–globule and globule–solid transitions by calculating the heat capacity C_V, and the results for 150-bond chain are given in Fig. 2b. When the contact energy decreases, the polymers have three main phases: the coil, the disordered globule, and the chain-folded 'crystalline' structures. Our results are in good agreement with previous results [56]. The critical phase transition points are located at $\varepsilon_C = -0.5$ and -3.2, respectively. The configuration is the coil structure for $\varepsilon_C > -0.5$, and it is the disordered globule structure for $\varepsilon_C < -0.5$. Thus, due to the coil-globule transition at $\varepsilon_C = -0.5$, the crossover behaviors for $\varepsilon_C < -0.5$ are more remarkable than that for $\varepsilon_C > -0.5$, as shown in Fig. 2a. Here the mean radius of gyration of polymer chain $R_g \equiv \sqrt{\langle R_g^2 \rangle}$ is also calculated, and our results for 150-bond polymer chains are $R_g = 9.28$ and 2.80 for contact energy $\varepsilon_C = 0$ and -1.0, respectively, which is 8.3 and 1.8 times larger than the nanopore size. We also calculate the shape factor $\langle \delta \rangle$, which is defined as [57,58]

$$\langle \delta \rangle = 1 - 3\left\langle \frac{\left(L_1^2 L_2^2 + L_1^2 L_3^2 + L_2^2 L_3^2\right)}{\left(L_1^2 + L_2^2 + L_3^2\right)^2} \right\rangle \tag{3}$$

where L_1, L_2, and L_3 are the principal components of the squared radius of gyration $R_g^2 = L_1^2 + L_2^2 + L_3^2$ of individual configurations taken along the principal axes of inertia, and the results are $\langle \delta \rangle = 0.05$ for compact chains with contact energy $\varepsilon_C = -1.0$ and $\langle \delta \rangle = 0.43$ for SAW chains ($\varepsilon_C = 0$). As $\langle \delta \rangle = 0.0$ means that the structure of chains is sphere, the compact chains with $\varepsilon_C = -1.0$ is sphere structure. The compact polymer must be unfolded when the chains translocate through the nanopre.

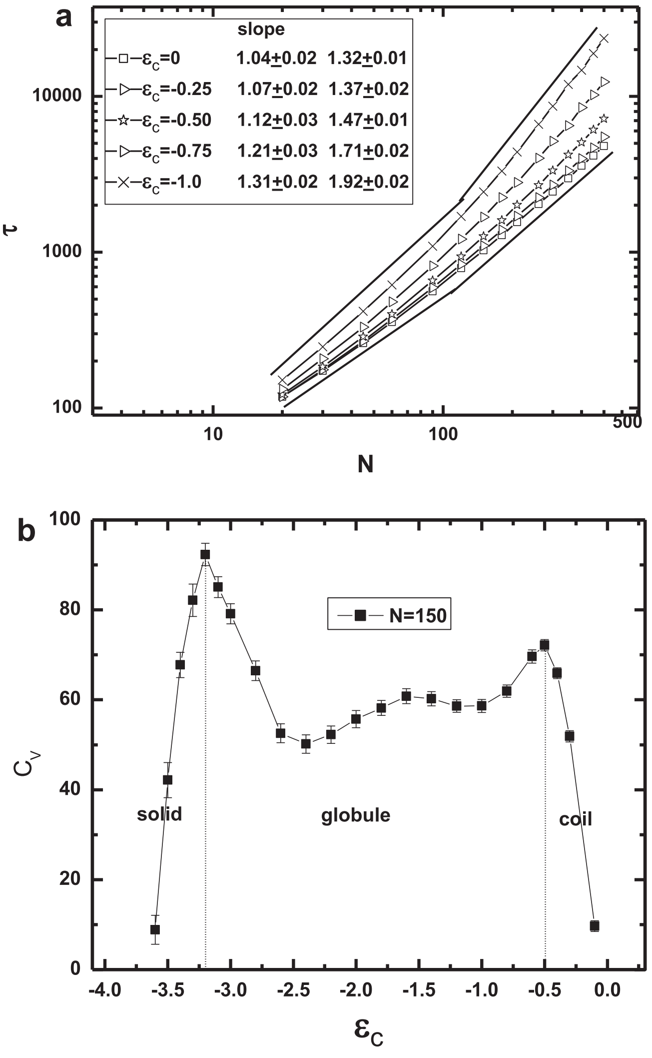

Fig. 2. (a) Mean translocation time τ as a function of chain length N with different contact energies. Here the electric field strength is $E = 1.0$ and the nanopore width is $L = 4$; (b) the heat capacity C_V as a function of ε_C.

The influences of the external electric field E on the translocation of compact chains are also studied. Fig. 3a and b show the dependence of τ on N with three different electric field strengths for the contact energies $\varepsilon_C = -0.5$ and -1.0, respectively. There are also crossover behaviors for all cases. In Fig. 3a, the scaling exponents of short chains are $\alpha = 1.15$, 1.12 and 1.08 for electric field strengths $E = 0.5$, 1.0 and 3.0, respectively. The scaling exponent decreases

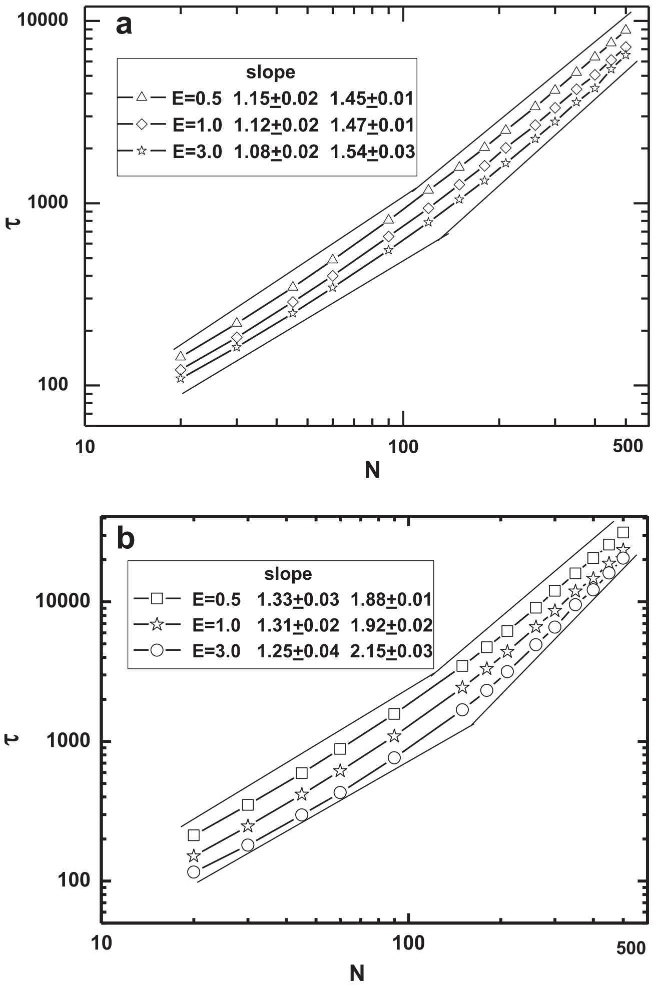

Fig. 3. Mean translocation time τ as a function of chain length N with different electric field strengths and different contact energies. (a) contact energy $\varepsilon_C = -0.5$; (b) contact energy $\varepsilon_C = -1.0$. Here $L = 4$.

when the electric field strength E is increased. On the contrary, the scaling exponents of long chains increase from 1.45 to 1.54 when the electric field is increased from 0.5 to 3.0. Similar results are also obtained in Fig. 3b.

The above results show the scaling exponent value decreases for short chains when the electric field is increased while it increases for long chains. The simulation results of Luo et al. [27] indicate that the density of monomers near the pore exit is much higher for a long chain than for a short chain. Therefore, the density of monomers in the right channel has little influence on the translocation velocity for short chains. The larger the external electric field is, the faster the chain translocates. At the late stage of translocation, the free energy difference between the chains in the left and the right parts will accelerate the translocation. It may be the reason why the values of scaling exponent decreases when the electric field is increased for short chains. For long chains, increasing the external force can speed up translocation velocity at the early stage, leading many monomers to get together quickly at the pore exit. Because there are the attractive interactions between monomers and without any electric field, it is difficult for translocated monomers to diffuse away from the pore exit for a short time, and these translocated monomers block the translocation of other monomers. Therefore, the scaling exponents of long chains increase when the electric field strength is increased, which is consistent with previous results [51].

3.2. *Effects of nanopore width on the average translocation time*

In order to investigate the influence of the nanopore width on the crossover behavior and the scaling exponent of average translocation time, we carry out three simulations for nanopore widths of $L = 1$, 8, and 12. At first, we study translocation behaviors for $L = 1$, and $L = 1$ means the width of the nanopore is one lattice spacing. In Fig. 4, there is no crossover behavior for compact chains at $E = 1.0$. The relation between the scaling exponent α and contact energy is different from that of $L = 4$. The scaling exponent of α for SAW chain ($\varepsilon_C = 0$) is 1.55, which is very close to the simulation and theoretical results of Dubbeldam et al. [22]. Lehtola et al. [59] also got similar result of $\alpha = 1.50 \pm 0.04$ at force $f = 1.0$ in 3D. Our result is also consistent with the scaling relationship of $\tau \sim N^{1+\nu}$ in 3D. In Fig. 4, the value of α decreases from 1.55 to 1.44 and then increases from 1.44 to 1.74 when contact energy decreases from 0 to -1.0. The different behavior of α as a function of contact energy ε_C can be explained by the coil-globule transition which can be seen in Fig. 2b. It is the coil structure for $\varepsilon_C > -0.5$, and the disordered globule structure for $\varepsilon_C < -0.5$. Thus, the chain configuration has great influence on the translocation process.

In Fig. 5a, the contact energy is $\varepsilon_C = -0.5$, and there are no crossover behaviors for $E = 0.5$ and 1.0. However, we can observe crossover behavior when the electric field strength is larger than or equal to 3.0. The scaling exponent α for short chains decreases a little and it increases a little for long chains when the electric field E is increased with $E > 3.0$. Similar results are also obtained for compact chains with $\varepsilon_C = -1.0$, as shown in Fig. 5b.

The nanopore is very short for $L = 1$, therefore the voltage drop between two ends of nanopore is very small, and it leads to a slow translocation. Under this condition, the translocated monomers have enough time to diffuse away from the vicinity of nanopore exit. Therefore, there is no hinder effect in the translocation process for both short and long chains, i.e., there is no crossover behavior at $E = 1.0$. What leads to the “V” tendency for the scaling exponent α when the contact energy decreases for $E = 1.0$ and $L = 1$? The compact chains with $\varepsilon_C > -0.5$ is the coil configuration before the translocation, and their free energy barriers are low. The electric field force is large enough to overcome their free energy barriers. Furthermore, the translocated monomers take the role of an attractive wall so that they can accelerate the translocation velocity. Therefore, the value of α decreases with contact energy decreases, which is consistent with the previous results [24]. When the contact energy ε_C is less than -0.5, the configuration is the globule

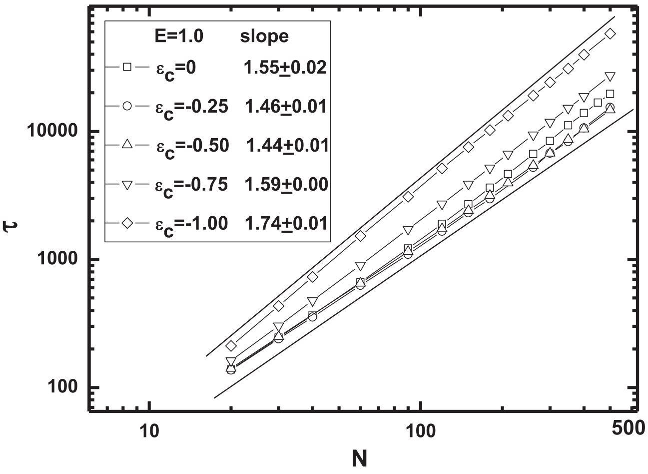

Fig. 4. Mean translocation time τ as a function of chain length N with different contact energies. Here $E = 1.0$ and $L = 1$.

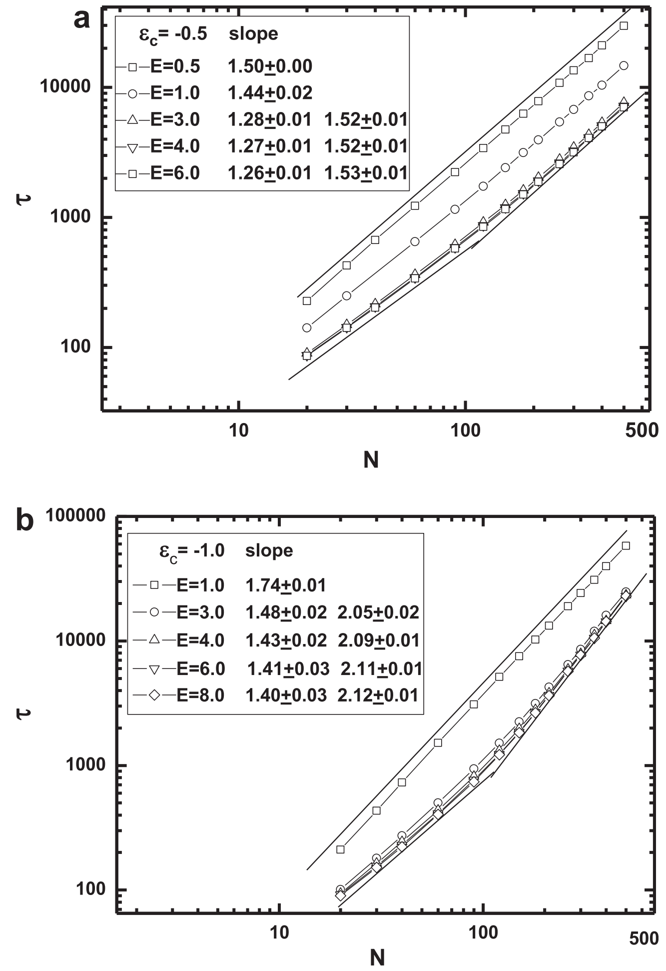

Fig. 5. Mean translocation time τ as a function of chain length N with different electric field strengths E and different contact energies. (a) contact energy $\varepsilon_C = -0.5$; (b) contact energy $\varepsilon_C = -1.0$. Here $L = 1$.

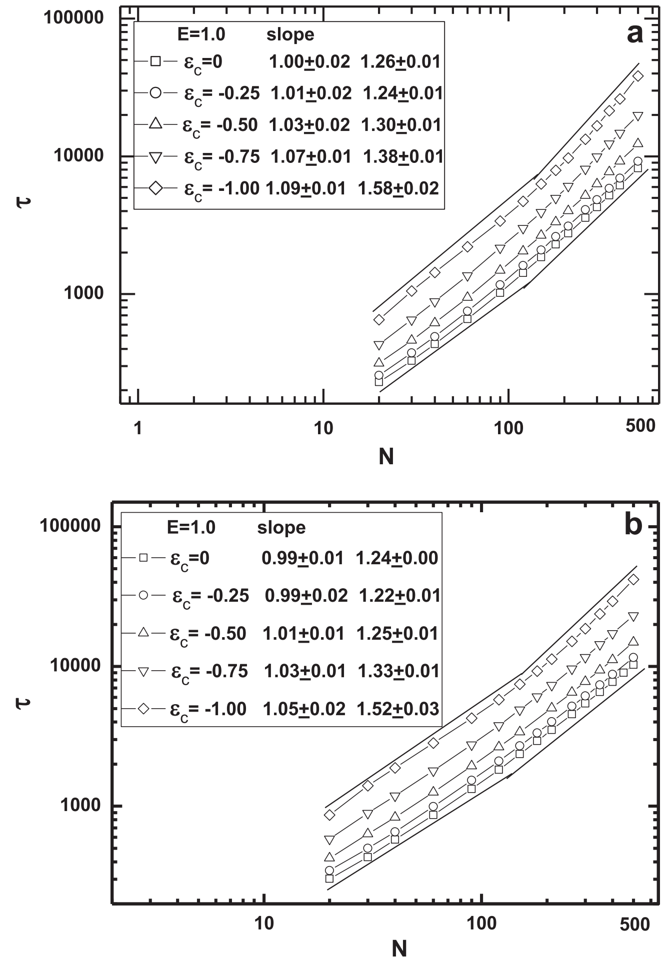

Fig. 6. Mean translocation time τ as a function of chain length N with different contact energies ε_C and different nanopore widths L. (a) $L = 8$; (b) $L = 12$. Here $E = 1.0$.

before the translocation, and their free energy barriers are higher. The electric field force is not enough to overcome the free energy barriers. The monomers of left part enter nanopore by biased diffusion, and the biased diffusion becomes very obvious. Therefore, the value of α increases with the contact energy decreases. When the electric field strengthens, the voltage drop increases, leading to large translocation velocities at the beginning. Moreover, monomers move only one unit lattice length to enter the right channel. Therefore, many monomers have entered the right channel quickly at the initial stage. The translocated monomers do not have enough time to diffuse away from the vicinity of nanopore exit, resulting in the decrease of translocation velocities. Hence we can observe the crossover behavior in Fig. 5 for large electric fields. From the simulation results we suggest that crossover behaviors are mainly caused by hinder effects, which is in agreement with previous studies.

We also consider larger pore widths of $L = 8$, and 12, and the results are shown in Fig. 6a and b, respectively. All cases have crossover behaviors, but they are less remarkable than those of $L = 4$. As the contact interaction ε_C decreases, the value of α for short chains increases monotonously, but for long chains it decreases a little first and then increases. The result of long chain is different from that of $L = 4$. We also note that the corresponding values of α for various cases are almost the same for $L = 8$ and 12. For short chains, the value of α is close to 1.0 for $L = 8$ and 12. For long chains, the value of α varies between 1.26 and 1.58 as well as 1.24 and 1.52 for $L = 8$ and 12, respectively. On one hand, the voltage drop increases with the increase of L and then more monomers are imposed the electric field force during the translocation, leading to a faster translocation. On the other hand, the chain needs to move a longer distance to enter the right part completely with the increase of L. As a result, it takes the chain a longer time to translocate through the nanopore. Hence, we think that the two factors should compete with each other during the translocation. Our simulation results may be useful for designing valid pore or membrane widths for protein translocation and sieving.

3.3. *The distribution of translocation time*

In this section, the translocation time distribution (TTD) of compact chains with $L = 4$ is discussed. Here the TTD is defined as the number of samples whose translocation times lie between t and $t + \Delta t$ $(0 < t < t_{\max})$. The result is based on the statistics of translocation time of 5000 independent samples, and it is very helpful for us to understand the translocation process. Huopaniemi et al. [60] found that the TTD shifts from the multi-peak distribution to Gaussian distribution when the electric field strength is increased. However, the TTD of compact chains is different from that of SAW chains, as shown in Fig. 7. Here ε_C is set as -1.0, and its equilibrium configuration is globule before the translocation. For weak electric field, the TTDs are Gaussian distribution for $N = 90$, 210, and 350, seen in Fig. 7a. The reason is that the electric field force is not strong

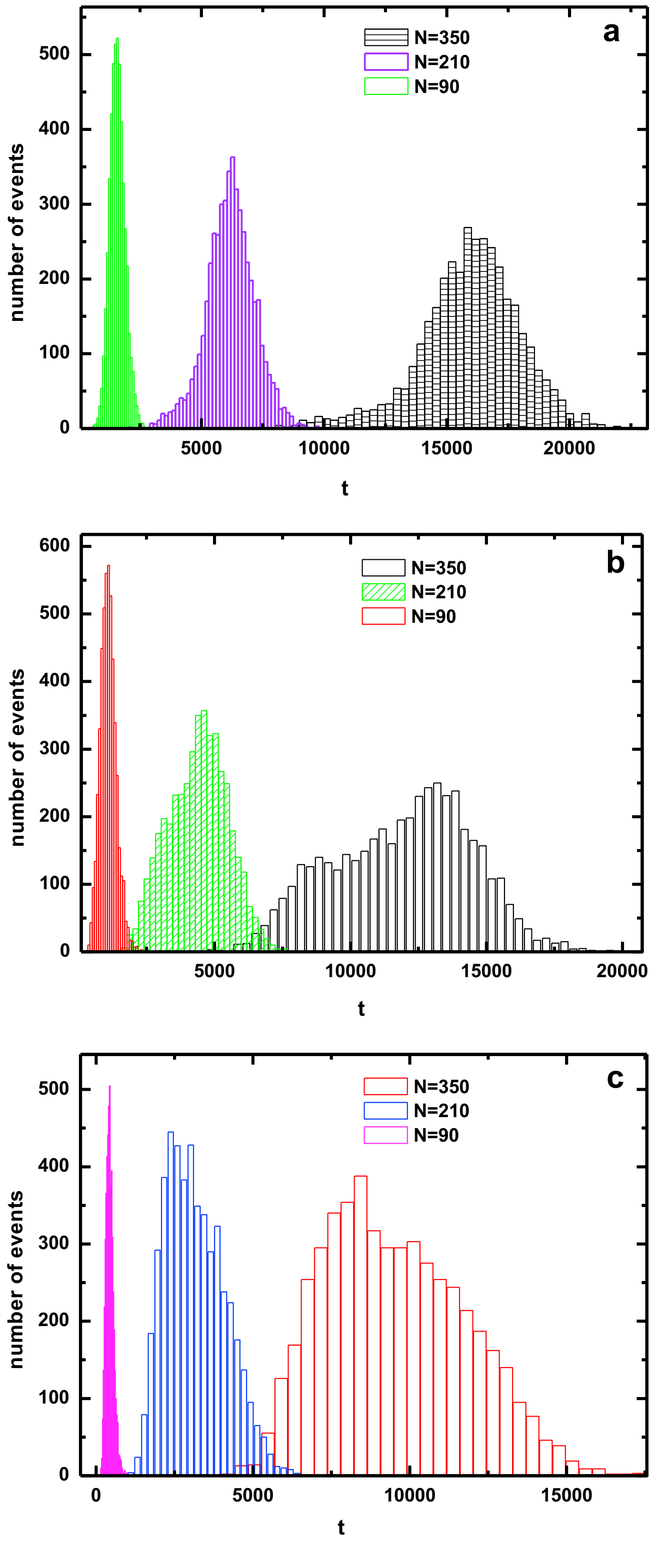

Fig. 7. Distributions of translocation time for compact chains with different chain lengths *N* and different electric field strengths *E*. (a) $E = 0.5$, (b) $E = 1.0$, and (c) $E = 3.0$. Here $\varepsilon_C = -1.0$.

enough to overcome the free energy barrier so that the compact chains translocate through the pore by biased diffusion. Because of the attractive interaction between the monomers for compact chains, the monomers, which are far away from the pore entrance, get together compactly in the vicinity of the pore entrance during the slow translocation. It leads to a little difference in the configuration of subchain in the left part among the independent samples before the first monomer enters the right part. Therefore, the translocation time distribution is the Gaussian distribution.

When the electric field strength is increased to $E = 1.0$, the TTDs do not satisfy Gaussian distribution in Fig. 7b. For $N = 90$, there is a short tail on the right. For $N = 210$ and 350, their TTDs are two-peak distributions. The main peak is on the right, while the sub-peak is on the left. However, the left peak of $N = 350$ is more obvious than that of $N = 210$. Peak distribution of long compact chain is completely contrary to SAW chains [39]. Because the electric field force is just large enough to overcome the free energy barrier, the influence of the local minimum free energy of the compact chain on the TTD becomes obvious. At $E = 3.0$, the translocation time distributions are very similar for different chain lengths, as shown in Fig. 7c. All of them have a tail on the right and it becomes more obvious for larger *N*. Maybe, the electric field is large enough to make the monomers translocate relatively fast at the beginning of the translocation. The influence of subchain configuration in the left part becomes weak. However, when most of monomers are in the right part, the monomers are hard to diffuse away from the pore exit within a short time. Therefore, the translocation velocity slows down greatly. The tendency of TTDs for short and long chains is different when the electric field is increased, and the TTDs of compact chains are different from that of SAW chains.

In order to investigate the effect of contact energy on the translocation time distribution, the simulations of 350-bond chains with different contact energies are carried out. Here *E* is set as 1.0. The TTD becomes wider and wider, and shifts from Gaussian distribution to multi-peak distribution with the contact energy decreases, as shown in Fig. 8. It is Gaussian distribution for $\varepsilon_C = 0$, and two-peak distribution for $\varepsilon_C = -0.5$. When the attractive interaction between the monomers increases again, the height of left peak increases and the difference in height between the left and right peaks decreases. It indicates that the contact energy has great influence on the TTD. Because of local minimum free energy, some configurations are relatively extendable, and the others are relatively compact before the translocation. Moreover, the free energy barrier rises when the attractive interaction between monomers becomes strong. As indicated in Ref. [54], the translocation process is dominated by the initial configuration of the chains. Therefore, the influence of the configuration on the translocation time

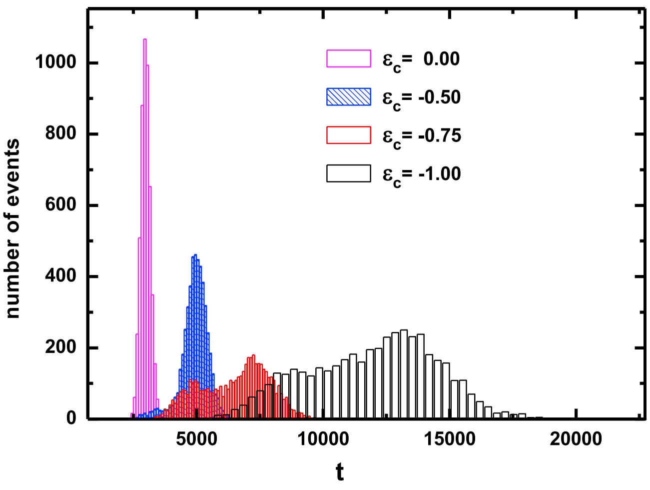

Fig. 8. Distribution of translocation time for 350-bond chain with different contact energies ε_C. Here $E = 1.0$.

becomes obvious during the driven translocation for compact chains. Because the configuration is the coil structure for $\varepsilon_C > -0.5$, and it is the disordered globule structure for $\varepsilon_C < -0.5$, the TTDs of compact chains are different from that of SAW chain.

4. Conclusions

In this work, we have investigated the translocation of compact chains through a small pore under an electric field using the 3D fluctuating bond model and dynamic Monte Carlo method. The effects of electric field strength (E), chain length (N), contact energy (ε_C) and nanopore width (L) on the scaling behavior of average translocation time and translocation time distribution are studied. There is the coil-globule transition at $\varepsilon_C = -0.5$. The contact energy has influence on the scaling exponent α of average translocation time. For short nanopore width L, the value of α depends on contact energy ε_C and nanopore width L. For long nanopore width L, the effects of nanopore width L on average translocation time can be ignored. For $L = 1$, there is no crossover behavior for SAW chains and compact chains at $E = 1.0$. However, the crossover behavior appears when the electric field E becomes very strong. For $L = 4$, there is very obvious crossover behavior. When L is increased to 8 or 12, the crossover behavior becomes weak, compared with the results of $L = 4$ and the value of scaling exponent α nearly keeps constant. Moreover, the value of α increases with ε_C decreases and the effects of electric field on α are obvious.

The TTD depends on the chain length (N), electric field (E), and contact energy (ε_C). For short chains, the TTD shifts from the Gaussian distribution to a right-skew distribution with the electric field E increases. For long chains, it has an interim process that its TTD is multi-peak distribution, and the TTD also depends on the contact energy and the TTD changes from Gaussian distribution to multi-peak distribution with contact energy decreasing from 0 to -1.0. We hope this study can help us to understand the complex mechanism of protein translocation, and will be useful for designing valid pore or membrane widths for the translocation and sieving of different proteins.

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