Effect of channel–protein interaction on translocation of a protein-like chain through a finite channel*

Sun Ting-Ting(孙婷婷)[a)†], Ma Hai-Zhu(马海珠)[a)], and Jiang Zhou-Ting(姜舟婷)[b)]

[a)] *School of Information and Electronic Engineering, Zhejiang Gongshang University, Hangzhou* 310018, *China*
[b)] *Department of Physics, China Jiliang University, Hangzhou* 310018, *China*

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We study the translocation of a protein-like chain through a finite cylindrical channel using the pruned-enriched Rosenbluth method (PERM) and the modified orientation-dependent monomer–monomer interaction (ODI) model. Attractive channels ($\varepsilon_{cp} = -2.0, -1.0, -0.5$), repulsive channels ($\varepsilon_{cp} = 0.5, 1.0, 2.0$), and a neutral channel ($\varepsilon_{cp} = 0$) are discussed. The results of the chain dimension and the energy show that $Z_0 = 1.0$ is an important case to distinguish the types of the channels. For the strong attractive channel, more contacts form during the process of translocation. It is also found that an external force is needed to drive the chain outside of the channel with the strong attraction. While for the neutral, the repulsive, and the weak attractive channels, the translocation is spontaneous.

Keywords: pruned-enriched Rosenbluth method, translocation, protein-like chain

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1. Introduction

The translocation of biopolymers (DNA and proteins) across nanopores or channels plays a critical role in numerous biological processes, such as the translocation of DNA and RNA across nuclear pores, the DNA packaging into viral capsids, gene swapping, the virus infection of cells, the translocation of protein through membrane channels,[1,2] and the translocation of nascent proteins inside the ribosomal tunnel or across the endoplasmic reticulum.[3−6] Moreover, translocation processes have various potential technological applications, such as rapid DNA sequencing, gene therapy, and controlled drug delivery.[7−9] Therefore, biopolymer translocation has attracted the attention of a large number of scientists.

Although the actual biological system is complicated due to many biological factors, a primitive model including a polymer chain and a small hole (or a channel) is always used to understand the basic physical process of translocation. There are a number of theoretical studies and simulations of polymer translocation.[10−28] Sung and Park[1] have studied the transport of a Gaussian chain under the special condition that the segment friction across the pore is proportional to the polymer length. Muthukumar[11] has treated the process with the classical nucleation theory in which the monomer friction is taken to be dictated by the ratchet potential associated with the pore. In another of his works,[12] the free energy barrier and the mean translocation time have been studied for the movement of a single Gaussian chain from one sphere to another larger sphere through a narrow pore. Recent simulation studies[13,14] have shown that it is possible to capture many essential features of the translocation process using an appropriate one-dimensional model. In fact, a number of simulation methods[15−36] are effectively used in polymer physics. In the translocation process, the external field,[15−20] the chemical potential gradient,[19,21] the confinement,[22] the adsorption,[23] and the unbiased translocation[20,24−27] have been considered.

In recent years, the study of protein translocation has been developed based on some protein-like models. For example, Zhang and Chen[28] have investigated the translocation of compact chains on a simple-cubic lattice. Only the attractive interaction between polymers and channels was considered, the repulsive chan-

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†Corresponding author. E-mail: Tingtingsun@mail.zjgsu.edu.cn

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nel was not taken into consideration. At the same time, in the process of compact polymers escaping from a small sphere through a hole, the free energy barrier was investigated.[35] The result was in accordance with the theoretical study. Later, we also used the orientation-dependent monomer–monomer interaction (ODI) model and the pruned-enriched Rosenbluth method (PERM) to simulate the process of the protein-like chain escaping from a finite channel.[37] An energy barrier was found in the work, but no free energy barrier was found. Only a neutral channel was considered in the former work, the important influence of the channel–protein interaction was not mentioned. However, some experimental results have implied that the interaction might play an important role in the chain translocation through small pores or narrow channels.[38,39]

A few studies show that protein translocation is significantly affected by the surrounding environments and the membrane–protein interactions. However, how channel–protein interaction affects translocation is not clear. Therefore, in the present work, we study another interesting problem, that is, how channel–protein interaction influences the translocation of a protein-like chain through a finite cylindrical channel by using the PERM method[35,37] with our previous modified ODI model.[40,41] The attractive and the repulsive channels are both considered in this work. The investigation shows how the dimension and the energy change in the process of translocation out of different channels. The rest of the present paper is organized as follows. In Section 2, we introduce the model as well as the simulation methods. In Section 3, we present our simulation results and some discussions. We draw some conclusions from the present study in Section 4.

2. Method of calculation

We use the modified ODI model,[21,22] which is based on the ODI model.[24] In this model, a protein-like chain is schematically viewed as a linear sequence, and the chains are constrained to be nearest-neighbors on a three-dimensional cubic lattice. Each lattice site can be occupied by only one monomer. The merit of our model is that the α-helical and the β-sheet structures can be taken into account simultaneously. Therefore, the model is much better in describing the real protein. In the model, the energy of the protein-like chain is assumed to contain four terms

$$E = \sum_{|i-j|\geq 3} \varepsilon_{\rm c}\delta(r_{ij}-a) + \sum_{\substack{|i-j|\geq 3 \\ \boldsymbol{r}_i+\boldsymbol{s}_i=\boldsymbol{r}_j}} \varepsilon_{\rm b}\delta(r_{ij}-a) + \sum_{i=1}^{N-1} A(\boldsymbol{s}_i\cdot\boldsymbol{s}_{i+1}) + \varepsilon_{\rm h} n_{\rm h}, \quad (1)$$

where r_{ij} is the distance between monomers i and j; a is the lattice spacing ($a = 1$ in our calculation); $\delta(x) = 1$ for $x = 0$, and $\delta(x) = 0$ for $x \neq 0$; $\boldsymbol{s}_i$ is the unit vector that represents the orientation of the monomer; $\boldsymbol{s}_i \cdot \boldsymbol{s}_{i+1}$ is the scalar product of the orientation vectors; $\varepsilon_{\rm c}$ is the energy of one contact; and $\varepsilon_{\rm b}$ corresponds to the hydrogen bond in the topological contact. Monomers i and j will form a contact if they are adjoining lattice sites but not adjacent along the chain. The first term on the right-hand side of Eq. (1) represents the total contact energy of the chain. Bearing in mind the conditions necessarily for the formation of the hydrogen bonds, we consider the value of $\varepsilon_{\rm b}$ to be negative if (i) one of the monomers is directed toward the other monomer (e.g., $\boldsymbol{r}_i + \boldsymbol{s}_i = \boldsymbol{r}_j$), and (ii) vectors $\boldsymbol{s}_i$ and $\boldsymbol{s}_j$ are parallel to each other simultaneously. In all other cases, $\varepsilon_{\rm b} = 0$. The second term on the right-hand side of Eq. (1) is the β-sheet energy. The third term (with A > 0), constructed in analogy to the Ising antiferromagnetic spin–spin interaction, describes the orientational dependence of the interaction between the nearest-neighbor monomers linked via peptide bonds, and reproduces an antiparallel orientation of the nearest-neighbor monomers. In the last term, $\varepsilon_{\rm h}$ is the energy of one helix, $n_{\rm h}$ is the number of the helices in the chain, $\varepsilon_{\rm h} n_{\rm h}$ represents the total energy of the helices. Therefore, the α-helical and the β-sheet energies are both considered in the conformational energy. In this paper, we use $\varepsilon_{\rm h} = -0.5$ and $\varepsilon_{\rm b} = -0.5$ (in units of kT, k is the Boltzmann constant, T is the temperature).

A new and effective simulation method called the pruned-enriched Rosenbluth method (PERM) is used here.[19,20] This algorithm has been used for simulating flexible chain polymers, and their results illuminate that this method is the most efficient one for simulating three-dimensional polymers on the simple-cubic lattice. The PERM can replace the enumeration calculation method, and it can be used to calculate the partition function. Therefore, the PERM was widely used in earlier simulations.[25,26]

Figure 1 shows the schematic diagram of a protein-like chain through a finite cylindrical channel along the Z axis. The radius of the channel is R. The length of the channel is L, which is twice of the chain length N. The channel walls are impenetrable. In our model, the first monomer of the protein-like chain will start from the center of the channel and extend to a place which is L distance away from the channel exit. The reason for adopting such a model is that many studies[6,27−28] have revealed that a tunnel running through the large ribosomal subunit is the path followed by the nascent polypeptide from the peptidyl transferase center to the exit. We count the total conformations with different values of Z and with different interactions between the channel and the protein chain. Our aim is to investigate how the protein-like chain escapes through the channel and how the size and the energy change in the process of translocation. Here, we use $N = 50$ and $L = 100$.

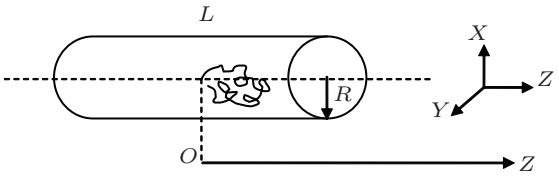


Fig. 1. Schematic diagram of protein-like chain confined in a finite cylindrical channel along the Z axis.

The partition function of the system is

$$\Omega = \sum_i \exp(-E_i/kT), \tag{2}$$

where $\sum_i$ is the sum of all conformations at different position Z. The average Helmholtz free energy of the protein-like chains can be obtained from the partition function

$$A = -kT \ln \Omega. \tag{3}$$

This parameter can supply much important thermodynamic information about the chains.[37,38] At the same time, the mean-square end-to-end distance, the mean-square radius of gyration, and the average energy can be deduced from the partition function.[35]

We define Z_0 as

$$Z_0 = \frac{Z_{\rm f}}{N}, \tag{4}$$

where $Z_{\rm f}$ is the Z coordinate of the first monomer, and the influence of chain length N is ignored. In our simulation, the value of Z_0 ranges from 0 to 1.5.

3. Results and discussion

3.1. Chain dimension and shape

Figure 2 presents the end-to-end distance per bond $\langle R^2\rangle/N$ versus Z_0 for the protein-like chains with different values of channel–protein interaction $\varepsilon_{\rm cp}$. Channel radius $R = 1$ is used. For the chain inside the channel, the values of $\langle R^2\rangle/N$ are 23.48, 2.49, 2.69, 5.48, 20.11, 42.81, and 46.30 respectively corresponding to $\varepsilon_{\rm cp}$ of −2.0, −1.0, −0.5, 0, 0.5, 1.0, and 2.0. It is shown that $\langle R^2\rangle/N$ has a minimum inside the weak attractive channel, and $\langle R^2\rangle/N$ increases as $\varepsilon_{\rm cp}$ increases from zero to a positive value (repulsive interaction). However, due to the strong attractive interaction, the monomers of the chain are attracted to the channel surface, therefore the dimension of the chain obviously increases. From these findings, it is obviously that the attractive and the repulsive channel–protein interactions both influence the chain dimension confined inside the channel.

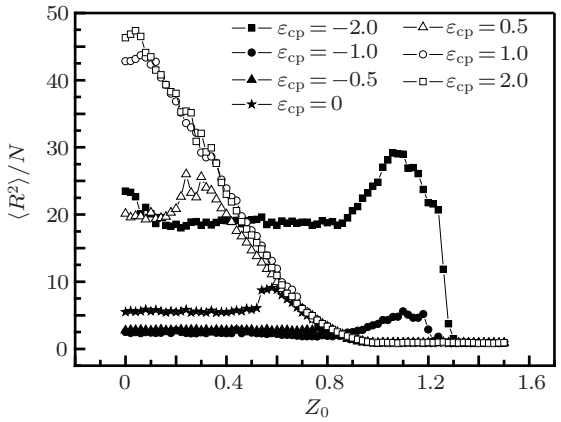


Fig. 2. Mean-square end-to-end distance per bond $\langle R^2\rangle/N$ vs. Z_0 for protein-like chains with different channel–protein interactions. Here, chain length $N = 50$ and channel radius $R = 1$.

We further investigate the change of the chain dimension during the translocation. For the neutral channel ($\varepsilon_{\rm cp} = 0$), it is found that $\langle R^2\rangle/N$ hardly changes when Z_0 is between 0 and 0.5 ($\langle R^2\rangle/N = 5.4$). It increases with Z_0 increasing from 0.5 to 0.6 ($\langle R^2\rangle_{\rm max}/N = 9.2$), and then decreases until $Z_0 = 1$ ($\langle R^2\rangle/N = 0.85$). This trend is similar to that of $\langle S^2\rangle/N$ in our earlier work.[37] Then, we find the values of repulsive interaction, $\varepsilon_{\rm cp} = 1.0$ and 2.0. The value of $\langle R^2\rangle/N$ is relatively large inside the channel, then increases slightly, and finally drops quickly to a small value at about $Z_0 = 1$ ($\langle R^2\rangle/N = 0.85$). The peaks are found to be at 0.04 and 0.06 for $\varepsilon_{\rm cp} = 1.0$

and 2.0, respectively. However, for the weak repulsive interaction ($\varepsilon_{\rm cp} = 0.5$), $\langle R^2\rangle/N$ keeps unchanged when Z_0 is between 0 and 0.2, then it has two peaks near $Z_0 = 0.3$. The trend behind it is quite similar to that in the case of other repulsive interactions. At the same time, the peak is not obvious for the weak attractive interaction ($\varepsilon_{\rm cp} = -0.5$). The value of $\langle R^2\rangle/N$ decreases as Z_0 increases to be larger than 0.76. For the strong attractive interaction ($\varepsilon_{\rm cp} = -1.0, -2.0$), $\langle R^2\rangle/N$ has maximum values at $Z_0 = 1.1$ ($\langle R^2\rangle/N = 5.70, 31.40$). At $Z_0 = 1.2$ and 1.3, $\langle R^2\rangle/N$ changes to 0.85. It shows that the strong channel–protein attractive interaction influences the chain dimension in the later process of the translocation ($Z_0 > 1.0$), while the repulsive, the neutral, and the weak attractive interactions affect the chain dimension in the early stage of the translocation ($Z_0 < 1.0$).

In the present simulations, the shape of the protein-like chain is observed by monitoring shape factor $\langle\delta^*\rangle$. The instantaneous shape of an individual configuration may be described by several ratios based on the principal components $L_1^2 \le L_2^2 \le L_3^2$ of $S^2 = L_1^2 + L_2^2 + L_3^2$, i.e., the orthogonal components of the squared radius of gyration taken along the principal axes of inertia.[39,40] The $\langle\delta^*\rangle$ is obtained by combining the components of S^2 to a single quantity that varies between 0 (sphere) and 1 (rod),[41,42]

$$\langle\delta^*\rangle = 1 - 3\left\langle \frac{L_1^2L_2^2 + L_2^2L_3^2 + L_3^2L_1^2}{(L_1^2 + L_2^2 + L_3^2)^2} \right\rangle. \qquad (5)$$

Figure 3 shows the shape factors $\langle\delta^*\rangle$ of the protein-like chains each as a function of Z_0 with $R = 1$. Different values of channel–protein interaction $\varepsilon_{\rm cp}$ are considered. It is shown that for $\varepsilon_{\rm cp} = -1.0$ and -2.0, the values of $\langle\delta^*\rangle$ are about 0.88 and 0.97 at $Z_0 < 1.0$. In the range of Z_0 from 1.0 to 1.1, they both have maximum values, which are 0.97 and 0.99, respectively. The values drop quickly until $Z_0 = 1.2$ and 1.3, where $\langle\delta^*\rangle$ is about 0.28. It is clear that for the strong attractive interaction, the influence on the chain shape happens when Z_0 is between 1.0 and 1.3. The chain shape changes from rod to sphere. However, it is found that for weak attraction ($\varepsilon_{\rm cp} = -0.5$), $\langle\delta^*\rangle$ is 0.89 when the chain is inside the channel. The value drops when $Z_0 > 0.7$, the conformation of the chain changes earlier compared to that of the strong attraction. When $Z_0 > 1.0$, $\langle\delta^*\rangle$ almost keeps unchanged. For neutral and repulsive channels, the trend is quite similar to that in the case of $\varepsilon_{\rm cp} = -0.5$. For the neutral channel, $\langle\delta^*\rangle$ of the chain inside the channel is 0.94. And $\langle\delta^*\rangle$ decreases when $0.6 < Z_0 < 1.0$. For the repulsive channel, $\langle\delta^*\rangle$ changes little when $Z_0 < 0.2$. It drops slowly when $Z_0 < 0.6$, then drops quickly until $Z_0 = 1.0$ ($\langle\delta^*\rangle = 0.28$). It also shows that $Z_0 = 1.0$ is an important case. As also shown in the figure, in different channels, $\langle\delta^*\rangle$ of the chain is always larger than 0.85. This means that the shape of the chain is flat inside any channel. It is also shown that the shape of the chain changes from flat to spherical much later in the strong attractive channel during the translocation compared to those in the other channels. On the other hand, for the weak attractive, the neutral and the repulsive channels, the shape is easily destroyed. Maybe it is because an entropy force drives the chain out of these channels.

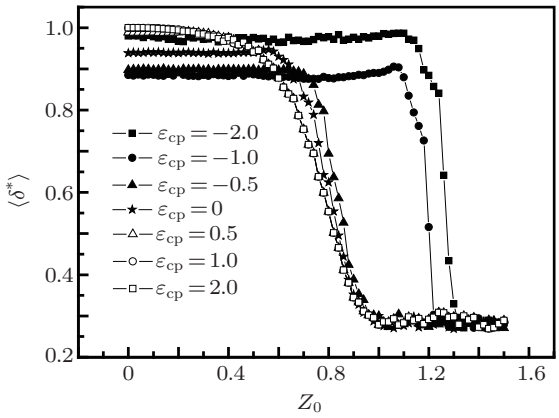


Fig. 3. Shape factor $\langle\delta^*\rangle$ vs. Z_0 for protein-like chains.

3.2. Thermodynamic properties

We now turn to study the thermodynamic properties of protein. Figure 4 shows the average energy $\langle U\rangle/N$ versus Z_0 for the protein-like chains with different channel–protein interactions. For repulsive interaction $\varepsilon_{\rm cp} = 0.5$, 1.0, and 2.0, $\langle U\rangle/N$ keeps to be a constant first, then increases from -0.10 to 0.48 at $0.4 < Z_0 < 1.0$. Finally, it keeps to be a constant value again. For the neutral channel ($\varepsilon_{\rm cp} = 0$), the value of $\langle U\rangle/N$ is -0.56 when $Z_0 < 0.52$, there is a peak at $Z_0 = 0.60$ ($\langle U\rangle/N = -0.21$), then it drops to -0.44 at $Z_0 = 1.00$. This energy barrier has been presented in our previous work.[37] The peak is an important turning point in the process of translocation. However, the peak is no longer seen in other channels. For $\varepsilon_{\rm cp} = -0.5$, $\langle U\rangle/N$ is -1.58 when $Z_0 < 0.7$. In the range of $0.7 < Z_0 < 1.0$, $\langle U\rangle/N$ increases. For $\varepsilon_{\rm cp} = -1.0$ and -2.0, the values of $\langle U\rangle/N$ are -2.80 and -6.00 when $Z_0 < 1.0$. They increase until $Z_0 = 1.2$ and $Z_0 = 1.3$, respectively.

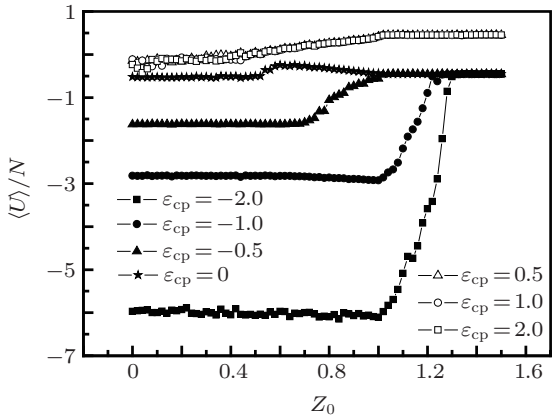


Fig. 4. Average energy per bond $\langle U\rangle/N$ vs. Z_0 for protein-like chains.

Our model contains many forms of energy, such as the contact energy, the α-helical energy, and the β-sheet energy. We further study these energies in the translocation processes for the different channels. First, we discuss the average contact energy $\langle U\rangle_c/N$ in Fig. 5. For relatively large attractive interactions ($\varepsilon_{cp} = -1.0, -2.0$), the curves of $\langle U_c\rangle/N$ each have a maximum at $Z_0 = 1.0$. When the adsorption of the channel is strong, the protein-like chain is restricted to the surface of the channel. With the Z_0 increasing, the monomers adsorbed on the surface gradually decrease. Thus, a minimum of $\langle U_c\rangle/N$ exists in the translocation process. It means that more contacts form. At $Z_0 > 1.0$, $\langle U_c\rangle/N$ increases until $Z_0 = 1.2$. However, when the adsorption is weak ($\varepsilon_{cp} = -0.5$), there exists a maximum in the curve of $\langle U_c\rangle/N$. This peak represents the looser structure existing during the translocation. The number of contacts becomes smaller. And the results of the other interactions are similar to those in the case of $\varepsilon_{cp} = -0.5$. Another important phenomenon is that the number of contacts increases for the strong attractive channel at the beginning of the translocation process, and it decreases for the other channels. As is known, more contacts mean that the structure of the chain is more stable. And the more stable structure makes is difficult for the protein-like chain to escape, which is concordant with the results of Figs. 2 and 3.

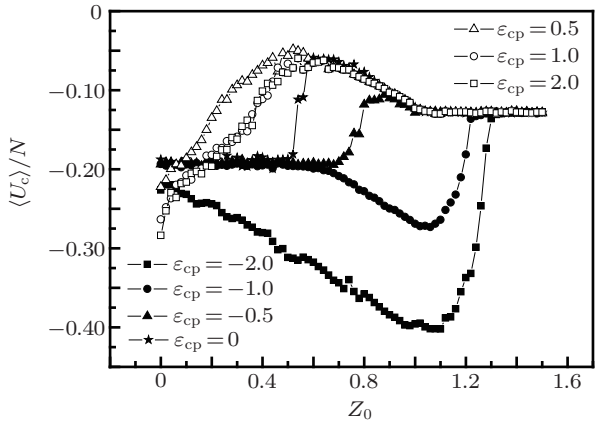


Fig. 5. Average contact energy per bond $\langle U_c\rangle/N$ vs. Z_0 for protein-like chains.

figure 6 presents the average α-helical energy per bond $\langle U_h\rangle/N$ as a function of Z_0. For a small channel radius, the values of $\langle U_h\rangle/N$ for $\varepsilon_{cp} = -1.0$ and -2.0 are -0.15 and -0.03 respectively when $Z_0 < 1.0$, and decrease when $Z_0 > 1.0$. Finally, they become -0.22 at $Z_0 = 1.22$ and 1.30, respectively. It means that the helical structure changes at $Z_0 > 1.0$ for the relatively strong attractive interaction. When $Z_0 < 1.0$, the helical structure is nearly not destroyed. Combining with the results of the chain shape, we conclude that the helical energy is the primary part of the total energy. The helix is very important for the stability of the chain. For the small attractive interaction ($\varepsilon_{cp} = -0.5$), the value of $\langle U_h\rangle/N$ drops from -0.17 ($Z_0 = 0.75$) to -0.22 ($Z_0 = 1.0$). We have also found a peak for the neutral channel at $Z_0 = 0.60$. Following the peak, $\langle U_h\rangle/N$ decreases abruptly till $Z_0 = 1.0$. A small peak also exists in the figure of $\varepsilon_{cp} = 0.5$. For $\varepsilon_{cp} = 1.0$ and 2.0, a long decreasing process of $\langle U_h\rangle/N$ happens when $Z_0 < 1.0$. Thus, the translocation becomes easier.

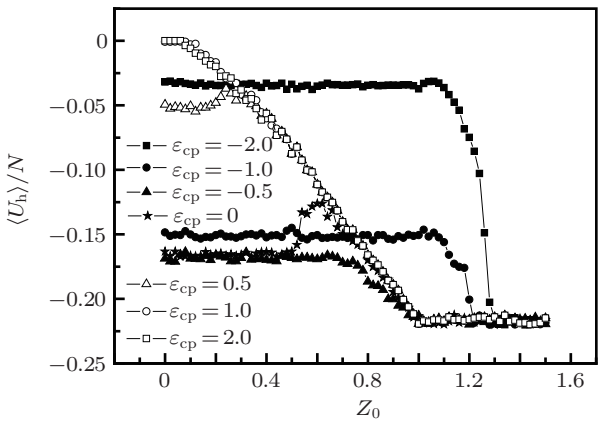


Fig. 6. Average helical energy per bond $\langle U_h\rangle/N$ vs. Z_0 for protein-like chains.

We also study the average sheet energy per bond $\langle U_b\rangle/N$ as a function of Z_0. Different channel–protein interactions are considered. The results are shown in Fig. 7. For the case of $\varepsilon_{cp} = -2.0$, $\langle U_b\rangle/N$ keeps unchanged at $Z_0 < 1.0$, then it drops until $Z_0 = 1.22$ ($\langle U_b\rangle/N = -0.07$). The curve of $\langle U_b\rangle/N$ for $\varepsilon_{cp} = -1.0$ has a minimum at $Z_0 = 1.0$. However, for $\varepsilon_{cp} = -0.5$, 0, and 0.5, there are peaks at $Z_0 = 0.88$, 0.66, and 0.33, respectively. While there

is no peak shown in the curves of $\varepsilon_{\rm cp} = 1.0$ and 2.0. The value drops when $0.2 < Z_0 < 1.0$.

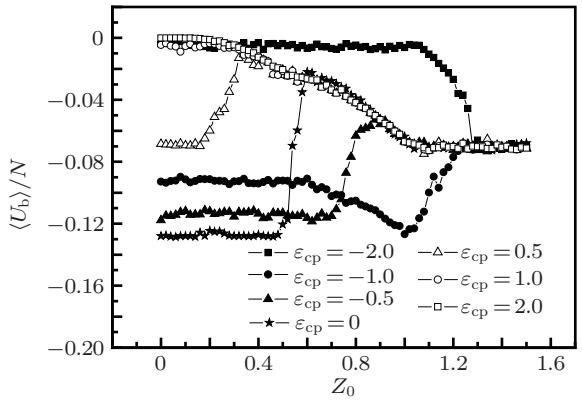


Fig. 7. Average sheet energy per bond $\langle U_{\rm b}\rangle/N$ vs. Z_0 for protein-like chains.

Next, the results of $\langle U_{\rm s}\rangle/N$ are presented in Fig. 8. It shows that for $\varepsilon_{\rm cp} = -1.0$ and -2.0, the values of $\langle U_{\rm s}\rangle/N$ increase when $Z_0 > 1.0$. For $\varepsilon_{\rm cp} = -0.5$, $\varepsilon_{\rm cp} = 0$, and $\varepsilon_{\rm cp} > 0$, the values of $\langle U_{\rm s}\rangle/N$ all change at $Z_0 < 1.0$.

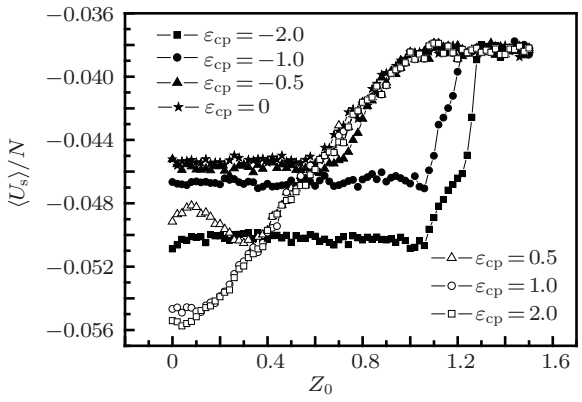


Fig. 8. Average spin–spin interaction energy per bond $\langle U_{\rm s}\rangle/N$ vs. Z_0 for protein-like chains.

Finally, the channel–protein interaction energy $\langle U_{\rm cp}\rangle/N$ is shown in Fig. 9. It is easy to find that the results of $\varepsilon_{\rm cp} = -1.0$ and -2.0 show increases at $1.0 < Z_0 < 1.22$ and $1.0 < Z_0 < 1.3$, respectively. At $Z_0 < 1.0$, the values of $\langle U_{\rm cp}\rangle/N$ inside the chain are -2.32 and -5.55 for $\varepsilon_{\rm cp} = -1.0$ and -2.0, respectively. For $\varepsilon_{\rm cp} = -0.5$, it increases from -1.1 ($Z_0 = 0.7$) to 0 ($Z_0 = 1.0$). For the weak repulsive interaction ($\varepsilon_{\rm cp} = -0.5$), $\langle U_{\rm cp}\rangle/N$ increases from -0.54 to 0. For $\varepsilon_{\rm cp} = 0$, $\langle U_{\rm cp}\rangle/N$ is certainly zero. However, for $\varepsilon_{\rm cp} = 1.0$ and 2.0, the value of $\langle U_{\rm cp}\rangle/N$ has a slight variation.

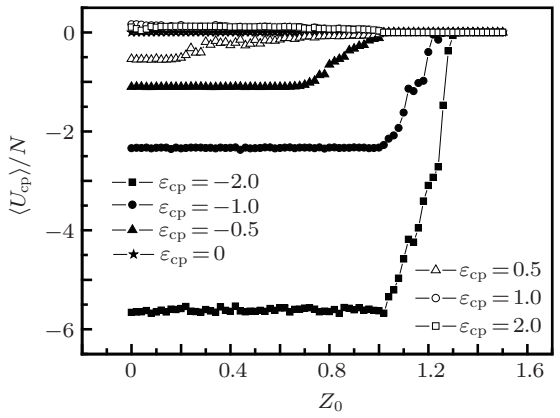


Fig. 9. Average channel–protein interaction energy per bond $\langle U_{\rm cp}\rangle/N$ vs. Z_0 for protein-like chains.

Another aspect that is worth mentioning is the free energy per bond A/N. A larger free energy means more conformations of the state. Figure 10 shows the results of A/N during the translocation process with channel radius $R = 1$. For strong attractive interactions ($\varepsilon_{\rm cp} = -1.0$ and -2.0), the values of A/N are -4.6 and -7.6, respectively. The A/N increases till $Z_0 = 1.20$ for $\varepsilon_{\rm cp} = -1.0$, and till $Z_0 = 1.35$ for $\varepsilon_{\rm cp} = -2.0$. It shows that for the strong attractive interaction, an external force is needed to drive the protein-like chain out of the channel. The translocation is not spontaneous. However, for the result of $\varepsilon_{\rm cp} = -0.5$, it is found that the value of A/N monotonically decreases from -3.5 ($Z_0 = 0.8$) to -3.7 ($Z_0 = 1.0$). This means that the number of conformations becomes larger when $0.8 < Z_0 < 1.0$. The translocation is spontaneous for $\varepsilon_{\rm cp} = -0.5$ as well as for the cases of other four interactions ($\varepsilon_{\rm cp} = 0$, 0.5, 1.0, and 2.0). This is because the slopes of the curves are all the same and negative. This means that the interior entropy drives the chain out of the channel. The decreasing ranges for the four interactions

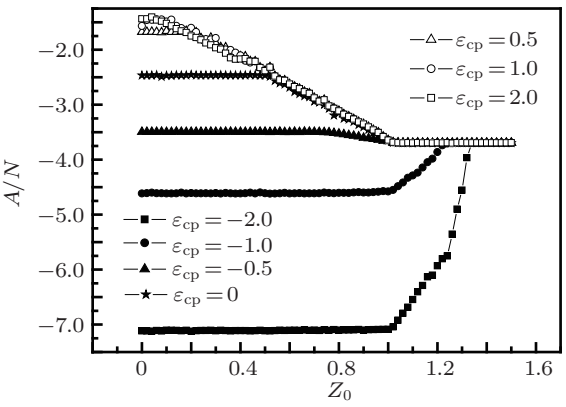


Fig. 10. Average Helmholtz free energy per bond A/N vs. Z_0 for protein-like chains.

are $0.5 < Z_0 < 1.0$, $0.17 < Z_0 < 1.0$, $0.05 < Z_0 < 1.0$, and $0.05 < Z_0 < 1.0$, respectively. If the repulsive interaction is stronger, the entropy driving process lasts longer. It is not difficult to conclude from the above figures that $Z_0 = 1.0$ is the turning point to distinguish the strong attractive channel from the other ones.

4. Conclusion

Using the pruned-enriched Rosenbluth method, we investigate the translocation of a protein-like chain through a finite cylindrical channel ($R = 1$). We find that the chain dimension changes mainly at $Z_0 > 1.0$ for the strong channel–protein interaction ($\varepsilon_{\rm cp} = -2.0, -1.0$), while for the other channels, it changes at $Z_0 < 1.0$. The turning point $Z_0 = 1.0$ is also observed in the investigation of the average energy and the other energies. Specifically, we study the free energy during the translocation. We show that the free energy increases at $Z_0 > 1.0$ for $\varepsilon_{\rm cp} = -2.0$ and -1.0. It means that an external force is needed to drive the translocation. However, for the other interactions, the free energy decreases at $Z_0 < 1.0$. It shows that the chain can spontaneously cross the chain without any external force. This is due to the interior entropy that drives the chain to the outside. These investigations may provide some insights into the translocation of proteins and DNA through channels or pores.

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