Polymer Translocation Induced by Adsorption

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Abstract

We study the translocation of a flexible polymer through a pore in a membrane induced by its adsorption on trans side of the membrane. When temperature $T$ is higher than $T_c$, the adsorption-desorption transition temperature, attractive interaction between polymer and membrane plays little role in affecting polymer conformation, leading to translocation time that scales as $\tau \sim L^3$ where $L$ is the polymer contour length. When $T < T_c$, however, the translocation time undergoes a sharp crossover to $\tau \sim L^2$ for sufficiently long polymers, following the second order conformational (adsorption) transition. The translocation time is found to exhibit the crossover around $T = T'_{c}$, which is lower than $T_c$ for polymers shorter than a critical length($N < N_c$).
I. INTRODUCTION

Biopolymers exhibit various transmembrane conformational states determined by their intrinsic properties as well as by the interactions with the surrounding environments. For example, polymer flexibility, capability of hydrogen bond formation between segments, and hydrophobic interaction with membrane play crucial roles in conformation of membrane-bound proteins. An important aspect of membrane-protein interaction can be found in the dynamics of proteins. As the experimental observations of protein translocation are available only in limited situations, theoretical investigations are also in a primitive stage. However, a few studies show that polymer translocation across the membrane is significantly affected by the surrounding environments and membrane-protein interactions. Theoretical studies have been focused on the driving mechanisms of polymer translocation across the membrane such as chemical potential asymmetry and its random modulation, chaperon bindings, and lipid molecular density imbalance. It was shown that a minute chemical potential bias per segment of the chain can bring about a significant effect on translocation, due to the long-chain connectivity. In this paper, we investigate the effect of attractive membrane-polymer interaction yielding adsorption transition as another possible driving mechanism.

To highlight the effects arising from long chain nature, we consider a rigid plane of negligible thickness with a hole small enough to allow only a single segment passage, as a minimal model of membrane with a translocation pore as shown Fig. 1. In this model, polymer segments interact with the membrane attractively in the trans side, while those in the cis side recognizes the membrane only as an impenetrable wall. No specific interaction between the segments and pore is assumed. Furthermore we neglect the mutual interaction.
between the segments because we are interested in the most dominant effects resulting from the chain connectivity. The attraction, if it is strong enough to bring about desorption-adsorption transition, would drive the polymer to the \textit{trans} side as shown in Fig. 1 to minimize the free energy.

The total free energy of the transmembrane polymer has two distinct contributions. One is the entropic contribution affected by the steric interaction with the membrane, and the other is the adsorption energy due to attraction in \textit{trans} side. At high temperatures, thermal fluctuation dominates and the polymer conformation is nearly the same as the case without attractive interaction. As the polymer is situated in nearly symmetric environments in this case, it is driven to either side of the membrane with equal probability. At temperatures below the adsorption-desorption transition temperature, on the other hand, polymer conformation in the \textit{trans} side becomes collapsed(adsorbed) and the polymer is driven spontaneously to the \textit{trans} side to minimize the total free energy. Near the transition temperature, however, competition between thermal fluctuation and membrane attraction determines the chain conformation, while the translocation dynamics is governed by the interplay between thermal diffusion and segmental energy bias due to interaction with membrane.

In section II, conformation of transmembrane polymer and the associated free energy are derived as a function of temperature and interaction potential parameters. In section III, we consider the dynamics of polymer translocation as a stochastic process crossing the free energy barrier, where the effects of attraction and temperature on translocation dynamics are discussed. Section IV gives summary and conclusion.
II. STATISTICAL MECHANICS OF A POLYMER ONE-END-ANCHORED ON ATTRACTIVE SURFACE

The transmembrane polymer can be regarded as two independent chains anchored at the spot of pore (Fig. 1). In this section, we consider the chain conformation and free energy of one-end-anchored chain to calculate the free energy of a transmembrane polymer. The Green’s function of a polymer $G(r, r'; n)$ is defined as the statistical weight of an $n$-segment polymer whose end positions are located at $r$ and $r'$ respectively. For a polymer with Kuhn length $b$, $G(r, r'; n)$ satisfies the following differential equation:

$$\left[ \frac{\partial}{\partial n} - \frac{b^2}{6} \nabla^2 \right] G(r, r'; n) = \delta(r - r').$$

(1)

In unbound free space it is reduced to a familiar Gaussian form:

$$G_0(r, r'; n) = \left[ \frac{2\pi nb^2}{3} \right]^{-3/2} \exp \left[ -\frac{3(r - r')^2}{2nb^2} \right].$$

(2)

For a polymer subjected to an attractive wall ($z = 0$ surface), the attractive potential effect can be incorporated in terms of the following boundary condition:

$$\left[ \frac{\partial}{\partial z} \log G(r, r'; n) \right]_{z=0} = c.$$ 

(3)

This boundary condition consideration is valid only for the case that the attractive interaction range is short enough compared with other length scales involved such as polymer radius of gyration or adsorption layer thickness. The $c$ is a convenient parameter descriptive of surface interaction the details of which this mesoscopic description usually bypasses. Although, for flexible chain, the Edwards equation is more adequate to describe the adsorbed state incorporating details of surface interaction, this mesoscopic description, also applicable
to semiflexible chains, can easily yield useful results for a full range of temperatures. For the cases of weak adsorption \( u_0 \ll k_B T \) and flexible chain \( a \gg b \) considered throughout this paper, we will use the Edwards equation to determine the interaction parameter \( c \) in terms of temperature, attraction strength \( (u_0) \) and range \( (a) \).

The Green’s function in half space \((z > 0)\) can be written as

\[
G(\mathbf{r}, \mathbf{r}'; n) = G_0(x, x'; n)G_0(y, y'; n)G(z, z'; n)
\]

where \( G_0(x, x'; n) \) and \( G_0(y, y'; n) \) are one dimensional Gaussian propagators analogous to Eq. 2, and the \( z \) component is given by

\[
G(z, z'; n) = \frac{\pi nb^2}{6} \left[ \frac{1}{2} \left\{ \exp \left\{ \frac{-3(z-z')^2}{2nb^2} \right\} + \exp \left\{ \frac{-3(z+z')^2}{2nb^2} \right\} \right\} \right]^{-1/2} \exp \left\{ \frac{-3(z+z')^2}{2nb^2} \right\} \text{erfc} \left\{ \frac{2nb^2}{3} \left( z + z' + cnb^2/3 \right) \right\} \]

where \( \text{erfc}(u) \equiv (2/\sqrt{\pi}) \int_u^\infty \exp(-u'^2)du' \) is the complementary error function, and

\[
w \equiv (n/6)^{1/2}bc.
\]

The \( z \) component of Green’s function has the following limiting behaviors:

\[
G(z, z'; n) = G_0(z, z'; n), \quad z, z' \to \infty,
\]

\[
G(z, z'; n) = \left[ \frac{2\pi nb^2}{3} \right]^{-1/2} \left[ \exp \left( \frac{-3(z-z')^2}{2nb^2} \right) - \exp \left( \frac{-3(z+z')^2}{2nb^2} \right) \right], \quad w \gg 1,
\]

as it should be. The latter is the ideal chain Green’s function in the presence of absorbing boundary at \( z = 0 \). Now that \( |w| \) is defined as the ratio of free polymer size \((\sim n^{1/2})\) and adsorbed layer thickness \((\sim |c|^{-1})\) for low temperature adsorbed states \((w < 0, c < 0)\), it can be regarded as a parameter describing the effects of surface attraction or temperature.
For high temperature desorbed states \( w > 0 \), \( w \) measures the strength of steric repulsion, which also entails the surface attraction effect.

The conformational partition function of a polymer with one end anchored on attractive surface is given by:

\[
Q(n) \equiv \lim_{z' \to 0} \int_0^\infty G(z, z'; n) dz
\]

\[
= \exp(w^2) \text{erfc}(w)
\]

\[
= \begin{cases} 
\pi^{-1/2} w^{-1}, & w \gg 1 \\
1 - 2\pi^{-1/2} w, & w \approx 0 \\
2 \exp(w^2), & w \ll -1,
\end{cases}
\]

where the bulk value of partition function \( q^n \) is omitted throughout this paper, where \( q \) is the partition function of a single segment. To see the conformational states of anchored polymer explicitly, let us see the conditional probability distribution of free end defined by

\[
P_n(z|z' = 0) \equiv \frac{1}{Q(n)} G(z, z' = 0; n),
\]

which has the following limiting forms:

\[
P_n(z|z' = 0) = \begin{cases} 
(nb^2/3)^{-1} z \exp(-3z^2/2nb^2), & w \gg 1 \\
(\pi nb^2/6)^{-1/2} \exp(-3z^2/2nb^2), & w = 0 \\
|c| \exp(-|c|z), & w \ll -1.
\end{cases}
\]

For \( w \gg 1 \), \( P_n(z|z' = 0) \) is equal to the distribution without attraction, which corresponds to the high temperature desorbed phase. On the other hand, for \( w \ll -1 \), \( P_n(z|z' = 0) \) represents the distribution for low temperature adsorbed phase of a polymer subject to a surface of sufficiently short range attraction. The distribution at the adsorption-desorption transition point corresponds to the case \( w = 0 \).
Using the partition function of a one-end-anchored polymer in Eq. 10, its free energy is given by

\[ F(n) = -k_B T \log Q(n) \] (14)

\[ = -k_B T \left[ w^2 + \log \text{erfc}(w) \right] \] (15)

\[ \simeq \begin{cases} 
(k_B T/2) \log n + \text{const}, & w \gg 1 \\
2k_B T n^{1/2} b c (6\pi)^{-1/2}, & w \simeq 0 \\
-k_B T n b^2 c^2/6 + \text{const}, & w \ll -1.
\end{cases} \] (16)

Note that the \( F(n) \) changes sign at \( w = 0 \), which corresponds to adsorption-desorption transition point. At high temperature \( (w \gg 1) \), we can see the polymer free energy, the value relative to that of free polymer, goes like \( \log n \) due to the anchorage effect. At low temperatures \( (w \ll -1) \), adsorption free energy scales as \( n \) involving segmental free energy as \( -k_B T n b^2 c^2/6 \).

Since the transmembrane polymer is composed of two independent one-end-anchored chains with length \( n \) and \( N - n \) in cis and trans side respectively(Fig. 1), its partition function is given by

\[ Q(n) \equiv Q_{cis}(N - n) Q_{trans}(n, c), \] (17)

where the effect of attraction appears only in the trans side partition function in terms of \( c \).

This partition function has the following limiting behaviors:

\[ Q(n) \sim \begin{cases} 
(N - n)^{-1/2} n^{-1/2}, & T \gg T_c \\
(N - n)^{-1/2}, & T = T_c \\
(N - n)^{-1/2} \exp(n b^2 c^2/6), & T \ll T_c.
\end{cases} \] (18)
The free energy as a function of translocation coordinate \( n \), defined as the number of segments in trans side, is, apart from additive constants,

\[
\mathcal{F}(n) = -k_B T \log Q(n)
\]

\[
= \frac{1}{2}k_B T \log(N - n) - k_B T \left[ \frac{nb^2c^2}{6} + \log \text{erfc} \left( \sqrt{\frac{n}{6bc}} \right) \right]
\]

\[
= \begin{cases} 
\frac{1}{2}k_B T \log [(N - n)n], & T \gg T_c \\
\frac{1}{2}k_B T \log(N - n), & T = T_c \\
\frac{3}{2}k_B T \log(N - n) - k_B T \frac{nb^2c^2}{6}, & T \ll T_c.
\end{cases}
\]

In Fig. 2, this free energy function is depicted for different values of \( c \). \( \mathcal{F}(n) \) exhibits nearly symmetric barrier for positive \( c(T > T_c) \), while it does exhibits a linearly slant shape for negative \( c(T < T_c) \). This signifies that the polymer is driven to the trans side due to the adsorption for \( c < 0 \). One remarkable point here is that \( \mathcal{F}(n) \) slants to the trans side at \( T = T_c \) even though the polymer in the trans side is not in its adsorbed state. The \( n \) segments in the trans side feel neither steric interaction nor attraction. The cancelation of these two effects makes the total free energy be determined only in terms of the \( N - n \) segments in the cis side.

**Determination of \( c \)**

In the previous section, the free energy of a transmembrane polymer is determined in terms of interaction parameter \( c \), which is defined as the logarithmic derivative of polymer Green's function at the surface(Eq. 3). To determine \( c \) in its adsorbed phase in terms of interaction potential parameters, we consider a microscopic model of flexible polymer weak adsorption in this subsection. As the polymer conformation in its adsorbed phase is not
affected by the anchorage, we will consider the adsorbed polymer without anchorage for simplicity.

Let us choose the interaction potential between a monomer and the membrane as

\[ v(r) = \begin{cases} 
-u_0, & 0 < z < a, \\
0, & z > 0, 
\end{cases} \tag{22} \]

where \( u_0 > 0 \) is the strength and \( a \) is the range of attraction. Under the conditions \( u_0 \ll k_B T \) and \( a \gg b \), the polymer Green’s function obey the Edwards equation

\[ \left[ -\frac{b^2}{6} \frac{\partial^2}{\partial z^2} + \beta v(z) \right] G(z, z'; n) = -\frac{\partial}{\partial n} G(z, z'; n). \tag{23} \]

It can be expanded as

\[ G(z, z'; n) = \sum_i \exp(-n\lambda_i)\psi_i(z)\psi_i(z') \tag{24} \]

where \( \lambda_i \) and \( \psi_i(z) \) are the eigenvalues and eigenfunctions of the Schrödinger-like equation,

\[ \left[ -\frac{b^2}{6} \frac{\partial^2}{\partial z^2} + \beta v(z) \right] \psi_i(z) = \lambda_i \psi_i(z), \tag{25} \]

subject to the boundary condition

\[ \psi_i(z = 0) = 0. \tag{26} \]

By solving this eigenvalue problem, we can get the adsorption-desorption transition temperature \( T_c \) and the value of \( c \) as a function of \( T \), \( a \) and \( u_0 \) for adsorbed state.

For \( T < T_c \), the ground state dominance approximation, \( G(z, z'; n) \simeq \exp(-n\lambda_0)\psi_0(z)\psi_0(z') \), works well for a long chain, where \( \lambda_0 \) is the lowest eigenvalue and \( \psi_0(z) \) is the corresponding eigenfunction of Eq. 25. The ground state eigenfunction in \( z \) direction is given by
\[ \psi_0(z) = \begin{cases} 
A \sin(kz), & 0 < z < a, \\
B \exp(-\kappa z), & z > a,
\end{cases} \tag{27} \]

where \( k = (6/b^2)^{1/2}(\beta u_0 + \lambda_0)^{1/2} \) and \( \kappa = (6/b^2)^{1/2}|\lambda_0|^{1/2} \) with \( \lambda_0 < 0 \) for \( T < T_c \). The transition temperature \( T_c \) can be determined as

\[ k_B T_c = \frac{24 u_0 a^2}{\pi^2 b^2}, \tag{28} \]

below which a bound state of negative eigenvalue exists. The continuity condition of \( \psi_0(z) \) and \( \psi_0'(z) \) at \( z = a \) gives the following relation:

\[ \kappa a = -ka \cot(ka) \tag{29} \]

which determines \( \lambda_0 \) for \( T < T_c \). The interaction parameter \( c \) for \( T < T_c \) can be defined as

\[ c \equiv \left[ \frac{1}{\psi_0(z)} \frac{\partial}{\partial z} \psi_0(z) \right]_{z=a} = -\kappa. \tag{30} \]

This microscopic definition of \( c \) can be identified with the previous definition if the interaction is short-ranged. From the solution of Eq. 29 and Eq. 30, \( c \) can be written as the following functional form for \( T \leq T_c \):

\[ c = -a^{-1}H(\alpha) \tag{31} \]

where \( \alpha \equiv (a/b)(6\beta u_0)^{1/2} \), and \( H(\alpha) \) is depicted in Fig. 3. As \( T \) approaches \( T_c \) from below, \( \alpha \) goes to \( \pi/2 \) and \( H(\alpha) \) goes to zero, which yields

\[ c \simeq -\frac{\pi^2 T_c}{8a} - T + O(T_c - T)^2, \tag{32} \]

for \( T \ll T_c \). At sufficiently low temperatures\((T \ll T_c)\), on the other hand, \( \alpha \gg 1 \) and \( H(\alpha) \simeq \alpha \). In this regime, \( c \) can be approximated as
\[ c \simeq -b^{-1}(6\beta u_0)^{1/2} \sim -T^{-1/2}, \quad (33) \]

which is independent of interaction range \( a \). Eq. [32] and Eq. [33] are useful to examine the temperature dependence of polymer descriptions derived from the boundary condition (Eq. 3), which will be demonstrated in the next section.

### III. DYNAMICS OF POLYMER TRANSLOCATION

As shown by us, the translocation of a polymer can be thought of as a one dimensional diffusive process of the translocation coordinate \( n \) crossing the effective potential \( \mathcal{F}(n) \). The probability density of \( n(t), P(n,t) \), is described by Fokker-Planck equation

\[ \frac{\partial}{\partial t}P(n,t) = \mathcal{L}_{FP}(n)P(n,t), \quad (34) \]

where \( \mathcal{L}_{FP}(n) \) is the Fokker-Planck operator given by

\[ \mathcal{L}_{FP}(n) \equiv \frac{1}{b^2} \frac{\partial}{\partial n}D(n) \exp[-\beta \mathcal{F}(n)] \frac{\partial}{\partial n} \exp[\beta \mathcal{F}(n)], \quad (35) \]

with \( D(n) \) defined as the whole chain diffusion coefficient. The translocation time of a polymer can be defined as the mean first passage time \( \tau(n;n_0) \), the time for diffusion from \( n_0 \) to \( n \), which satisfies

\[ \mathcal{L}_{FP}^\dagger(n_0)\tau(n;n_0) = -1, \quad (36) \]

where \( \mathcal{L}_{FP}^\dagger(n_0) \) is the backward Fokker-Planck operator given by

\[ \mathcal{L}_{FP}^\dagger(n_0) \equiv \frac{1}{b^2} \exp[\beta \mathcal{F}(n_0)] \frac{\partial}{\partial n_0}D(n_0) \exp[-\beta \mathcal{F}(n_0)] \frac{\partial}{\partial n_0}. \quad (37) \]

Using the following boundary conditions
\[ \frac{\partial}{\partial n_0} \tau(n; n_0 = 1) = 0 \quad (38) \]
\[ \tau(n; n_0 = N - 1) = 0, \quad (39) \]

the solution of the above backward equation (Eq. 36) can be obtained and the polymer translocation time is determined as

\[ \tau \equiv \tau(N - 1; 1) \quad (40) \]

\[ = b^2 \int_1^{N-1} dn \frac{1}{D(n)} e^{\beta F(n)} \int_1^n dn' e^{-\beta F(n')} \quad (41) \]

By putting the diffusion coefficient \( D(n) \) to be a constant \( D \) for simplicity, the translocation time as a function of \( w \) is shown in Fig. 4, where a drastic change in \( \tau \) occurs near \( w = 0 \). Because \( w \) or \( c \) is expected to be a monotonic function of temperature as shown in Eq. 31 and Fig. 3, Fig. 4 can be understood as a sharp dynamic crossover induced by temperature change. Note that \( \tau \sim |w|^{-2} \sim |c|^{-2} \) for \( T \ll T_c \), while \( \tau \) changes smoothly only by a small amount for \( T > T_c \).

The Fig. 5 is a plot of \( \tau \), which is obtained using the free energy (Eq. 20) with \( c \) given by Eq. 31, as a function of \( N \) for four different temperatures ranging from \( T \gg T_c \) to \( T \ll T_c \). For \( T \gg T_c \), i.e., \( \beta u_0 \simeq 0 \), the transmembrane polymer does not feel attractive interaction and translocation time (Eq. 41) is reduced to

\[ \tau \simeq \frac{\pi^2}{8} \left[ \frac{L^2}{2D} \right] \sim L^3, \quad (42) \]

where \( L = Nb \) is the contour length of the polymer and the diffusion coefficient is given by \( D = k_B T/(N\gamma) \), with segmental hydrodynamic friction coefficient \( \gamma \) following the Rouse model. In this high temperature regime, translocation time is proportional to \( L^3 \) (Fig. 5, A), which is the same result as the case without the attractive interaction.
As the temperature is lowered, the free energy curve tends to slant down to the right and the prefactor of $\tau$ decreases smoothly until $T = T_c$ as shown in Fig. 4. At $T = T_c$, the translocation time becomes

$$\tau = \frac{2}{3} \left[ \frac{L^2}{2D} \right] \sim L^3,$$  \hspace{1cm} (43)

where the prefactor is reduced from $\pi^2/8$ to $2/3$. In this case, the steric interaction in the trans side is canceled off by the attractive interaction, which drives the polymer to the trans side, but $\tau$ is still proportional to $L^3$ (Fig. 5, B). Assuming $D$ increases as $T$ increases like $D \sim T^\alpha$ with $\alpha > 0$,

$$\frac{\tau(T \gg T_c)}{\tau(T = T_c)} \sim \frac{3\pi^2}{16} \left( \frac{T_c}{T} \right)^\alpha \ll 1.$$  \hspace{1cm} (44)

Thus, as can be seen in A and B of Fig. 5, the $\tau$ increases as $T$ decreases to $T_c$, which results from the suppression of thermal diffusion. The $\tau$ attains its maximum at $T = T_c$, since for $T < T_c$, the polymer adsorption speeds the translocation as discussed below.

For $T \ll T_c$, $c$ behaves as $c \sim -T^{-1/2}$ (Eq. 33) and the translocation time (Eq. 11) is given by

$$\tau \sim \left[ \frac{L^2}{2D} \right] \frac{2}{Nb^2c^2/6} \left[ \frac{L^2}{2D} \right] \frac{2}{N\beta u_0} = \left[ \frac{L^2}{2D} \right] \frac{2}{N\beta u_0} \sim L^2,$$  \hspace{1cm} (45)

(46)

(47)

(48)

which is depicted in Fig. 5, D. In this low temperature regime, the free energy of transmembrane polymer is dominated by the attraction energy which is linearly proportional to $n$,.
where the prefactor of $n$ can be interpreted as the energy per segment in trans side, or transmembrane segmental energy bias that features as “chemical potential difference” between the two sides of membrane.

We find that the crossover of scaling behavior from $\tau \sim L^3$ to $\tau \sim L^2$ sharply occurs around $T = T_c$, which can also be inferred from Fig. 4. The conditions for the crossover can be analyzed in detail as follows using the Edwards equation approach for $T < T_c$. As shown by us, segmental energy bias approximately larger than $k_BT/N$ can bring about the crossover in translocation from $\tau \sim L^3$ to $\tau \sim L^2$ due to chain connectivity(cooperativity). For the adsorption-driven translocation when $T < T_c$, the condition for the crossover can be written as

$$|\lambda_0| \gtrsim \frac{1}{N}, \quad (49)$$

where $\lambda_0$, the lowest eigenvalue in Eq. 23, is the segmental free energy in units of $k_BT$ in adsorbed state. This condition(Eq. 49) for $T$ near $T_c$ can be converted to

$$T \lesssim T'_c(N) = T_c \left[1 - \frac{8a}{\pi^2} \left( \frac{6}{Nb^2} \right)^{1/2} \right], \quad (50)$$

where the relation $\lambda_0 = -b^2H^2(\alpha)/6a^2$(see Eq. 31) was used. This condition implies that the crossover occurs at $T'_c$ smaller than $T_c$ for finite chain length $N$. That is, for $T'_c < T < T_c$, $\tau \sim L^3$ although the transmembrane polymer is adsorbed in trans side. For a numerical example for the difference between $T_c$ and $T'_c$, we consider the case, $a/b = 10$ and $N = 60000$, which yields $T'_c \approx 0.9T_c$. The C of Fig. 5 depicts this situation. For temperatures less than $T_c$, the condition of Eq. 49 yields the critical chain length

$$N_c(T) \simeq \frac{384a^2}{\pi^4b^2} \left( \frac{T_c - T}{T_c} \right)^{-2} \quad (51)$$
around which the crossover from \( \tau \sim L^3 \) to \( \tau \sim L^2 \) occurs. Indeed this \( N_c \) is consistent with
the crossover point in C of Fig. 5.

Table 1 summarizes the conditions for the crossover and associated chain conformations
for diverse temperatures and chain length. The meaning of two critical temperatures \( T_c, T'_c \)
as well as the critical chain length \( N_c \) for chain cooperativity, can be understood as follows.
The segmental free energy \( \lambda_0(T) \) vanishes at \( T = T_c \), while \( N|\lambda_0(T)| \) becomes larger than 1
for \( T \lesssim T'_c \) or \( N \gtrsim N_c \), which are the conditions for a cooperative, facilitated translocation
driven by an energetic bias. In this study, we do not incorporate the solvent effect which
will induce interaction between segments and thus affect the polymer free energy function
significantly. Yet the crossover in \( \tau \) is seen to occur irrespective of excluded volume effect,
as a consequence of the long-chain nature of the polymer interacting with the membrane.\[6\]
Incorporation of the effect will modify only \( T_c \) and \( T'_c \).

IV. SUMMARY AND CONCLUSION

We considered the dynamics of flexible polymer translocation as a diffusive process cross-
ing the free energy barrier which we derived in section II. The translocation dynamics is
found to be strongly correlated with transmembrane chain conformation, both of which are
varied depending upon the competition between thermal fluctuation and attractive polymer
interaction with the membrane. The polymer adsorption-desorption transition point(\( T_c \))
divides the length scaling regimes of translocation time, \( \tau \sim L^3 \) and \( \tau \sim L^2 \), for sufficiently
long chains(\( N > N_c \)). However, for shorter chains(\( N < N_c \)), a crossover of two regimes
is found to occur at a lower temperature, \( T'_c \), although the conformational transition still
occurs at the same transition temperature, \( T_c \). We used the mesoscopic theory of polymer
adsorption using the machinery of boundary condition, supplemented by the microscopic Edwards equation approach to consider the case of flexible chain weak adsorption in detail. This theory can be adapted to the more biologically-relevant situations of semiflexible chain strong adsorption, if the interaction parameter can be appropriately given.

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FIGURES

FIG. 1. Translocation of a polymer through a pore. Polymer segments are adsorbed in the trans side due to the attractive interaction at sufficiently low temperatures.

FIG. 2. Free energy $\mathcal{F}(n)$ as a function of translocation coordinate $n$. (A. $bc = 1.0$, B. $bc = 0$, C. $bc = -0.5$, D. $bc = -1.0$)

FIG. 3. $H(\alpha)$ versus $\alpha \equiv (a/b)(6\beta u_0)^{1/2}$. At $T = T_c(\alpha = \pi/2)$, $H(\alpha) = 0$ and $c \equiv -a^{-1}H(\alpha) = 0$. For $T \ll T_c(\alpha \gg 1)$, $H(\alpha) \simeq \alpha$ and $c \simeq -b^{-1}(6\beta u_0)^{1/2}$ (dotted line).

FIG. 4. Translocation time $\tau$ normalized by $\tau_0 \equiv L^2/(2D)$ versus $|w|$, with $w \equiv bc(N/6)^{1/2}$, (A. $c > 0(T > T_c)$, B. $c < 0(T < T_c)$). Note that $\tau/\tau_0 \sim w^{-2}$ for $T \ll T_c$. Inset: The same figure in linear scale, where sharp transitional behavior occurs at $c = 0(T = T_c)$.

FIG. 5. Translocation time $\tau$ in units of $\tau_1 \equiv \gamma b^2/u_0$ versus chain length $N$, where $a = 10b \ll Nb$, (A. $T = 10T_c$, B. $T = T_c$, C. $T = 0.9T_c$, D. $T \ll T_c$). $\tau \sim L^3$ for A and B, and $\tau \sim L^2$ for D. Crossover between them can be seen for C near $N = N_c$ as the chain length varies.
Table 1. Length scaling behavior of polymer translocation time $\tau$ and associated chain conformations as a function of temperature and chain length.

| Temperature Range | Shorter Chain ($N < N_c$) | Longer Chain ($N > N_c$) |
|-------------------|----------------------------|--------------------------|
| $T > T_c$         | $\tau \sim L^3$ (desorbed) | $T > T_c$ $\tau \sim L^3$ (desorbed) |
| $T_c' < T < T_c$  | $\tau \sim L^3$ (adsorbed) | $T < T_c$ $\tau \sim L^2$ (adsorbed) |
| $T < T_c'$        | $\tau \sim L^2$ (adsorbed) |                          |
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Fig. 5, Park, Polymer Translocation ...