

## Tunneling effects on the current and the mobility for coupled random walks

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**Abstract** A model based on coupled random walks (CRW) is proposed to investigate the current and the frequency-dependent mobility. The system is composed of particles, hopping from mode  $j$  at site  $m$  to mode  $i$  at site  $m'$  under a driving force,  $E(t)$ . We get an expression for the current in which the mobility depends on a "tunneling factor" and the difference of energy levels. The frequency-dependent mobility depends on the cell structure as well as the tunneling factor.

### 1. Introduction

Stochastic descriptions have been realized to be important for studying dynamical systems<sup>1</sup>. Specifically the approach based on random walks (RW) has been extensively utilized<sup>2-6</sup>. Montroll and Weiss<sup>2</sup> proposed the continuous-time RW (CTRW) considering the individual jumps specified by a time dependent distribution. This formalism provided many applications and models<sup>4-6</sup>. For transport phenomena in a medium with traps, there are trapping or hopping models<sup>4</sup> including repeated capture and release. Recently, Kehr and Haus<sup>5</sup> studied the relation between the CTRW and the trapping models. Furthermore, Zwerger and Kehr<sup>6</sup> gave a more general model to investigate the influence of the internal state on the frequency-dependent mobility. In this model, however, the particle can make a transition to neighboring sites, only when it is on the top of a potential barrier.

### *Tunneling effects on the current and the mobility...*

In previous papers<sup>7,8</sup>, one of the present authors proposed the coupled RW to take into account the couplings or interactions between the walker (particle) and the environment (medium and the other particles). On stochastic descriptions for the hopping among potential wells, it is necessary that successive jumps are uncorrelated and particles are supposed to remain long enough.

The purpose of this paper is to propose a model based on coupled random walks (CRW) having a "tunneling" effect. The tunneling effect represents direct transitions between sites at the same modes, *not located at top modes* corresponding to the usual tunneling effect on the energy description. In the CRW, the jumping probabilities (JP) (transitions) between sites are "correlated\*" through the normalization of the JP, while the successive jumps are not correlated directly with weight functions. To clarify the effect, we derive a general expression of the current, and the frequency dependent mobility is studied.

## **2. Coupled random walks**

Here we assume that the particle (walker) in a well resides long enough at each mode. The time scale (step) that the particle's stay is short enough in a macroscale such that we can define modes, corresponding to energy levels having intervals  $\Delta E_1, \Delta E_2, \dots, \Delta E_n, \dots$ . The latter condition leads us to describe a propagation in terms of the transition probabilities specified by the energy intervals:  $\Delta E_1, \Delta E_2, \dots$

We give the model of the CRW expressed in a form similar to the trapping models. The CRW is expressed by a set of coupled recursion relations in which the walker makes a site-to-site and/or mode-to-mode jump in the range  $-L \leq m \leq L$ . Let  $W^{(i)}(m, N)$  be the probability that the walker starting from the origin arrives at site  $m$  on a mode  $i$  after  $N$  steps. The recursion relation for  $W^{(i)}(m, N)$  is written in the form

$$W^{(i)}(m, N) = P_{N-1}^{+(i)}(M|m-1)W^{(i)}(m-1, N-1) + P_{N-1}^{-(i)}(m|m+1)W^{(i)}(m+1, N-1)$$

$$\begin{aligned}
 & + \sum_{j=1}^{i-1} R_{N-1}^{+(i,i-j)}(m) W^{(i-j)}(m, N-1) \\
 & + \sum_{j=1}^{M-i} R_{N-1}^{-(i,i+j)}(m) W^{(i+j)}(m, N-1) \\
 & (i = 1, 2, \dots, M)
 \end{aligned} \tag{2.1}$$

and  $W^{(i)}(m = \pm L, N) = 0$  and  $W^{(i)}(m, N)$  is normalized as follows

$$\sum_m \sum_i W^{(i)}(m, N) = 1 \tag{2.2}$$

where mode  $i$  represents the sequence number of energy intervals at each site, and  $P_{N-1}^{\pm(i)}(m|m \mp 1)$  and  $R_{N-1}^{\pm(i,i \mp j)}(m)$  are jumping probabilities normalized as

$$P_N^{+(i)}(m+1|m) + P_N^{-(i)}(m-1|m) + \sum_{j=1}^{M-i} R_N^{+(i+j,i)}(m) + \sum_{j=1}^{i-1} R_N^{-(i-j,i)}(m) = 1 \tag{2.3}$$

(see fig. 1).

Note here that the jumping probabilities are correlated through the normalization eq.(2.3), while the successive jumps are uncorrelated.

Following the previous papers<sup>7,8</sup>, we convert the recursion relation eq. (2.1) into the corresponding continuous form. The system we consider here is a lattice walk of particles. To this end, we introduce only a continuous time  $t$  defined by

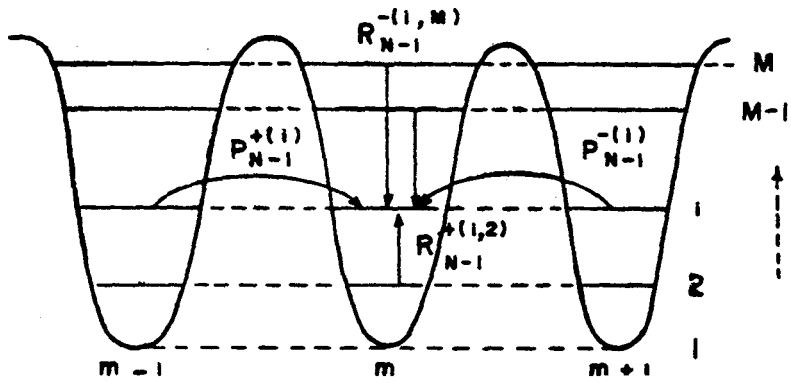
$$t = N\Delta t \quad (\Delta t : \text{unit time}) \tag{2.4}$$

and use a set of continuous functions for  $t$  but discrete ones for  $i$  and  $m$ .<sup>\*</sup> The time region we consider here is assumed to be long enough such that we can describe the stochastic motions of a particle in a well  $t \ll \tau$ , but  $\tau$  is small enough that we can define energy intervals  $\Delta E$ ; ( $i = 1, 2, \dots$ ).

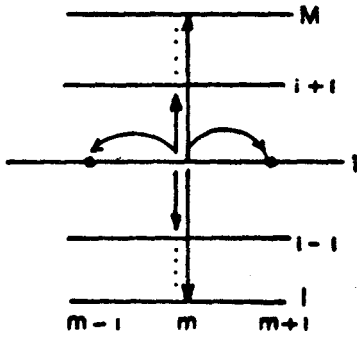
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<sup>\*</sup> Here we use the same notations for the continuous functions  $W^{(i)}(m, t)$ ,  $P_{t-\Delta t}^{(i)}(m|m-\alpha.1)$  and  $r_{t-\Delta t}^{(i,i-\alpha.j)}(m)$  for  $\alpha = \$. , -, 0$  corresponding to  $W^{(i)}(m, N)$ ,  $P_{N-1}^{\alpha(i)}(m|m-\alpha.1)$  and  $R_{N-1}^{\alpha(i,i-\alpha.j)}(m)$ , respectively.

Tunneling effects on the current and the mobility...



( a )



( b )

Fig. 1 - Coupled random walks. (a) Graphical representation of eq. (2.1). (b) Normalization of jumping probabilities given by eq. (2.3).

S.J. Lee and H. Hara

After expanding the recursion relation (2.1) of a continuous form around  $t = 0$ , we get a master equation

$$\begin{aligned} \frac{\partial W^{(i)}(m, t)}{\partial t} &= \sum_{\alpha(=+-)}^I P_t^{\alpha(i)}(m|m - \alpha.1)W^{(i)}(m - \alpha.1, t) \\ &+ \sum_{\alpha}^I \left( \sum_{j=1}^{M_+^{(\alpha)}} R_t^{\alpha(i, i-\alpha.j)}(m)W^{(i-\alpha.j)}(m, t) \right) - \sum_{\alpha}^I P_t^{\alpha(i)}(m + \alpha.1|m)W^{(i)}(m, t) \\ &- \sum_{\alpha}^I \left( \sum_{j=1}^{M_-^{(\alpha)}} R_t^{\alpha(i+\alpha.j, i)}(m)W^{(i)}(m, t) \right) + O(\Delta t) \end{aligned} \quad (2.5)$$

with

$$\sum_{\alpha}^I P_t^{\alpha(i)}(m + \alpha.1|m) + \sum_{\alpha}^I \left( \sum_{j=1}^{M_-^{(\alpha)}} R_t^{\alpha(i+\alpha.j, i)}(m) \right) = 1 \quad (2.6)$$

where

$$\begin{aligned} P_t^{\alpha(i)}(m|m - \alpha) &\equiv \frac{1}{\Delta t} \left[ P_N^{\alpha(i)}(m|m - \alpha.1) \right]_{N=t/\Delta t} \\ R_t^{\alpha(i, i-\alpha.j)}(m) &\equiv \frac{1}{\Delta t} \left[ R_N^{\alpha(i, i-\alpha.j)}(m) \right]_{N=t/\Delta t} \end{aligned} \quad (2.7)$$

and

$$M_{\pm}^{(\alpha)} = \frac{\mathbf{M}}{2}(1 \mp \alpha.1) - \frac{1}{2}(1 \pm \alpha.1) \pm \alpha.i \quad (\mathbf{a} = +, -) \quad (2.8)$$

and a prime on C means to omit  $\mathbf{a} = 0$  in the sum. In the derivation of eq. (2.5), we have used the normalization eq. (2.3) and the fact that the jumping probabilities  $P_N^{\alpha(i)}$  and  $R_N^{\alpha(i, j)}$  are of the order of  $\Delta t$ . The master eq. (2.5) is a general expression corresponding to the set of basic equations for the trapping models due to Kehr et al.<sup>5,6</sup>. In the present master equation, the jumps between sites are taken into account considering modes corresponding to the intermediate energy intervals of the potential barriers as shown in fig. (1a). Also note that "hopping rates" are related themselves with the normalization eq. (2.6).

*Tunneling effects on the current and the mobility...*

**3. Tunneling** (shift) factor

As seen in **fig. 1**, the **mode i** corresponds to an energy interval of the particle motions in the **trapping** model or hopping model. In this paper, we **call** the energy intervals "energy levels", for simplicity, and we **call** the top energy interval  $i = M$  the "hopping level". To take into account the jumping processes between **sites**  $P_t^{\pm(i)}(m \pm 1|m)$  occurred at the intermediate energy levels, we introduce a shift factor  $T^{(i)}$  defined by

$$P_t^{\pm(i)}(m \pm 1|m) = P_t^{\pm(M)}(m \pm 1|m)T^{(i)} \tag{3.1}$$

for each  $i$ , see **fig. (2a)** and  $T^{(M)} = 1$ . Processes described by the shift factor are corresponding to the tunneling effect. **Fig. (2b)** shows that the shift factor depends on thickness,  $a$ , and heights of potential barrier,  $\eta_i$  and  $V$  from the corresponding energy levels  $i$  and  $1$ .

In the following analysis, we **study** hopping models in which the  $T^{(i)}$  (which will be discussed shortly) is specified by

(I) Exponential type ( $\eta_i a^2 > 1$ )

$$T^{(i)} = \frac{(V - \eta_i)\eta_i}{(V - \eta_M)\eta_M} \exp(-2a\sqrt{\eta_i - \eta_M}) \tag{3.2a}$$

and

$$T^{(i)} = \frac{(V - \eta_M) + V^2 a^2 / 4}{(V - \eta_i) + V^2 a^2 / 4} \cdot \frac{(V - \eta_i)}{(V - \eta_M)} \tag{3.2b}$$

where

$$\eta_i = V - i, \quad (\eta_1 \leq V), \quad (i = 2, 3, \dots, M) \tag{3.3}$$

$\eta_i$  and  $V (= \eta_1)$  express the height of the potential barrier from energy levels  $i$  ( $\neq 1$ ) and  $1$ . The parameter  $a$  denotes thickness of the potential barrier.

In the derivation of the forms expressed by eqs. (3.2) and (3.3), we have used the fact that the one-dimensional square potential of barrier height  $V$  and thickness  $a$  gives the transmission coefficient  $T$  :

$$T = \left( 1 + \frac{V^2 \sinh a\sqrt{V - \epsilon}}{4\epsilon(V - \epsilon)} \right)^{-1} \tag{3.4}$$

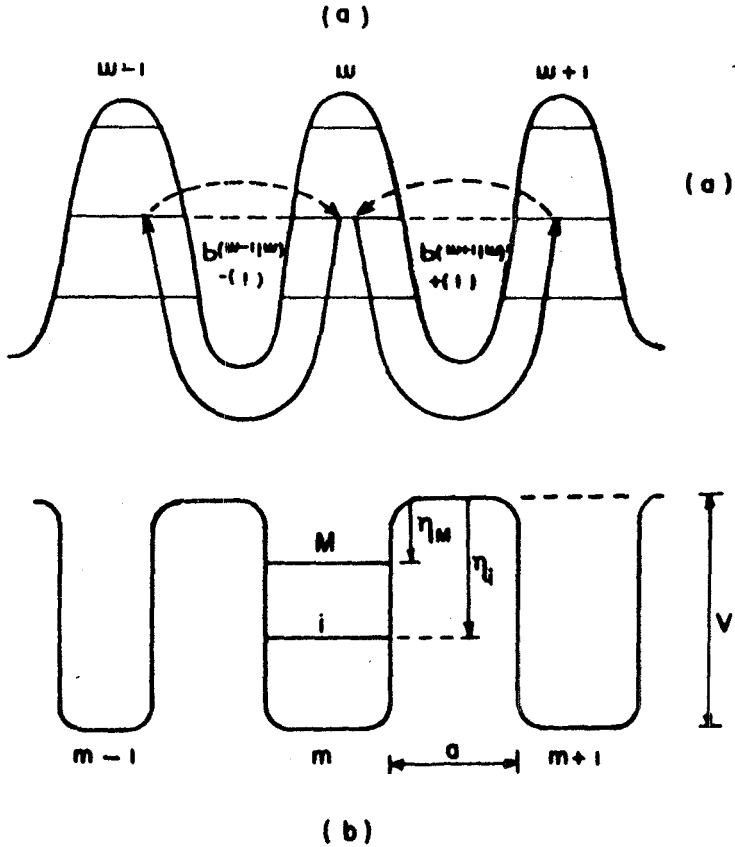


Fig. 2 - Tunneling (shift) factor. (a) Tunneling effects of potential barrier. (b) Specification of potential barrier by geometrical factor  $a$  and  $V$ .

where  $\epsilon$  is the energy of an incident particle having wave number  $k$ <sup>9</sup>. Replacement  $V - \epsilon \rightarrow \eta_i$  ( $\epsilon = i$ ) yields asymptotic forms:

$$T^{(i)} \sim \frac{16(V - \eta_i)\eta_i}{V^2} \exp(-2\sqrt{\eta_i}a) \left( 1 + \frac{16(V - \eta_i)\eta_i}{\exp(2\sqrt{\eta_i}a)V^2} - \frac{2}{\exp(2\sqrt{\eta_i}a)} \right)^{-1} \quad (\sqrt{\eta_i}a > 1) \quad (3.5a)$$

and

$$T^{(i)} \sim \frac{4(V - \eta_i)}{4(V - \eta_i) + V^2 a^2} \quad , \quad (\sqrt{\eta_i}a < 1) \quad (3.5b)$$

**Tunneling effects on the current and the mobility...**

according to **whether** the magnitude of  $(\sqrt{\eta_i}a)$  is **greater** than unity or **less** than unity. The shift (**tunneling**) factors eq.(3.2a) or eq. (3.2b) are obtained from the ratio of eq.(3.5a) or eq. (3.5b) to the corresponding expression for  $\eta_M$ .

Fig. 3 shows the models of the tunneling factors for the exponential type I **and** the fractional type II, respectively.

In fig. 4 we **explicitly** show the behavior of  $T^{(i)}$  for **two** different cases. Here, for **convenience**, we took,  $V = 4$ ,  $\eta_i \in [1, 4]$   $\eta_M = 1$  and  $a = 2$  ( $a = 1/5$ ) for the case I (case II).

For a case in which the height of **chain** of the potential barriers is **iffere**nt from **site** to **site**, we have to generalize the tunneling factor in eq. (3.1) as **follows**

$$P_t^{\pm(i)}(m \pm 1|m) = P_t^{\pm(M)}(m \pm 1|m)T^{(i)}(m) \tag{3.6}$$

where

$$T_{(m)}^{(i)} = \frac{[V(m) - \eta_i(m)]\eta_i(m)}{[V(m) - \eta_M(m)]\eta_M(m)} \exp(-2a\sqrt{\eta_i(m) - \eta_M(m)}) \text{ for (I)} \tag{3.7a}$$

$$T_{(m)}^{(i)} = \frac{V(m) - \eta_M(m) + V^2(m) a^2/4}{V(m) - \eta_i(m) + V^2(m) a^2/4} \cdot \frac{V(m) - \eta_i(m)}{V(m) - \eta_M(m)} \text{ for (II)} \tag{3.7b}$$

and an argument  $m$  in  $V$  and  $\eta_i$  implies that  $V$  and  $\eta$  depend on **site**  $m$ .

**4. Current for coupled random walks**

To get a general expression for current in which tunneling factors are explicitly expressed, we rewrite the recursion relation (2.1) in which **particles** are hopping from energy **level**  $j$  at **site**  $m'$  to energy **level** at **site**  $m$  under a driving force. Instead of eq. (2.1) we get the recursion relation

$$W^{(i)}(m, N) = \sum_{m'} \sum_j P_{N-1}^{(i,j)}(m|m')W^{(j)}(m', N-1) \tag{4.1}$$

$$\sum_{m'} \sum_j P_{N-1}^{(j,i)}(m'|m) = 1 \tag{4.2}$$



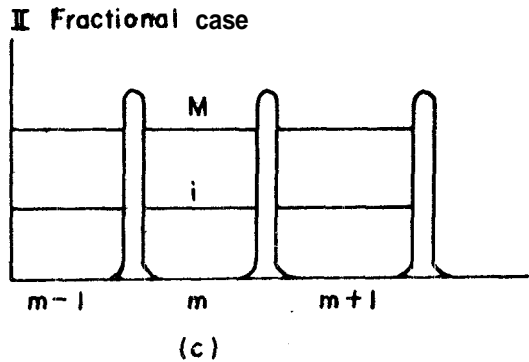
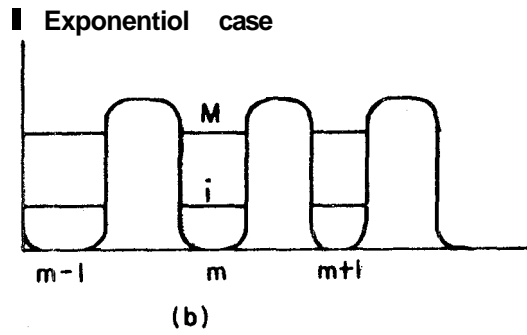
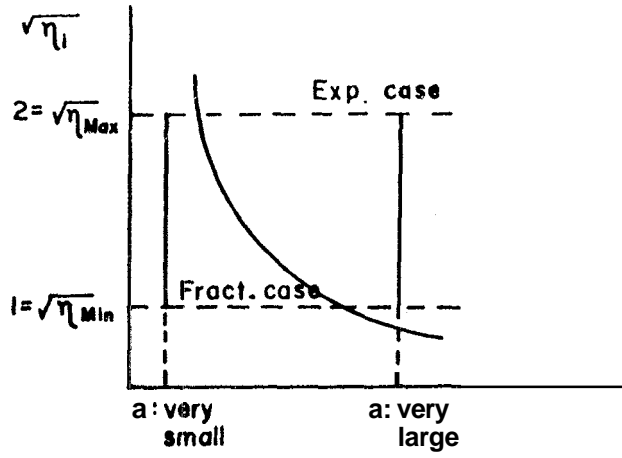


Fig. 3 - Models of tunneling (shift) factor. (a) Exponential type. (b) Fractional type.

Tunneling effects on the current and the mobility...

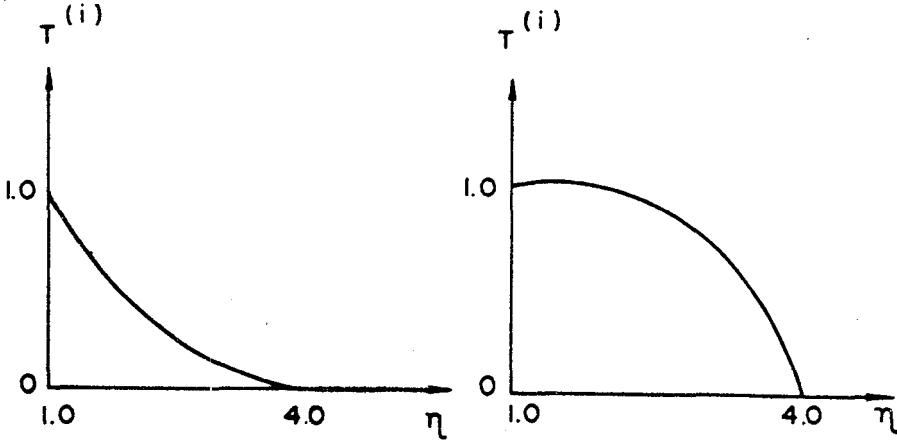


Fig. 4 - Behaviors of  $T^{(i)}$ . (a) Exponential type. (b) Fractional type. In the evaluation, we have put  $V = 4$ ,  $\eta_i \in [1, 4]$ ,  $\eta_M = 1$  and  $a = 2$  ( $a = 1/5$ ) for the case (I) (case (II)).

where the jumping probabilities  $P_{N-1}^{(i,j)}(m|m')$ 's are reduced to the  $P_{N-1}^{\pm(i)}(m|m \mp 1)$  for  $j = i$  and  $m' = m \pm 1$  or  $R_{N-1}^{\mp(i,j)}(m)$  for  $m' = m$ .

The continuum limit of eq. (4.1) yields

$$\frac{\partial W^{(i)}(m, t)}{\partial t} = \Delta m J^{(i)}(m, t) \tag{4.3}$$

$$\Delta m J^{(i)}(m, t) = J^{(i)}(m + 1, t) - J^{(i)}(m, t) \tag{4.4}$$

$$J^{(i)}(m, t) = \sum_j \left[ P_i^{(i,j)}(m + 1|m)W^{(j)}(m, t) - P_i^{(j,i)}(m - 1|m)W^{(i)}(m, t) \right] \tag{4.5}$$

From eq. (4.5) the current  $J(t)$  per particle is expressed by

$$J(t) = \sum_i \sum_m J^{(i)}(m, t) \tag{4.6}$$

For  $j = i$  in eq. (4.5),  $J(t)$  is found to be equivalent to the expression

$$J(t) = \sum_m (m \partial W(m, t) / \partial t)$$

which is used by Zwerger and Kehr<sup>6</sup> [ZK].

The expression (4.6) with (4.5) is a general expression very convenient for modelling the current in terms of the jumping probabilities  $P_t^{(i,j)}(m|m')$ . For a restricted case with  $j = i$  in eq.(4.5), the  $J(t)$  expressed by the tunneling factor eq. (3.1) reads

$$J(t) = \sum_m \left( \left[ P_t^{+(M)}(m+1|m) - P_t^{-(M)}(m-1|m) \right] \times \left( 1 - \sum_{i \neq M} \frac{T^{(i)}W^{(i)}(m,t)}{W^{(M)}(m,t)} \right) \right) W^{(M)}(m,t) \quad (4.7)$$

The contributions having  $T^{(i)}W^{(i)}(m,t)/W^{(M)}(m,t)$  represent a "local current" due to the jumping processes occurring at intermediate level  $i$  of potential barrier at site  $m$  under the driving force  $E(t)$ .

We consider a transport process on the hopping level  $M$  in which the mobility  $B(t)$  of the particles (ions) having the charge  $e$ , under the driving force  $E(t)$  is defined by

$$J(t) = W_{eq}^{(M)} e \int_{-\infty}^t B(t-t') E(t') dt' \quad (4.8)$$

where  $W_{eq}^{(M)}$  is the thermal equilibrium value of  $W^{(M)}(t)$ , that is the number density of particles.

Here we suppose that under the driving force  $E(t)$  the jumping probabilities  $P_t^{(i)}(m|m')$ 's (=  $P_t^{(i,j)}(m|m')$ ) are specified by

$$\frac{P_t^{+(M)}(m+1|m)}{P_t^{-(M)}(m-1|m)} = \exp(-\beta(\mu_M^+ - \mu_M^-)) = \exp(\beta e E(t)) = 1 + \beta e E(t) \quad (4.9)$$

$$\mu_M^\pm = \mu\left(m \pm \frac{1}{2}\right) = E_0 \pm \frac{eE}{2}, \quad \left(\beta = \frac{1}{k_B T}\right) \quad (4.10)$$

where  $\mu(m \pm 1/2)$  is a chemical potential at intermediate site  $m \pm 1/2$ ,  $E_0$  is an activation energy, and  $T$  is the temperature. We define a hopping rate

Tunneling effects on the current and the mobility...

$$\gamma = P_t^{+(M)}(m+1|m) + P_t^{-(M)}(m-1|m) \left( = 1 - R_t^{(M-1,M)}(m|m) \right) \quad (4.11)$$

Firstly, we consider a very weak driving force  $\beta e E(t) \ll 1$ . We have

$$P_t^{\pm}(m \pm 1|m) = \frac{\gamma}{2}(1 \pm e\beta E(t)) + O(E^2) \quad (4.12)$$

For a special case in which the  $m$ -dependence of a ratio  $W^{(i)}(m, t)/W^{(M)}(m, t)$  is omitted

$$\frac{W^{(i)}(m, t)}{W^{(M)}(m, t)} \equiv f(i, M; t) \quad (4.13)$$

We can simplify the expression for  $J(t)$  in eq. (4.7)

$$J(t) = \frac{\gamma e E(t)}{2k_B T} W^{(M)}(t) \left[ 1 + \sum_{i \neq M} T^{(i)} f(i, M; t) \right] \quad (4.14)$$

where

$$W^{(M)}(t) = \sum_m W^{(M)}(m, t) \quad (4.15)$$

Here note that the current is expressed by the contributions on the hopping level  $M$ .

In the linear response to force  $E(t)$ , we can replace  $W^{(i)}(t)$  by  $W_{eq}^{(i)}$ , the **thermal equilibrium value** of  $W^{(i)}(t)$  before applying the external field  $E(t)$ . The expression for  $J(t)$  then becomes

$$J(t) = \frac{\gamma_{\text{eff}} e E(t)}{2k_B T} W_{eq}^{(M)} \quad (4.16)$$

where

$$\gamma_{\text{eff}} = \gamma \left[ 1 + \sum_{i \neq M} T^{(i)} f_{eq}(i, M) \right], \quad (4.17)$$

$$f_{eq}(i, M) \equiv W_{eq}^{(i)} / W_{eq}^{(M)}$$

and the mobility  $B$  corresponding to the expression in eq. (4.8) is then

$$B = \frac{\gamma_{\text{eff}}}{2k_B T} W_{eq}^{(M)} \quad (4.18)$$

Specifically, when we assume that  $f_{eq}(i, M)$  is expressed in a form  $\exp(-\beta(\epsilon_i - \epsilon_M))$ ,  $\gamma_{\text{eff}}$  reads

$$\gamma_{\text{eff}} = \gamma \left[ 1 + \sum_{i(\neq M)} T^{(i)} \exp(-\beta(\epsilon_i - \epsilon_M)) \right] \quad (4.19)$$

The mobility shows no frequency dependence and reveals that its variation depends on two factors: one is the tunneling factor  $T^{(i)}$  and the other is the difference of energy levels  $\epsilon_i, \epsilon_M$ .

### 5. Frequency-dependent mobility

We consider a case that yields frequency dependent mobility. In the case that the driving force  $E(t)$  is assumed to change energy levels at each site, the force modifies a chain of potential barriers, and eventually forms a repeated structure of cells. To this end, we start the general expression for  $J(t)$ , corresponding to eq. (4.7),

$$J(t) = \sum_m \left[ P_t^{+(M)}(m+1|m) \tilde{T}^+(m) - P_t^{-(M)}(m-1|m) \tilde{T}^-(m) \right] W^{(M)}(m, t) \quad (5.1)$$

with

$$\tilde{T}^{\pm(i)}(m) = \mathbf{i} \dagger \sum_{i(\neq M)} T^{\pm(i)}(m) f(\mathbf{i}, M) \quad (5.2)$$

where new notations  $T^{\pm(i)}(m)$  are introduced instead of the tunneling factor  $T^{(i)}(m)$  in eq. (3.6) to distinguish energy level shifts in  $P_t^{\pm(i)}(m \pm 1|m)$  and  $P_t^{\pm(M)}(m \pm 1|m)$  due to the driving force

$$P_t^{\pm(i)}(m \pm 1|m) = P_t^{\pm(M)}(m \pm 1|m) T^{\pm(i)}(m)$$

here we assume that the chain of potential barriers is characterized by a set of cells with repeated structures and the processes are specialized by the "balance condition" appearing in the cell under  $E(t)$ , see fig. 5.

*Tunneling effects on the current and the mobility...*

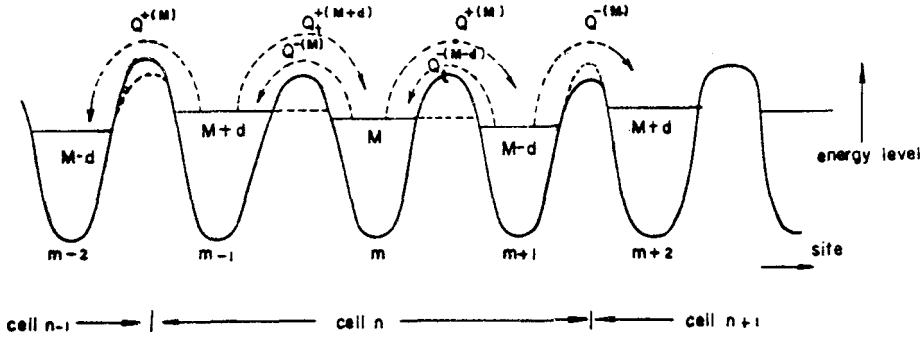


Fig. 5 - The appearing cell structures due to the driving force, the repeated structures yield frequency-dependent mobility. Each cell is specified by a set of jumping probabilities of hopping levels, probabilities and tunneling factors.

Namely, each cell is specified by a set of jumping probabilities of hopping levels  $P_t^{\pm(M)}(m \pm 1|m)$ , the probabilities  $W^{(M)}(m, t)$  and an "effective" tunneling factor  $\tilde{T}_n^{\pm}(m)$

$$P_t^{+(M)}(m' + 1|m') = Q_n^{+(M+d)}(t), \quad (m' = m - 1) \tag{5.3a}$$

$$P_t^{+(M)}(m' + 1|m') = Q_n^{+(M)}, \quad (m' = m) \tag{5.3b}$$

$$P_t^{+(M)}(m' + 1|m') = Q_n^{-(M)}, \quad (m' = m + 1) \tag{5.3c}$$

$$P_t^{-(M)}(m' - 1|m') = Q_n^{+(M)}, \quad (m' = m - 1) \tag{5.4a}$$

$$P_t^{-(M)}(m' - 1|m') = Q_n^{-(M)}, \quad (m' = m) \tag{5.4b}$$

S.J. Lee and H. Hara

$$P_t^{-(M)}(m' - 1|m') = Q_n^{-(M-d)}(t), \quad (m' = m \mp 1) \quad (5.4c)$$

$$W^{(M)}(m', t) = W_n^{(M \pm d)}(t), \quad (m' = \mp 1) \quad (5.5a)$$

$$W^{(M)}(m', t) = W_n^{(M)}(t), \quad (m' = m) \quad (5.5b)$$

and'

$$\tilde{T}^+(m') = T_n, \quad (m' = m \pm 1, m) \quad (5.6)$$

Jumping probabilities  $Q_n^{\pm(M \pm d)}$  are  $t$ -dependent ones, while  $Q_n^{\pm(M)}$  are constant ones. An index  $n$  of  $Q_n$ ,  $W_n$  and  $T_n$  represents that the quantities are defined in the  $n$ -th cell. Superscripts  $(M \pm d)$  of  $Q_n^{\pm(M \pm d)}(t)$  and  $W_n^{(M \pm d)}$  denote energy levels modified by the driving force  $E(t)$ .

Eqs. (5.3c) and (5.4a) represent the balance condition mentioned above: slopes and shapes of **outer** potential barriers of the cell are supposed to **regulate** the jumping probabilities  $P_t^{\mp(M \pm d)}(m \mp 2|m \mp 1)$  as follows

$$\begin{aligned} P_t^{-(M+d)}(m-2|m-1)W^{M+d}(m-1, t)\tilde{T}^-(m-1) \\ = P_t^{+(M)}(m+1|m)W^{(M)}(m, t)\tilde{T}^+(m) \end{aligned} \quad (5.7)$$

$$\begin{aligned} P_t^{+(M-d)}(m+2|m+1)W^{M-d}(m+1, t)\tilde{T}^+(m+1) \\ = P_t^{-(M)}(m-1|m)W^{(M)}(m, t)\tilde{T}^-(m) \end{aligned} \quad (5.8)$$

In other words, transition rates between energy levels  $(M-d)$  at cell  $n$  or  $n-1$  and  $(M+d)$  at cell  $n+1$  or  $n$ , respectively, are regulated by changing shape to match transition rates between energy levels  $M$  and  $M \pm d$ . From eq. (5.6), we can rewrite  $\tilde{T}^{\pm}(m \pm k) = T_n$  for  $k = 1, 0$ .

Here note that the  $Q_n^{\pm(M \pm d)}(t)$  depend on the  $E(t)$  as follows

$$\frac{Q_n^{+(M+d)}(t)}{Q_n^{-(M-d)}(t)} = \exp(-\beta[\mu_n^+ - \mu_n^-]) = \exp(\beta eE(t)) = 1 + \beta eE(t) \quad (5.9)$$

$$\mu_n^{\pm} = \mu\left(m \pm \frac{1}{2}\right) = E_0 \pm \frac{eE}{2}$$

*Tunneling effects* on the current and the *mobility*...

$m$  is a site in cell  $n$ , whereas the  $Q^{\pm(M)}$  are independent from  $E(t)$ : center sites of each cell are neutral points. For a special case in which  $R_t(m \mp 1)$  have separate forms:  $R_t(m \mp 1) = R \pm \Delta R_t$  we note that  $Q_t^{\pm(M \mp d)}$  (or  $Q^{\pm(M)}$ ) and  $W_n^{(M \pm d)}$  (or  $W_n^{(M)}(t)$ ) are related by

$$Q_t^{(M+d)} + Q^{+(M)} = 1 - (R - \Delta R_t) \quad (5.10a)$$

$$Q^{+(M)} + Q^{-(M)} = 1 - R \quad (5.10b)$$

$$Q^{-(M)} + Q_t^{-(M-d)} = 1 - (R + \Delta R_t) \quad (5.10c)$$

from  $\sum_{\alpha} P_t^{\alpha}(m' \pm \alpha.1|m') = 1$  for  $m' = m \mp 1$  and  $m$ . When  $R_t(m \pm 1)$  and  $R_t(m)$  are  $m$ -independent these relations lead us to define the hopping rate  $\gamma$  in eq.(4.11) by

$$\gamma' = Q_t^{+(M+d)} + Q_t^{-(M-d)} (= 1 - R) \quad (5.11)$$

The hopping rate and the relation eq. (5.9) give us

$$Q_n^{\pm(M \pm d)}(t) = \frac{\gamma'}{2} \left( 1 \pm \frac{\beta e E(t)}{2} \right) + O(E^2) \quad (5.12)$$

After considering contributions for  $m \pm 1$ , and  $m$  in the  $n$ -th cell, and taking account of eqs. (5.6), (5.7) and (5.8), substitutions of eqs. (5.3a)-(5.5b) into eq.(5.1) lead us to

$$J(t) = \sum_n \left[ Q_n^{+(M+d)}(t) W^{(M+d)}(t) - Q_n^{-(M-d)}(t) W^{(M-d)}(t) \right] T_n \quad (5.13)$$

Consideration of eq.(5.12) in eq.(5.13) yields an expression of  $J(t)$  for the present model

$$\begin{aligned} J(t) = & \frac{\gamma'}{2} \sum_n \left[ (W_n^{(M+d)}(t) - W_n^{(M-d)}(t)) \right. \\ & \left. + \frac{E(t)}{2} (W_n^{(M+d)}(t) + W_n^{(M-d)}(t)) \right] T_n \end{aligned} \quad (5.14)$$



S.J. Lee and H. Hara

The  $J(t)$  has an expression similar to the ZK model, except for the presence of the tunneling factor,  $T_n$  and cell structure. The first terms  $(W_n^{(M+d)}(t) - W_n^{(M-d)}(t))T_n$  in eq. (5.14) contain implicitly the contribution of order  $E(t)$ . To get the explicit form, we have to solve a set of master equations in each cell. The second term contains  $E(t)$  explicitly, hence we can replace  $(W_n^{(M+d)}(t) - W_n^{(M-d)}(t))$  by the corresponding equilibrium ones.

The master equation for  $W_n^{(M\pm d)}(t)$  and  $W_n^{(M)}(t)$  becomes

$$\dot{\hat{W}}_n = Q\hat{W}_n, \quad \hat{W}_n = \begin{pmatrix} W_n^{(M-d)}(t) \\ W_n^{(M)}(t) \\ W_n^{(M+d)}(t) \end{pmatrix} \quad (5.15)$$

$$Q = \begin{pmatrix} -Q_t^{-(M-d)} + S_b^{(M-d)} & \tilde{Q}^{+(M)} - Q^{-(M)} & 0 \\ Q_t^{-(M-d)} & -(Q^{-(M)} + Q^{+(M)}) + S_b^{(M)} & Q^{+(M+d)} \\ 0 & \tilde{Q}^{-(M)} - Q^{+(M)} & -Q_t^{+(M+d)} + S_b^{(M+d)} \end{pmatrix} \quad (5.16)$$

where

$$S_\eta^{(M+k)} = \eta Q_t^{+(M+k-1)} - Q_t^{-(M+k)}, \quad (k = \pm d) \quad (5.17a)$$

$$S_\eta^{(M+k)} = \eta Q^{+(M-1)} - Q^{-(M)}, \quad (k = 0) \quad (5.17b)$$

$$\tilde{Q}^{\pm(M)} \equiv Q^{\pm(M)}(1 + \delta^\mp) \quad (5.18)$$

Parameters  $b$  and  $\delta^\pm$  are defined by

$$bW_n^{(N+k)} = W_n^{(M+k-1)} \quad (5.19a)$$

$$\delta^\pm W_n^{(N+k)} = W_{n\pm 1}^{(M+k)} \quad (5.19b)$$

to get the master equation for hopping levels  $M \pm d$ ,  $M$  and within the  $n$ -th cell.

Notations  $R^{*(M+k)}$  denote jumping probabilities (vertical transition rates) between energy levels  $R^{\pm(M+k, M+k\mp 1)}$  in eq. (2.3).

Tunneling *effects* on the current and the mobility...

The parameter  $b$  converts energy level and the parameter  $\delta^\pm$  adjust the  $W_{n\pm 1}^{(M+k)}(t)$  to the  $W_n^{(M+k)}(t)$ , ( $k = \pm d, 0$ ). Zeros in elements  $Q_{13}$  and  $Q_{31}$  are obtained by applying the conditions eqs.(5.7) and (5.8) in eq. (5.6), and eq. (5.19b). To specify the unknown parameters, we put a new condition that k-surmmation of  $W_n^{(k)}(t)$ 's over  $M \pm d$  and  $M$  leads to a constant, a conserved quantity: in each cell, the probability is conserved. The condition yields relations among the jumping probabilities referred to in eq. (5.15)

$$S_b^{(M-d)} = 0 \quad (5.20a)$$

$$Q^{-(M)}(\delta^- - 1) + Q^{+(M)}(\delta^+ - 1) + S_b^{(M)} = 0 \quad (5.20b)$$

$$S_b^{(M+d)} = 0 \quad (5.20c)$$

In the following analysis, we put

$$S_b^{(M+k)} = 0, \quad (k = \pm d, 0) \quad (5.21)$$

This means that the difference of respective energy levels are smaller than the displacements of hopping levels due to  $E(t)$ . Consideration of the requirements of eqs. (5.8), (5.19a) and eq. (5.19b) in eq. (5.16) and the statements below eq. (5.14), leads us to rewrite eq. (5.15) into

$$\dot{\hat{W}} = G_0 \hat{W} + eG_1 E(t) \hat{W}_{eq} \quad (5.22)$$

$$G_0 = \frac{\gamma'}{2} \begin{pmatrix} -1 & \frac{2}{\gamma'}(\tilde{Q}^{+(M)} - Q^{-(M)}) & 0 \\ 1 & -\frac{2}{\gamma'}(Q^{+(M)} + \tilde{Q}^{-(M)}) & 1 \\ 0 & \frac{2}{\gamma'}(\tilde{Q}^{-(M)} - Q^{+(M)}) & -1 \end{pmatrix} \quad (5.23)$$

$$G_1 = \frac{\beta e \gamma'}{4} \begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & 1 \\ 0 & 0 & -1 \end{pmatrix} \quad (5.24)$$

and  $\hat{W}_{eq}$  is the solution to the  $\hat{W} = 0$ .

The Fourier transform of eq. (5.14) then reads

$$J(\omega) = \frac{\gamma'_{eff}}{2} W_{eq} \left[ \frac{W_n^{(M+d)}(\omega) - W_n^{(M-d)}(\omega)}{W_{n,eq}} + E(\omega) \right] \quad (5.25)$$

*S.J. Lee and H. Hara*

where  $A(\omega)$  denotes the Fourier transform of  $A(t)$  defined by

$$A(\omega) = \int_{-\infty}^{\infty} A(t)e^{i\omega t} dt \quad (5.26)$$

$$\gamma'_{\text{eff}} = \gamma' \left[ 1 + \sum_{i(\neq M)} T^{(i)} \frac{W_{eq}^{(i)}}{W_{eq}^{(M)}} \right] = \gamma' \left[ 1 + \sum_{i(\neq M)} T^{(i)} \eta^{M-i} \right] \quad (5.27)$$

$$W_{eq}^{(M)} = N_0 W_{n,eq}$$

and  $N_0$  is the number of cells.

In the second expression of (5.27), we have used eq. (5.19a) with eq. (5.27) and the Fourier transform of eq. (4.8). We can express  $B(\omega)$  as follows

$$B(\omega) = \frac{\gamma'_{\text{eff}}}{2k_B T} W_{eq}^{(M)} [1 + V(\omega)] \quad (5.28)$$

where  $V(\omega)$  is the frequency-dependent velocity given by

$$\begin{aligned} V(\omega) &= -\frac{k_B T}{eE(\omega) \hbar} \left( W_n^{(M+d)}(\omega) - W_n^{(M-d)}(\omega) \right) \\ &= \frac{\gamma'}{2} \cdot \frac{1}{i\omega - \frac{\gamma'}{2}} \\ &= \frac{\gamma'}{2} \cdot \frac{1}{i\omega - \frac{\gamma'}{2}} \quad (\omega \rightarrow \infty) \\ &= 0 \quad (\omega \rightarrow 0) \end{aligned} \quad (5.29)$$

The frequency-dependent velocity  $V(\omega)$  becomes zero as  $\omega \rightarrow 0$  ( $t \rightarrow 0$ ), while  $V(\omega)$  becomes minus one as  $\omega \rightarrow 0$  ( $t \rightarrow \infty$ ), and then  $B(\omega)$  becomes zero, as  $\omega \rightarrow 0$ , as  $\omega \rightarrow 0$ . The present special case describes a frequency-dependent process. In the evaluation, we have put the conditions for transition rates: eq. (5.7) and eq. (5.8) with eq. (5.6); and used the parameters eq. (5.19a) and eq. (5.19b). Furthermore, we have assumed that eq. (5.21) holds and used the eq. (5.18b) in which  $S_n^{(M)} = 0$  from eq. (5.19). The expression  $B(\omega)$  has no

### *Tunneling effects on the current and the mobility...*

contribution due to the cell structure through  $\delta^+$  and  $\delta^-$  as seen in eq. (5.29). So we have the very simple expression for  $V(\omega)$ , but from eq. (5.1) we can study more general cases.

Closing this section, we remark that Pietronero and Strassler<sup>10</sup> have proposed a model in which hoppings of the particles are modulated by an additional harmonic variable.

## **6. Concluding remarks**

Based on the coupled random walks (CRW), the expression for the current was obtained for trapping or hopping model. In the present treatment, jumping probabilities (transitions) between sites appear through intermediate energy levels of the potential barrier. The processes are called tunneling effects, different from the usual trapping models<sup>6</sup>, in which the particles are hopping only when they are on the top of the potential barrier. In the CRW, we regard a particle as the walker whose potential barrier and energy levels are modified by the driving force  $E(t)$ . As a factor representing the tunneling effects, we discussed typical cases: (1) Exponential type and (2) Fractional type. These functional forms are expressed by the geometrical parameters  $\eta_i$  and  $a$  for the potential barrier, see eq. (3.2a) and eq. (3.2b).

The expression of  $J(t)$  given by eq. (4.7) is a general expression in which tunneling effects are considered. By changing the role of arguments in  $T^{(i)}$ , we can regard the  $T^{(i)}$  as representing "higher order direct hopping" as shown in fig. 6.

For a model of frequency-dependent mobility, we considered a system in which cell structures appear due to the driving force  $E(t)$ . This feature and inclusion of tunneling factor are different points from the ZK model<sup>6</sup>. In the analysis, we have truncated the master equation within a cell by introducing the parameters. The problems related to hopping or trapping rate have been studied by using electrical network<sup>11</sup> or scattering theory analogy<sup>12</sup>. Recently Fujisaka and Grossman<sup>13</sup>, and Inoue<sup>14</sup> have reported hopping processes having chaotic behaviors by solving non-linear difference equations. In place of eq.(5.15), if we start with the expression

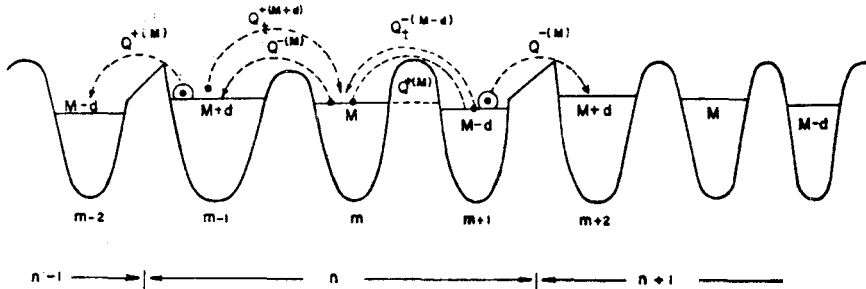


Fig. 6 - Graphical representation of "higher order direct hopping"

$J(t)$  in which the jumping probabilities  $P_N^\alpha$ 's are specified by a non-linear mapping  $F$ ,

$$P_N^\alpha = F(P_{N-1}^\alpha; K) \tag{6.1}$$

the processes then show chaotic behavior by varying the parameter  $K$  <sup>15</sup>.

Finally, we remark that energy levels of the particle correspond to the walker's mode in the original CRW. The expression  $J(t)$  then can be directly applied to the diffusion processes in ecological problems<sup>16</sup> by reinterpreting the factor  $T^{(i)}$  as a factor representing these phenomena.

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*S.J. Lee and H. Hara*

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#### Resumo

Um modelo baseado em caminhos aleatórios acoplados é proposto para investigar os fenômenos de corrente e mobilidade dependente da frequência. O sistema é composto por partículas, saltando do modo  $j$  no sítio  $m$  para o modo  $i$  no sítio  $m'$  sob a ação de um termo forçante,  $E(t)$ . Obtemos uma expressão para a corrente na qual a mobilidade depende de um "fator de **tunelamento**" e da diferença entre os níveis energéticos. A mobilidade dependente da frequência é função da estrutura de célula, bem como do fator de tunelamento.