Analysis of Equivalent Distorted Ratchet Potentials

Yiming Cheng[1], **Robert M. Miura**[1,2]

[1] Department of Mathematical Sciences
New Jersey Institute of Technology
Newark, NJ 07102

yc34@njit.edu, miura@njit.edu

[2] Department of Biomedical Engineering
New Jersey Institute of Technology
Newark, NJ 07102

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Yiming Cheng[1] and Robert M. Miura[1,2]
Departments of Mathematical Sciences[1]
and of Biomedical Engineering[2]
New Jersey Institute of Technology
Newark, NJ 07102

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Abstract

Different kinds of charged particles undergoing Brownian motion can be separated by subjecting them periodically to an asymmetrical spatially periodic electric field, sometimes referred to as a Brownian ratchet. It has been found numerically that equal fluxes of particles can be obtained from two different potentials under special distortions. Although a simple physical explanation for this equivalency can be given, there is no corresponding mathematical proof. Here, we pose the mathematical problem and discuss the difficulty in carrying out the analytical proof.

1. Introduction. Separation technology is becoming more and more important in biotechnology for certain processes such as separation of microscopic particles undergoing Brownian motion [1],[2]. These particles can be separated by subjecting them periodically to an asymmetrical spatially periodic electric field, sometimes referred to as a Brownian ratchet. Numerically, it was found that two different potentials are equivalent under special distortions [3],[4], in that they produce the same fluxes of particles. A simple physical explanation for this equivalency can be given; however, the analytical proof of this equivalency remains elusive. The corresponding mathematical problem is described in some detail, and it is shown where the difficulty lies in the analysis.

2. Mathematical Modeling. Consider a potential that is fluctuating between two states. State 1 is a constant potential and state 2 is denoted $V(x)$ (see Figure 1). In state i, i = 1,2, the probability of finding over-damped Brownian particles in the differential length dx centered at position x at time t is denoted by $p_i(x,t)$, and the velocity of the particles is denoted by $u_i(x,t)$. These quantities are governed by

$$\frac{\partial p_1(x,t)}{\partial t} = -\frac{\partial u_1}{\partial x} - r_1 p_1 + r_2 p_2, \tag{1}$$

$$\frac{\partial p_2(x,t)}{\partial t} = -\frac{\partial u_2}{\partial x} + r_1 p_1 - r_2 p_2, \tag{2}$$

$$u_1 = -\frac{\partial p_1}{\partial x}, \quad u_2 = -\frac{\partial p_2}{\partial x} - p_2 V'(x), \tag{3}$$

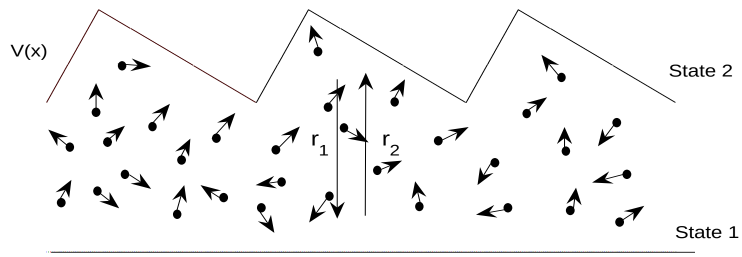

Figure 1: Fluctuating potential ratchet with rate constants r_1 and r_2, and Brownian particles.

where r_1 and r_2 are the rate constants for the fluctuating potential. We want to know the steady state velocity of the Brownian particles in the system if the probabilities satisfy the normalization condition

$$\int_0^1 [p_1(x) + p_2(x)]dx = 1. \tag{4}$$

From (1)–(3), we obtain the steady state equations

$$\begin{aligned} \frac{d^2p_1(x)}{dx^2} - r_1p_1(x) + r_2p_2(x) &= 0, \quad (5) \\ \frac{d^2p_2(x)}{dx^2} + V'(x)\frac{dp_2(x)}{dx} + V''(x)p_2(x) + r_1p_1(x) - r_2p_2(x) &= 0 \quad (6) \end{aligned}$$

where $V'(x)$ and $V''(x)$ are the first- and second-order derivatives, respectively, of the potential in state 2 (the potential in state 1 is constant, so it does not appear in the equations).

The total steady state transport flux of the system is given by

$$u(x) = u_1(x) + u_2(x) = -\frac{dp_1}{dx} - \frac{dp_2}{dx} - p_2V'(x). \tag{7}$$

At steady state, (5) and (6) yield

$$\frac{du}{dx} = 0, \tag{8}$$

that is, the steady state velocity is constant in space. This is what we call the long time velocity of the Brownian particles in the system.

Consider a regular ratchet consisting of two sides, see Figure 2. Now consider two distorted potentials. One, denoted V_1, has the left-hand side of the regular ratchet replaced by a kinked piecewise linear potential defined by the slope parameters, γ_1 and γ_2, respectively. The second potential, denoted V_2, has a left-hand side that is symmetric to the first distorted ratchet about the mid-point of the left arm of the regular ratchet. That is, the left-hand kinked potential is defined by the slope parameters, γ_2 and γ_1, respectively. The right-hand side is defined by the slope parameter, γ_3.

When the two periodic potentials are specified, as illustrated in Figure 2, it has been found numerically that these two potentials (the solid and dashed lines) produce equal fluxes of particles [3],[4]. The physical explanation is shown in Figure 3.

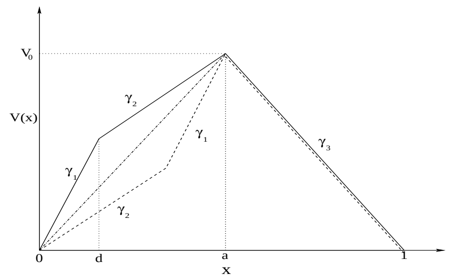

Figure 2: Equivalent potentials defined by the slope parameters γ_1, γ_2, and γ_3.

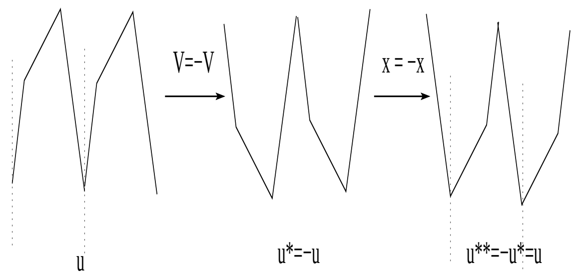

Figure 3: Physical explanation.

3. Mathematical Analysis.

The mathematical conjecture is that if there are two different potentials $V_1(x)$ and $V_2(x)$ where $V_2(x)$ is the "inverted" image of $V_1(x)$ where γ_1 and γ_2 are reversed (see Figure 2), then we obtain the same solution u(x) provided the potentials are periodic and the probabilities satisfy the normalization condition (4).

Although this conjecture has been confirmed numerically, there is no mathematical proof. The difficulty is that for (5)–(7), there is no simple analytical solution for the velocity in terms of the potential, even though the potential is simple. Also, it has been found numerically that if the left arm of the regular ratchet is replaced by a sinusoidal potential, then the reflected potentials also produces the same velocity. Here, we only consider the potentials shown in Figure 2.

The linear differential equations (5) – (6), have constant coefficients in each linear region, (i.e., region 1: $0 < x < d$; region 2: $d < x < a$; region 3: $a < x < 1$). Therefore, we can solve the equations analytically. The characteristic equation for (5) and (6) in region j is given by

$$s(s^3 + \gamma_j s^2 - (r_1 + r_2)s - r_1\gamma_j) = 0. \tag{9}$$

One root of (9) is always zero, and the other three non-zero roots are denoted by $\lambda_{jk},\ k = 1, 2, 3$. Thus, we have the solutions

$$p_{1j}(x) = c_{j0} + \sum_{k=1}^{3} c_{jk} e^{\lambda_{jk} x}, \tag{10}$$

$$p_{2j}(x) = \frac{r_1}{r_2} c_{j0} + \sum_{k=1}^{3} \frac{r_1 - \lambda_{jk}^2}{r_2} c_{jk} e^{\lambda_{jk} x} \tag{11}$$

where $p_{ij}(x)$ is the probability density in state i in region j. From the above, we obtain $u_{ij}(x)$, the velocity in state i in region j,

$$u_{1j}(x) = -\sum_{k=1}^{3} c_{jk} \lambda_{jk} e^{\lambda_{jk} x}, \tag{12}$$

$$u_{2j}(x) = -\frac{\gamma_j r_1 c_{j0}}{r_2} - \frac{\sum_{k=1}^{3} (r_1 - \lambda_{jk}^2)(\lambda_{jk} + \gamma_j) c_{jk} e^{\lambda_{jk} x}}{r_2}. \tag{13}$$

In region j, we can calculate the $\bar{u}_j(x) = u_{1j}(x) + u_{2j}(x)$ using (12) and (13) to obtain

$$\bar{u}_j(x) = -\frac{\gamma_j r_1 c_{j0}}{r_2}. \tag{14}$$

At steady state, there are 12 unknown functions given by p_{1j}, p_{2j}, u_{1j}, and u_{2j} where $j = 1, 2, 3$. The quantities $p_1(x)$ and $p_2(x)$, as well as $u_1(x)$, $u_2(x)$, are continuous at $x = 0, d$, and a, and

$$u = \bar{u}_j \qquad\qquad \text{in region j.} \tag{15}$$

Thus, $u(x)$ is continuous, and we have :

$$-\frac{r_2}{r_1}u = \gamma_1 c_{10} = \gamma_2 c_{20} = \gamma_3 c_{30}. \tag{16}$$

From the continuity of $p_1(x)$, $p_2(x)$, $u_1(x)$, and $u_2(x)$, there are 12 matching conditions, some of which may be dependent. However, if we use the two equations from (16), we can reduce the 12 matching conditions to 9 independent equations. Together with the above two conditions, we have 11 independent equations. Another independent equation is the normalization condition (4), leading to

$$\begin{aligned} dc_{10} \quad &+ \quad \sum_{k=1}^{3}(\frac{1}{\lambda_{1k}} - \lambda_{1k})(e^{\lambda_{1k}d} - 1)c_{1k} + (a-d)c_{20} + \sum_{k=1}^{3}(\frac{1}{\lambda_{2k}} - \lambda_{2k}) \\ \bullet(e^{\lambda_{2k}a} - e^{\lambda_{2k}d})c_{2k} \quad &+ \quad (1-a)c_{30} + \sum_{k=1}^{3}(\frac{1}{\lambda_{3k}} - \lambda_{3k})(e^{\lambda_{3k}} - e^{\lambda_{3k}a})c_{3k} = \frac{r_2}{r_1+r_2}. \end{aligned} \tag{17}$$

This equation can be simplified further to

$$\begin{aligned} dc_{10} + \sum_{k=1}^{3}\frac{e^{\lambda_{1k}d} - 1}{\lambda_{1k}}c_{1k} + (a-d)c_{20} + \sum_{k=1}^{3}\frac{e^{\lambda_{2k}a} - e^{\lambda_{2k}d}}{\lambda_{2k}}c_{2k} \\ +(1-a)c_{30} + \sum_{k=1}^{3}\frac{e^{\lambda_{3k}} - e^{\lambda_{3k}a}}{\lambda_{3k}}c_{3k} = \frac{r_2}{r_1+r_2}. \end{aligned} \tag{18}$$

Thus, we obtain the system of equations

$$A\begin{pmatrix} \overrightarrow{c_1} \\ \overrightarrow{c_2} \\ \overrightarrow{c_3} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \overrightarrow{r} \end{pmatrix} \quad \text{where} \quad \overrightarrow{r} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \frac{r_1}{r_1+r_2} \end{pmatrix}, \quad \overrightarrow{c_i} = \begin{pmatrix} c_{i0} \\ c_{i1} \\ c_{i2} \\ c_{i3} \end{pmatrix}, \tag{19}$$

and A is a 12×12 matrix.

For the distorted ratchet, V_2, case, the difference is that the piecewise-linear branches in the first two regions are exchanged and d becomes $g = a - d$. Thus, we obtain the linear system for the inverted image just by exchanging γ_1 and γ_2, λ_{1k} and λ_{2k} , and d and $a - d$. We then can write $A = A(d, \gamma_1, \gamma_2, \lambda_{1k}, \lambda_{2k})$, and we get another linear system with $B^* = A(a - d, \gamma_2, \gamma_1, \lambda_{2k}, \lambda_{1k})$. After simplification, we obtain the system of equations

$$B\begin{pmatrix} \overrightarrow{d_1} \\ \overrightarrow{d_2} \\ \overrightarrow{d_3} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \overrightarrow{r} \end{pmatrix} \quad \text{where} \quad \overrightarrow{d_i} = \begin{pmatrix} d_{i0} \\ d_{i1} \\ d_{i2} \\ d_{i3} \end{pmatrix},$$

B is a 12×12 matrix and the entries in B are the same as in A, except in different positions. Similar to 16, we have

$$-\frac{r_2}{r_1}\tilde{u} = \gamma_2 d_{10} = \gamma_1 d_{20} = \gamma_3 d_{30}. \tag{20}$$

We want to prove the velocity is the same for these two cases, that is, $u = \tilde{u}$. From (15) and (20), we need to prove one of the following three equalities is true:

$$c_{10} = d_{20}, \qquad c_{20} = d_{10}, \qquad c_{30} = d_{30}. \tag{21}$$

Here we try to prove $c_{10} = d_{20}$ by Cramer's rule. So $c_{10} = \frac{|A_c|}{|A|}$, and $d_{20} = \frac{|B_c|}{|B|}$, where A_c is the matrix obtained by deleting the first column and last row from A, and B_c is the matrix, obtained by deleting the fifth column and last row from B. Numerically, we found that

$$|A| = |B|, \qquad |A_c| = |B_c|. \tag{22}$$

Thus, it is reasonable to try to prove (22) analytically. To prove $|A_c| = |B_c|$, we use block matrix elimination to prove the equality

$$|XY - Z| = |YX - Z| \tag{23}$$

where

$$\begin{aligned} X &= P_1\Lambda_1 P_1^{-1}, & (24)\\ Y &= P_2\Lambda_2 P_2^{-1}, & (25)\\ Z &= P_3\Lambda_3 P_3^{-1}. & (26) \end{aligned}$$

Here, the Λ_j are arbitrary diagonal matrices and P_j is given by

$$P_j = \begin{pmatrix} 1 & 1 & 1 \\ \lambda_{j1} & \lambda_{j2} & \lambda_{j3} \\ \lambda_{j1}^2 & \lambda_{j2}^2 & \lambda_{j3}^2 \end{pmatrix}$$

To prove $|A| = |B|$. We can expand each determinant by the row or column that has the fewest nonzero entries. Then, we obtain the simpler relationship

$$\begin{aligned} |A| &= \gamma_2(\gamma_3 - \gamma_1|A1| + \gamma_1(\gamma_2 - \gamma_3)|A2| + \gamma_3(\gamma_2 - \gamma_1)|A3|, & (27)\\ |B| &= \gamma_2(\gamma_1 - \gamma_3|B1| + \gamma_1(\gamma_3 - \gamma_2)|B2| + \gamma_3(\gamma_1 - \gamma_2)|B3| & (28) \end{aligned}$$

where the Ai and Bi, $i = 1, 2, 3$, are 9×9 matrices. Furthermore, if we assume that $|A| = |B|$, then we obtain the equation

$$\gamma_2(\gamma_3 - \gamma 1)(|A1| + |B1| + |A3| + |B3|) = \gamma 1(\gamma 3 - \gamma_2)(|A2| + |B2| + |A3| + |B3|). \tag{29}$$

We can verify the equation numerically for all $a, d, k_1, k_2, \gamma_1, \gamma_2, \gamma_3$. So far analytical proofs of (23) and (27) have eluded us.

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