Limit properties of periodic one dimensional hopping model

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Abstract

Periodic one dimensional hopping model is useful to study the motion of microscopic particles, which lie in thermal noise environment. The mean velocity $V_N$ and diffusion constant $D_N$ of this model have been obtained by Bernard Derrida [J. Stat. Phys. 31 (1983) 433]. In this research, we will give the limits $V_D$ and $D_D$ of $V_N$ and $D_N$ as the number $N$ of mechanochemical states in one period tends to infinity by formal calculation. It is well known that the stochastic motion of microscopic particles also can be described by overdamped Langevin dynamics and Fokker-Planck equation. Up to now, the corresponding formulations of mean velocity and effective diffusion coefficient, $V_L$ and $D_L$ in the framework of Langevin dynamics and $V_P, D_P$ in the framework of Fokker-Planck equation, have also been known. In this research, we will find that the formulations $V_D$ and $V_L, V_P$ are theoretically equivalent, and numerical comparison indicates that $D_D, D_L$, and $D_P$ are almost the same. Through the discussion in this research, we also can know more about the relationship between the one dimensional hopping model and Fokker-Planck equation.

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1 Introduction

Many physical \cite{1,2} and biochemical phenomena, especially for the motion of motor protein \cite{3,4,5,6}, can be described by the periodic one dimensional hopping model. In this model, the particle jumps along a periodical linear track from one binding site to next one through the sequence of $N$ mechanochemical states \cite{7,8}. The particle in state $j$ can jump forward to state $j + 1$ with the rate $u_j$, or jump backward to state $j - 1$ with the rate $w_j$. After moving $N$ sites forward the particle comes to the same mechanochemical state but shifted by a step size distance $L$ (for motor protein kinesin $L = 8.2\text{nm}$). The dynamics of particle motion is described by the standard rate equations of occupation probabilities $p_j(t)$

$$\frac{\partial p_j(t)}{\partial t} = u_{j-1}p_{j-1}(t) + w_{j+1}p_{j+1}(t) - [u_j + w_j]p_j(t)$$  \hspace{1cm} (1)

where

$$p_{lN+j}(t) = p_j(t) \quad u_{lN+j} = u_j \quad w_{lN+j} = w_j \quad l \in \mathbb{Z}$$  \hspace{1cm} (2)

At steady state,

$$u_{j-1}p_{j-1} + w_{j+1}p_{j+1} - [u_j + w_j]p_j = 0 \quad 0 \leq j \leq N$$  \hspace{1cm} (3)

It’s solution is

$$p_j = \frac{r_j}{R_N}$$  \hspace{1cm} (4)

where

$$r_j = \frac{1}{u_j}\left[1 + \sum_{k=1}^{N-1} \prod_{i=j+1}^{j+k} \frac{w_i}{u_i}\right] \quad R_N = \sum_{j=0}^{N-1} r_j$$  \hspace{1cm} (5)
This model has been extensively studied \([9,10]\) and its mean velocity \(V_N\) and diffusion constant \(D_N\) has been obtained explicitly \([11]\). 

\[
V_N = \frac{L}{R_N} \left[ 1 - \prod_{j=0}^{N-1} \frac{w_i}{u_i} \right] \\
D_N = \frac{L}{N} \left[ \frac{LU_N + VS_N}{R_N^2} - \frac{(N+2)V}{2} \right]
\]  

(6)

where

\[
S_N = \sum_{j=0}^{N-1} s_j \sum_{k=0}^{N-1} (k+1) r_{k+j+1} \quad U_N = \sum_{j=0}^{N-1} u_j r_j s_j \quad s_j = \frac{1}{u_j} \left[ 1 + \sum_{k=1}^{N-1} \prod_{i=j+1}^{j+k} w_i \right]
\]

Besides one dimensional hopping model, the stochastic motion of particle also can be modelled by Langevin dynamics \([12,13]\) and Fokker-Planck equation \([14,8,15,16]\). Intuitively, the Langevin dynamics and Fokker-Planck equation can be regarded as infinite mechanochemical states case of periodic one dimensional hopping model. In the framework of Langevin dynamics, the particle position is governed by the following Langevin equation

\[
\xi \frac{dx(t)}{dt} = -\frac{\partial \phi(x)}{\partial x} + \sqrt{2k_B T} \xi f_B(t)
\]  

(7)

where \(\xi\) is viscous friction coefficient, \(k_B\) is Boltzmann’s constant. \(\phi(x) = \Phi(x) - F_{\text{ext}} x\), \(F_{\text{ext}}\) is external load, \(\Phi\) is a (tilted) periodic potential with period \(L\). \(T\) is absolute temperature and \(f_B(t)\) is Gaussian white noise. Based on the relation between the effective diffusion coefficient and the first two moments of the mean first passage time (MFPT), the mean velocity and effective diffusion coefficient can be expressed in quadratures \([17,18]\)

\[
V_L = \frac{1 - e^{-\Delta \phi \Delta \phi}}{\int_0^L dx I_+(x)} L \\
D_L = \frac{\int_0^L dx I_2^2(x)I_-(x)}{\left[ \int_0^L dx I_+(x) \right]^2} DL^2
\]  

(8)

where

\[
I_\pm = \pm \frac{e^{\pm \phi(x)/K_B T}}{D} \int_x^{x \mp L} dy e^{\mp \phi(y)/K_B T}
\]  

(9)

\(\Delta \phi \triangleq \phi(L) - \phi(0)\) and \(D\) is the free diffusion constant which satisfies the Einstein relation \(\xi D = k_B T\).
At the same time, the stochastic motion of particle can be modelled by the Fokker-Planck equation \[14, 15, 16\]

\[
\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left[ \rho \frac{\partial \phi}{\partial x} + D \frac{\partial \rho}{\partial x} \right]
\]

\[0 \leq x \leq L\] (10)

where \(\rho(x, t)\) is the probability density for finding particles at position \(x\) and time \(t\).

At steady state,

\[
\frac{\partial}{\partial x} \left[ \rho \frac{\partial \phi}{\partial x} + D \frac{\partial \rho}{\partial x} \right] = 0
\]

\[0 \leq x \leq L\] (11)

It’s solution is (see \[14, 17, 19\])

\[
\rho(x) = \frac{J \exp \left(-\phi(x) \frac{k_B T}{\Delta} \right)}{D \left[1 - \exp \left(\frac{\Delta \phi}{k_B T} \right)\right]} \left(\int_x^{x+L} \exp \left(\frac{\phi(y)}{k_B T} \right) dy\right)
\]

(12)

where

\[
J = \frac{D \left[1 - \exp \left(\frac{\Delta \phi}{k_B T} \right)\right]}{\int_0^L \exp \left(-\phi(x) \frac{k_B T}{\Delta} \right) \left(\int_x^{x+L} \exp \left(\frac{\phi(y)}{k_B T} \right) dy\right) dx}
\]

(13)

is the probability flux. So the mean velocity of particles is

\[
V_F = LJ = \frac{DL \left[1 - \exp \left(\frac{\Delta \phi}{k_B T} \right)\right]}{\int_0^L \exp \left(-\phi(x) \frac{k_B T}{\Delta} \right) \left(\int_x^{x+L} \exp \left(\frac{\phi(y)}{k_B T} \right) dy\right) dx}
\]

(14)

In \[20\] we have known that the formulation of the effective diffusion coefficient is

\[
D_F = J \left[\int_0^L \left(\rho(x) \Delta \phi - L \rho(x) \Delta \phi \right) dx\right]
\]

\[- \frac{JL}{\exp \left(-\phi(x) \frac{k_B T}{\Delta} \right)} \left[\int_x^{x+L} \rho^2(z) \exp \left(\frac{\phi(z)}{k_B T} \right) dz\right] dx\]

(15)

As we have mentioned, the continuous models (Langevin equation and Fokker-Planck equation) can be regarded as infinite mechanochemical states cases of the discrete model, i.e. the periodic one dimensional hopping model. Therefore, the mean velocity and effective diffusion coefficient of continuous cases can be obtained directly by calculating the limits of which in discrete case \[6\]. In the following, we will obtain the limits \(V_D\) and \(D_D\) of \(V_N\) and \(D_N\) by formal calculation. Theoretically, \(V_D\) and \(V_L, V_P\) are equivalent. Though \(D_D\) and \(D_L, D_P\) are not theoretically equivalent, since \(D_N, D_L\) and \(D_P\) are all obtained under some assumptions, numerical results indicate that the differences among them are very small.

4
2 The limit of velocity of the hopping model

Firstly, we consider the large mechanochemical state \( N \) limit of the velocity of one dimensional hopping model.

Due to the detailed balance

\[
\frac{w_{i+1}}{u_i} = \frac{\exp \left( \frac{\phi(x_{i+1})}{k_B T} \right)}{\exp \left( \frac{\phi(x_i)}{k_B T} \right)} = \exp \left( \frac{\Delta \phi_i}{k_B T} \right)
\]

(16)

where \( x_i = \frac{iL}{N} \), \( \Delta \phi_i = \phi(x_{i+1}) - \phi(x_i) \), one can know that

\[
r_j = \frac{1}{u_j} \left[ 1 + \sum_{k=1}^{N-1} \prod_{i=j+1}^{j+k} \frac{w_i}{u_i} \right]
\]

\[
= \frac{1}{u_j} + \sum_{k=1}^{N-1} \frac{1}{u_{j+k}} \prod_{i=j+1}^{j+k} \frac{w_i}{u_i}
\]

\[
= \frac{1}{u_j} + \sum_{k=1}^{N-1} \frac{1}{u_{j+k}} \prod_{i=j+1}^{j+k} \exp \left( \frac{\Delta \phi_{i-1}}{k_B T} \right)
\]

\[
= \frac{1}{u_j} + \sum_{k=1}^{N-1} \frac{1}{u_{j+k}} \exp \left( \frac{\phi(x_{j+k}) - \phi(x_j)}{k_B T} \right)
\]

\[
= \sum_{k=0}^{N-1} \frac{1}{u_{j+k}} \exp \left( \frac{\phi(x_{j+k}) - \phi(x_j)}{k_B T} \right)
\]

(17)

In the large \( N \) limit, \( u_j \approx D_N \left( \frac{N}{L} \right)^2 = D_N / (\Delta x)^2 \) (for detailed discussion, see \([21, 6]\)).

Therefore

\[
r(x_j) \approx \frac{N}{L} \int_0^L \frac{1}{u(x_j + z)} \exp \left( \frac{\phi(x_j + z) - \phi(x_j)}{k_B T} \right) dz
\]

\[
= \frac{N}{L} \int_{x_j}^{x_j + L} \frac{1}{u(z)} \exp \left( \frac{\phi(z) - \phi(x_j)}{k_B T} \right) dz
\]

\[
\approx \frac{1}{D_N \left( \frac{N}{L} \right)} \int_{x_j}^{x_j + L} \exp \left( \frac{\phi(z) - \phi(x_j)}{k_B T} \right) dz
\]

(18)

consequently

\[
R_N = \sum_{j=0}^{N-1} r_j \approx \frac{1}{D_N \left( \frac{N}{L} \right)} \int_{X_j}^{x_j + L} \exp \left( \frac{\phi(z) - \phi(x_j)}{k_B T} \right) dz
\]

\[
\approx \frac{1}{D_N} \int_0^L \left[ \int_{X_j}^{x_j + L} \exp \left( \frac{\phi(z) - \phi(x_j)}{k_B T} \right) dz \right] dx
\]

(19)
Thanks to the periodicity of the transition rates \( u_j \) and \( w_j \),

\[
\prod_{j=0}^{N-1} \frac{w_j}{u_i} = \prod_{j=0}^{N-1} \frac{w_{i+1}}{u_i} = \exp \left( \frac{\phi(x_N) - \phi(x_0)}{k_B T} \right) = \exp \left( \frac{\Delta \phi}{k_B T} \right) \quad (20)
\]

From (2) (19) (20), it is easy to obtain

\[
V_D := \lim_{N \to \infty} V_N = \frac{\overline{D} L \left[ 1 - \exp \left( \frac{\Delta \phi}{k_B T} \right) \right]}{\int_{0}^{L} \int_{x}^{x+L} \exp \left( \frac{\phi(z) - \phi(x)}{k_B T} \right) dz \, dx} \quad (21)
\]

where \( \overline{D} = \lim_{N \to \infty} \overline{D}_N \). One can easily verify that, if \( \overline{D} = D \) then \( V_D = V_L = V_F \) (see (8) (14)). In the following, we always assume that \( \overline{D} = D \).

### 3 The limit of effective diffusion coefficient of the hopping model

Using the similar discussion as in the above section, it can be easily verified that

\[
s_j = \frac{1}{u_j} \left[ 1 + \sum_{k=1}^{N-1} \prod_{i=j-k}^{j-1} \frac{w_i}{u_i} \right]
\]

\[
= \frac{1}{u_j} \left[ 1 + \sum_{k=1}^{N-1} \prod_{i=j-1}^{j-k} \exp \left( \frac{\Delta \phi_i}{k_B T} \right) \right]
\]

\[
= \frac{1}{u_j} \left[ 1 + \sum_{k=1}^{N-1} \exp \left( \frac{\phi(x_j) - \phi(x_{j-k})}{k_B T} \right) \right]
\]

\[
= \frac{1}{u_j} \sum_{k=0}^{N-1} \exp \left( \frac{\phi(x_j) - \phi(x_{j-k})}{k_B T} \right) \quad (22)
\]

In the large biochemical state number \( N \) limit,

\[
s(x_j) \approx \frac{N}{L} \frac{1}{u(x_j)} \int_{0}^{L} \exp \left( \frac{\phi(x_j) - \phi(x_j - z)}{k_B T} \right) dz
\]

\[
= \frac{N}{L} \frac{1}{u(x_j)} \int_{x_j-L}^{x_j} \exp \left( \frac{\phi(x_j) - \phi(z)}{k_B T} \right) dz \quad (23)
\]

\[
\approx \frac{1}{\overline{D} L} \int_{x_j-L}^{x_j} \exp \left( \frac{\phi(x_j) - \phi(z)}{k_B T} \right) dz
\]
For the sake of the simplicity, we define

\[
\begin{align*}
    f(x) &= \int_x^{x+L} \exp \left( \frac{\phi(z) - \phi(x)}{k_B T} \right) dz \\
    g(x) &= \int_{x-L}^x \exp \left( \frac{\phi(x) - \phi(z)}{k_B T} \right) dz
\end{align*}
\]  

(24)

It can be readily verified that

\[
\begin{align*}
    R_N &\approx \frac{1}{D_N} \int_0^L f(x) dx \\
    r(x_j) &\approx \frac{f(x_j)}{D_N \left( \frac{N}{L} \right)} \\
    s(x_j) &\approx \frac{g(x_j)}{D_N \left( \frac{N}{L} \right)} \\
    U_N &= \sum_{j=0}^{N-1} u_j r_j s_j \\
    &= \sum_{j=0}^{N-1} \frac{1}{D_N} f(x_j) g(x_j) = \frac{N}{L D_N} \int_0^L f(x) g(x) dx
\end{align*}
\]  

(25)

Moreover

\[
\begin{align*}
    \sum_{k=0}^{N-1} (k+1) r_{k+j+1} &\approx \sum_{k=0}^{N-1} (k+1) f(x_{k+j+1}) \frac{1}{D_N \left( \frac{N}{L} \right)} \\
    &= \sum_{k=0}^{N-1} x_{k+1} f(x_j + x_{k+1}) \frac{1}{D_N \left( \frac{N}{L} \right)} \approx \frac{N}{L D_N} \int_0^L z f(x_j + z) dz
\end{align*}
\]  

(27)

so

\[
\begin{align*}
    S_N &= \sum_{j=0}^{N-1} s_j \sum_{k=0}^{N-1} (k+1) r_{k+j+1} \\
    &\approx \sum_{j=0}^{N-1} \left[ \frac{g(x_j)}{D_N \left( \frac{N}{L} \right)} \right] \left[ \frac{N}{L D_N} \int_0^L z f(x_j + z) dz \right] \\
    &= \frac{1}{D^2} \sum_{j=0}^{N-1} g(x_j) \int_0^L z f(x_j + z) dz \\
    &\approx \frac{N}{L D^2} \int_0^L \left[ g(x) \int_0^L z f(x + z) dz \right] dx
\end{align*}
\]  

(28)
Substituting (21) (25) (26) (28) into (6), one obtains

$$D_N = \frac{L}{N} \left[ \frac{L U_N + V S_N}{R_N^2} - \frac{(N + 2)V}{2} \right]$$

$$= \frac{L}{N} \left[ L \left[ 1 - \exp \left( \frac{\Delta \phi}{k_B T} \right) \right] \frac{N}{L D N} \int_0^L g(x) \int_0^L \rho(x + z) dz \, dx \right]$$

$$+ \frac{L}{N} \left[ \frac{N}{L D N} \int_0^L f(x) g(x) dx \right] \frac{N}{L D N} \int_0^L f(x) dx \right] - \frac{(N + 2)D_N L}{2} \left[ 1 - \exp \left( \frac{\Delta \phi}{k_B T} \right) \right]$$

$$= L D_N \left[ \frac{1 - \exp \left( \frac{\Delta \phi}{k_B T} \right)}{f_0^L f(x) dx} \right] \frac{N}{L D N} \int_0^L f(x) dx \right] - \frac{(N + 2)L}{2} \left[ \frac{1 - \exp \left( \frac{\Delta \phi}{k_B T} \right)}{f_0^L f(x) dx} \right]$$

$$+ \int_0^L f(x) g(x) dx \left[ \frac{f_0^L f(x) dx}{f_0^L f(x) dx} \right] - \frac{(N + 2)L}{2} \left[ \frac{1 - \exp \left( \frac{\Delta \phi}{k_B T} \right)}{f_0^L f(x) dx} \right]$$

$$= 2N \int_0^L f(x) dx \left[ \frac{1 - \exp \left( \frac{\Delta \phi}{k_B T} \right)}{f_0^L f(x) dx} \right] - \frac{(N + 2)L}{2} \left[ \frac{1 - \exp \left( \frac{\Delta \phi}{k_B T} \right)}{f_0^L f(x) dx} \right]$$

Substituting (31) into (30), we finally get the limit of the effective diffusion coefficient

$$D_D := \lim_{N \to \infty} D_N$$

$$= J L \int_0^L \rho(x) g(x) dx \left[ 1 - \exp \left( \frac{\Delta \phi}{k_B T} \right) \right] + \frac{J^2 L \int_0^L g(x) \int_0^L \rho(x + z) dz \, dx}{D \left[ 1 - \exp \left( \frac{\Delta \phi}{k_B T} \right) \right]} - \frac{1}{2} J L^2$$

$$= V \int_0^L \rho(x) g(x) dx \left[ 1 - \exp \left( \frac{\Delta \phi}{k_B T} \right) \right] + \frac{J V \int_0^L g(x) \int_0^L \rho(x + z) dz \, dx}{D \left[ 1 - \exp \left( \frac{\Delta \phi}{k_B T} \right) \right]} - \frac{1}{2} V L$$
By the way, the limit of the randomness parameter $RAN D_N = \frac{2DV}{VN L}$ is

$$
\lim_{N \to \infty} RAN D_N = \frac{2 \int_0^L \rho(x)g(x)dx}{L\left[1 - \exp\left(\frac{\Delta\phi}{k_B T}\right)\right]} + \frac{2J \int_0^L \left[g(x) \int_0^L z\rho(x + z)dz\right] dx}{DL\left[1 - \exp\left(\frac{\Delta\phi}{k_B T}\right)\right]} - 1 \tag{33}
$$

### 4 Numerical results and discussion

As we have known that the limit $V_D$ of velocity of the hopping model is the same as $V_L$ and $V_F$. However, it is easy to understand that $D_D$ would be different from $D_L$, $D_F$ because they are obtained under different assumptions.

To indicate the accuracy of the formulation (32), we present the numerical results of the formulations (8), (15) and (32) in Figure 1 and 2. From the numerical results we can find that the formulation (32) is accurate enough, especially for the cases with small external force $F_{ext}$. Which implies that the methods used to derived the formulation (32) is reasonable. From the derivation we also can know more about the relationship between discrete models and continuous models of stochastic motion of microscopic particles.

In conclusion, we have provided an analytical formulation of effective diffusion coefficient of the stochastic motion of microscopic particles. The numerical comparison with the formulation obtained in the framework of the overdamped Langevin dynamics and Fokker-Planck equation indicates that our analytical formulation is very accurate. Moreover, the methods used in this research can be further used to get more results about the stochastic motion. Through the discussion in this research, the relationship between continuous models and discrete models has also been made clear.

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Figure 1: **Left:** figures of effective diffusion coefficient as a function of free diffusion coefficient $D := k_B T / \xi$, where the red line is obtained by the formulation (15), the green stars are obtained by the formulation (8) and the blue circles are obtained by the formulation (32). **Right:** the difference between the formulations (32), (8) and (15), where $D_F$ denote the results of formulation (15), $D_L$ denote the results of the formulation (8) and $D_D$ denote the results of the formulation (32). In the simulation, the potential $\Phi(x) = U_0 \sin(2\pi x / L) - F_{\text{ext}} x$ and $\xi = U_0 = L = 1$ (see [18]), $F_{\text{ext}} = 0.5$. 
Figure 2: **Left:** the relationship between the effective diffusion coefficient and the external force $F_{\text{ext}}$. **Right:** the differences between the formulations (8) (15) and (32). In the simulation, the potential $\Phi(x) = U_0\sin(2\pi x/L) - F_{\text{ext}}x$ and $\xi = U_0 = L = 1$ (see [18]).

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