Effective Diffusion and transport coherence in presence of inhomogeneous temperature: Piecewise linear potential

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We compute the effective diffusion coefficient of a Brownian particle in a piece-wise linear periodic potential and subject of spatially inhomogeneous temperature, otherwise known as the Büttiker-Landauer motor. We obtain analytical expressions for the current and diffusion coefficients and compare with numerical results.

I. INTRODUCTION

A Brownian particle moving in a periodic potential and subject to a spatially non-uniform temperature profile gives rise to a net current, acting like a Brownian motor. This device is autonomous since it is entirely driven by thermal fluctuations. Several properties of such a Brownian motor, such as current, heat and thermodynamic efficiency have been studied.

Another important performance characteristic of such a Brownian device is the transport coherence as measured by the Peclet number, which is the ratio of the thermal velocity times the period of the substrate potential and the effective diffusion coefficient of the motor. It is desirable to design motors which produce the maximum velocity with the minimum dispersion i.e. small diffusion coefficient.

While the net current of such a Brownian ratchet has been derived for an overdamped system in the works of Landauer, Van Kampen and Büttiker the determination of the effective diffusion coefficient had remained a challenging task until the early twenty-first century. Reimann et al. first determined the effective diffusion coefficient for

\[ T(x) = \begin{cases} T_H, & \text{for } 0 \leq x < \alpha L \\ T_C, & \text{for } \alpha L \leq x < L \end{cases} \]

Both Potential and Temperature profiles are periodic i.e. \( U(x + L) = U(x) \) and \( T(x + L) = T(x) \).

\[ U(x) = \begin{cases} \frac{U_0 x}{\alpha L}, & \text{for } 0 \leq x < \alpha L \\ \frac{U_0(L-x)}{(1-\alpha)L}, & \text{for } \alpha L \leq x < L \end{cases} \]

\[ \alpha \text{ is the potential asymmetry parameter, } U_0 \text{ is the barrier height and } L \text{ is the spatial period of the potential. Without loss of generality we consider } U_0 = 1 \text{ and } L = 1. \]

The Langvin equation used to study the motion of the Brownian particle is given by,

\[ m\ddot{x} = -\gamma \dot{x} - U'(x) + \sqrt{2 k_B T(x) \gamma \xi(t)} \]  \hspace{1cm} (1)

We set \( k_B = 1 \) and \( \gamma = 1 \).

In the overdamped limit, we ignore the inertial term. However, for temperature dependent on position, an additional term needs to be added as pointed out in earlier works. As per the Stratonovich interpretation, the overdamped Langevin equation is given by,

\[ \dot{x} = -U'(x) - \frac{1}{2} \frac{dT(x)}{dx} + \sqrt{2 T(x) \gamma \xi(t)} \]  \hspace{1cm} (2)

Here, \( < \xi(t) > = 0 \) and \( < \xi(t) \xi(t') > = \delta(t - t') \). We set \( \gamma = 1 \). This equation will be understood according to the Stratonovich interpretation.

The Fokker-Planck equation corresponding to this overdamped Langevin equation is given by,
\[ \frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ U'(x)P(x,t) \right] + \frac{\partial^2}{\partial x^2} \left[ T(x)P(x,t) \right] \]  

(3)

The current is given by,

\[ \langle \dot{x} \rangle = \frac{x(t_f) - x(t_s)}{t_f - t_s} \]  

(4)

where, \( t_s \gg 1 \) is the time taken to reach the steady state and \( t_f \) is the final time up to which the simulations are carried out.

The effective diffusion coefficient is computed as per the following relation:

\[ D_{eff} = \frac{\langle (x(t_f) - x(t_s))^2 \rangle - \langle x(t_f) - x(t_s) \rangle^2}{2(t_f - t_s)} \]  

(5)

Our numerical calculations are carried out as per the Stochastic Euler-Maruyama algorithm.

The analytical calculation were carried out as per the following formulas provided in Ref. [? ].

\[ \langle \dot{x} \rangle = L \frac{1 - \exp(\psi(L))}{\int_0^L dx I_+(x)/g(x)} \]  

(6)

where, \( g(x) = \sqrt{T(x)} \) and

\[ I_+(x) = \exp(-\psi(x)) \int_x^{x+L} dy \exp(\psi(y))/g(y) \]  

(7)

We can also determine the Peclet number which determines the coherence of transport. It’s given by,

\[ Pe = L \langle \dot{x} \rangle / D_{eff} \]  

(10)

We also carried out numerical simulations to test the validity of our analytical results using the Euler-Maruyama algorithm. The time-step chosen was \( h = 0.001 \) and the number of realizations was 5000.

### III. EXACT EXPRESSIONS

The first step to solve this model is to recognize that the non-uniform temperature breaks the symmetry and simultaneously results in a non-equilibrium condition, the minimal ingredient to produce directed motion. In order to break the left right symmetry there should be a phase difference between them. Due to the spatial dependence of the temperature profile the noise term is multiplicative and Brownian particles subject to such a temperature profile move under the influence of the generalized potential given by,

\[ \psi(x) = \int_0^x dx' \left[ U'(x') + (1/2)T'(x') \right]/T(x') \]  

(11)

The condition to achieve directed transport (\( \langle \dot{x} \rangle \neq 0 \)) is for this potential to have an effective bias such that \( \psi(L = 1) - \psi(0) \neq 0 \).

For the piecewise linear potential and piecewise constant temperature profile, it is simple to calculate \( \psi(x) \), which is given by,
Using a suitable transformation of variables one can convert the overdamped Langevin equation with multiplicative noise to one with additive noise. The required transformation is given by,

$$y(x) = \int_0^x \frac{dz}{\sqrt{T(z)}} \tag{12}$$

and the corresponding Langevin equation is given by,

$$\dot{y} = \frac{\dot{x}}{\sqrt{T(x)}} - \frac{d\phi(y)}{dy} + \sqrt{2\xi(t)} \tag{13}$$

where,

$$\phi(y) = \int_0^y dy^* \frac{U'[x(y^*)] + (1/2)T'[x(y^*)]}{\sqrt{T[x(y^*)]}} \tag{14}$$

and $\phi(y) = \psi|x(y)|$.

For our potential and temperature profiles, the relation between the original and transformed coordinates is given by,

$$\psi(x) = \begin{cases} \frac{U_0}{T_C} + \frac{U_0(x+1-\alpha)}{\alpha T_C}, & \text{for } -1 \leq x < -1 + \alpha \\ -\frac{U_0 y}{(1-\alpha)T_C} + \frac{1}{2} \log\left(\frac{T_C}{T_H}\right), & \text{for } -1 + \alpha \leq x < 0 \\ \frac{U_0 y}{\alpha T_H}, & \text{for } 0 \leq x < \alpha \\ \frac{U_0}{T_H} + \frac{U_0(x-\alpha)}{(1-\alpha)T_C} + \frac{1}{2} \log\left(\frac{T_C}{T_H}\right), & \text{for } \alpha \leq x < 1 \\ \frac{2U_0}{T_H} - \frac{U_0}{T_C} + \frac{U_0(x-1-\alpha)}{(1-\alpha)T_C} + \frac{1}{2} \log\left(\frac{T_C}{T_H}\right), & \text{for } 1 \leq x < 1 + \alpha \\ \frac{2U_0}{T_H} - \frac{U_0}{T_C} - \frac{U_0(x-1-\alpha)}{(1-\alpha)T_C} + \frac{1}{2} \log\left(\frac{T_C}{T_H}\right), & \text{for } 1 + \alpha \leq x < 2 \\ \end{cases}$$

Finally, the effective potential in the transformed coordinates is given by,

$$y = \begin{cases} \frac{\alpha-1}{\sqrt{T_C}} - \frac{\alpha-x-1}{\sqrt{T_H}}, & \text{for } -1 \leq x < -1 + \alpha \\ \frac{x}{\sqrt{T_C}}, & \text{for } -1 + \alpha \leq x < 0 \\ \frac{x}{\sqrt{T_H}}, & \text{for } 0 \leq x < \alpha \\ \frac{1}{\sqrt{T_H}} + \frac{x-\alpha}{\sqrt{T_C}}, & \text{for } \alpha \leq x < 1 \\ \frac{1}{\sqrt{T_H}} + \frac{1-\alpha}{\sqrt{T_C}} + \frac{(x-1)}{\sqrt{T_H}}, & \text{for } 1 \leq x < 1 + \alpha \\ \frac{2\alpha}{\sqrt{T_H}} + \frac{1-\alpha}{\sqrt{T_C}} + \frac{(x-1-\alpha)}{\sqrt{T_H}} & \text{for } 1 + \alpha \leq x < 2 \end{cases}$$
The period of $\phi(y)$ is $L_y = \frac{4\pi}{B} + \frac{1}{\sqrt{4B}}$.

The effective diffusion coefficient computed as per the transformed dynamics with additive noise is given by,

$$D_{eff,y} = \frac{\int_0^{L_y} dx[I_-(x)]^2 I_+(x)/L_y}{[\int_0^{L_y} dx I_-(x)/L_y]^3}$$

(15)

and

$$I_\pm(x) = \mp e^{\pm \phi(x)} \int_x^{x \pm L_y} dy e^{\mp \phi(y)}$$

(16)

The velocity in the transformed coordinates is given by,

$$v_y = \frac{1 - e^{\phi(L_y)}}{[\int_0^{L_y} dx I_-(x)/L_y]}$$

(17)

The relation between the effective diffusion coefficient and the particle current in the original and transformed coordinates is given by,

$$D_{eff} = \frac{D_{eff,y}}{L_y^2}, \quad \langle \dot{x} \rangle = \frac{v_y}{L_y}$$

(18)

We will calculate the effective diffusion coefficient using Eq. 8. The Integral in the denominator is given by,

$$I_d = \int_0^\alpha dx e^{-\psi(x)} \int_x^{x+1} dy e^{\psi(y)} + \int_0^1 dx e^{-\psi(x)} \int_x^{x+1} dy e^{\psi(y)} = A + B$$

(19)

such that

$$A = \int_0^\alpha dx e^{-\psi(x)} \int_x^{x+1} dy e^{\psi(y)}/\sqrt{T(y)}$$

(20)

and,

$$B = \int_0^1 dx e^{-\psi(x)} \int_x^{x+1} dy e^{\psi(y)}/\sqrt{T(y)}$$

(21)

$$A = \int_0^\alpha \frac{\ln x}{x} \frac{1}{\sqrt{T_H}} \left[ \int_x^{x+1} \frac{\ln y}{y} \frac{1}{\sqrt{T_C}} + \int_1^y \frac{\ln y}{y} \frac{1}{\sqrt{T_H}} \right]$$

(22)

and,

$$B = \int_0^1 \frac{\ln x}{x} \frac{1}{\sqrt{T_C}} \left[ \int_x^{x+1} \frac{\ln y}{y} \frac{1}{\sqrt{T_H}} + \int_1^{x+1} \frac{\ln y}{y} \frac{1}{\sqrt{T_H}} \right]$$

(23)

Here,

$$a_{11} = \int_x^\alpha \frac{\ln x}{x} \frac{1}{\sqrt{T_H}} = -\frac{\alpha \sqrt{T_H}}{U_0} \left( e^{\alpha T_H} - e^{\alpha T_H} \right)$$

(24)
\[ a_{12} = \int_{-\infty}^{\alpha} \frac{e^{\frac{U_0}{T_H}}}{\sqrt{T_C}} - \frac{\frac{U_0(x-a)}{T_C} + \frac{1}{2} \log(T_C)}{\frac{\frac{U_0(x-a)}{T_C} + \frac{1}{2} \log(T_C)}{\frac{U_0(x-a)}{T_C} + \frac{1}{2} \log(T_C)}} \right] \left( e^{\frac{\frac{U_0}{T_H}}{\alpha - \frac{U_0}{T_H}}} - e^{\frac{\frac{U_0}{T_H}}{\alpha - \frac{U_0}{T_H}}} \right) e^{-\frac{U_0}{T_C}} - 1 \] (25)

and,

\[ a_{13} = \int_{1}^{x+1} \frac{e^{\frac{U_0}{T_H}}}{\sqrt{T_H}} \left( e^{\frac{\frac{U_0}{T_H}}{\alpha - \frac{U_0}{T_H}}} - e^{\frac{\frac{U_0}{T_H}}{\alpha - \frac{U_0}{T_H}}} \right) e^{-\frac{U_0}{T_C}} \] (26)

Similarly,

\[ b_{11} = \frac{(\alpha - 1)T_C}{U_0 \sqrt{T_H}} \left( -e^{\frac{-\frac{U_0}{T_H}}{\alpha - \frac{U_0}{T_H}}} e^{\frac{\frac{U_0}{T_H}}{\alpha - \frac{U_0}{T_H}}} \right) e^{-\frac{U_0}{T_C}} \] (27)

\[ b_{12} = \frac{\alpha \sqrt{T_H}}{U_0} e^{\frac{\frac{U_0}{T_H}}{\alpha - \frac{U_0}{T_H}}} e^{-\frac{U_0}{T_C}} \] (29)

\[ b_{13} = \frac{(\alpha - 1)T_C}{U_0 \sqrt{T_H}} \left( e^{\frac{\frac{U_0}{T_H}}{\alpha - \frac{U_0}{T_H}}} - 2 \right) e^{-\frac{U_0}{T_C}} \] (28)

\[ A = -\frac{\alpha}{U_0^2} \left( \left( -T_C + T_H - U_0 \right) \alpha + T_C \right) e^{-\frac{\frac{U_0}{T_C}}{\alpha - \frac{U_0}{T_C}}} \] (30)

\[ B = \alpha - \frac{1}{U_0^2} \left( \left( -T_C + T_H - U_0 \right) \alpha + T_C \right) e^{-\frac{\frac{U_0}{T_C}}{\alpha - \frac{U_0}{T_C}}} \] (31)

Then \( I_d \) is given by,

\[ I_d = \frac{1}{U_0^2} \left( \left( T_C - T_H + 2U_0 \right) \alpha - T_C - U_0 \right) e^{-\frac{\frac{U_0}{T_C}}{\alpha - \frac{U_0}{T_C}}} \] (32)

The numerator in the expression for effective diffusion coefficient can be written as,

\[ num = \int_{0}^{\alpha} \frac{e^{-\frac{\frac{U_0}{T_H}}{\alpha - \frac{U_0}{T_H}}}}{\sqrt{T_H}} \left[ \int_{x}^{x+L} dy \frac{\exp(\psi(y))}{\sqrt{T(y)}} \right]^2 \left( \int_{x-L}^{x} dy \frac{\exp[-\psi(y)]}{\sqrt{T(y)}} \right) + \int_{\alpha}^{1} \frac{e^{-\frac{\frac{U_0}{T_H}}{\alpha - \frac{U_0}{T_H}}}}{\sqrt{T_C}} \left[ \int_{x}^{x+L} dy \frac{\exp(\psi(y))}{\sqrt{T(y)}} \right]^2 \left( \int_{x-L}^{x} dy \frac{\exp[-\psi(y)]}{\sqrt{T(y)}} \right) \] (33)
such that,

\[
\text{num} = \int_{\alpha}^{x} \frac{1}{T_H} \left( a_{11} + a_{12} + a_{13} \right)^2 \left( \int_{x-L}^{x} \frac{\exp[-\psi(y)]}{\sqrt{T(y)}} \, dy \right) + \int_{x}^{1} \frac{1}{T_C} \left( b_{11} + b_{12} + b_{13} \right)^2 \left( \int_{x-L}^{x} \frac{\exp[-\psi(y)]}{\sqrt{T(y)}} \, dy \right)
\]

(34)

For \( 0 \leq x < \alpha \),

\[
P = \int_{x-1}^{x} \frac{\exp[-\psi(y)]}{\sqrt{T(y)}} = p_{11} + p_{12} + p_{13}
\]

(35)

where,

\[
p_{11} = \alpha \frac{\sqrt{T_H}}{U_0} \left( e^{\frac{\nu_0(\alpha-x)}{\tau_H}} - 1 \right) e^{-\frac{\nu_0}{\tau_H}}
\]

(36)

\[
p_{12} = -\frac{\sqrt{T_H}(\alpha-1)}{U_0} \left( e^{\frac{\nu_0}{\tau_C}} - 1 \right) e^{-\frac{\nu_0}{\tau_H}}
\]

(37)

For \( \alpha \leq x < 1 \),

\[
Q = \int_{x-1}^{x} \frac{\exp[-\psi(y)]}{\sqrt{T(y)}} = q_{11} + q_{12} + q_{13}
\]

(39)

where,

\[
q_{11} = \int_{0}^{x-1} \frac{\exp[-\psi(y)]}{\sqrt{T(y)}} \, dy = \frac{(\alpha - 1) \sqrt{T_H}}{U_0} \left( e^{\frac{\nu_0(\alpha-1)}{\tau_H}} - 1 \right)
\]

(40)

\[
q_{12} = \int_{0}^{\alpha} \frac{\exp[-\psi(y)]}{\sqrt{T_H}} = \alpha \frac{\sqrt{T_H}}{U_0} \left( e^{\frac{\nu_0}{\tau_H}} - 1 \right) e^{-\frac{\nu_0}{\tau_H}}
\]

(41)

\[
q_{13} = \int_{\alpha}^{x} \frac{\exp[-\psi(y)]}{\sqrt{T_C}} = -\frac{(\alpha - 1) \sqrt{T_H}}{U_0} \left( e^{\frac{\nu_0(\alpha-x)}{\tau_C}} - 1 \right) e^{-\frac{\nu_0}{\tau_H}}
\]

(42)

Finally, we have

\[
\text{num} = \int_{0}^{\alpha} \frac{\exp[-\psi(y)]}{\sqrt{T_H}} \left( a_{11} + a_{12} + a_{13} \right)^2 (p_{11} + p_{12} + p_{13}) + \int_{x}^{1} \frac{1}{T_C} \left( b_{11} + b_{12} + b_{13} \right)^2 (q_{11} + q_{12} + q_{13})
\]

(43)

The final expression is obtained as,

\[
\text{num} = \text{num}_1 + \text{num}_2
\]

(44)
\[ \text{num1} = \frac{1}{\sqrt{T_H}} (\varphi_0^3 + \frac{\alpha T_H}{U_0} \exp\left(\frac{U_0}{T_H}\right) - 1) \left[ \varphi_0^2 \hat{\varphi}_1 \varphi_c + \varphi_1 \varphi_c (2 \varphi_0^2 + \varphi_1 \hat{\varphi}_1 \varphi_c^2 \exp\left(\frac{U_0}{T_H}\right)) \right] 
\]
\[ + 2 \alpha \varphi_0 \varphi_1 \varphi_c^2 \exp(U_0/T_H) + \varphi_0 \varphi_1 \varphi_c^2 \frac{\alpha T_H}{2U_0} (\exp(2U_0/T_H) - 1) \]  
\[ \text{num2} = \mu_0^2 \lambda_0 (1 - \alpha) T_C \left[ \exp\left(\frac{2U_0}{T_C}\right) - 1 \right] + \xi_1 (1 - \alpha) T_C \left[ \exp\left(\frac{U_0}{T_C}\right) - 1 \right] + \xi_0 (1 - \alpha) \]
\[ + \mu_2 \lambda_1 \frac{\alpha - 1}{U_0} \exp\left(-\frac{U_0}{T_C}\right) - 1 \]  
\[ (45) \]

The numerator is then given by \( \text{num} = \text{num1} + \text{num2} \). The effective diffusion coefficient then obtained as
\[ D_{eff} = \frac{\text{num}}{I_d^3} \]  
\[ (47) \]

The various terms are provided in the Appendix. The current is calculated as,
\[ <\dot{x}> = L \left[ 1 - \exp(\psi(L)) \right] \]  
\[ (48) \]

In the low temperature limit, the particle current and effective diffusion coefficient can be obtained in terms of the transition rates in forward and reverse directions given by,
\[ r_f = \frac{1}{\alpha} \frac{1}{\alpha T_H Y^2 + (\alpha - 1) T_C Z} \]  
\[ (49) \]
where,
\[ Y = \exp\left(\frac{U_0}{2T_H}\right) - \exp\left(\frac{U_0}{2T_C}\right) \]  
\[ (50) \]
and,
\[ Z = (\exp(-\frac{U_0}{T_C}) - 1)(\exp(\frac{U_0}{T_H}) - 1) \]  
\[ (51) \]
and,
\[ r_b = \frac{1}{1 - \alpha} \frac{1}{\alpha T_H X + (1 - \alpha) T_C R^2} \]  
\[ (52) \]
where,
\[ X = (1 - \exp(-\frac{1}{T_H}))(\exp(\frac{1}{T_C}) - 1) \]  
\[ (53) \]
and,
\[ R = \exp\left(\frac{U_0}{2T_C}\right) - \exp(-\frac{U_0}{2T_C}) \]  
\[ (54) \]
So, the current and effective diffusion coefficient are given by,
\[ <\dot{x}> = r_f \alpha - r_b (1 - \alpha) \]  
\[ (55) \]

and,
\[ D_{eff} = \frac{r_f \alpha + r_b (1 - \alpha)}{2} \]  
\[ (56) \]

**Results.** In Fig. 2, we plot the current as a function of the asymmetry parameter. In Fig. 3 we show the effective diffusion coefficient as a function of the temperature of the hot bath. Fig. 4 shows the Peclet number. Good agreement is obtained between theory and simulation result.

![Fig. 3: (Color online) Effective diffusion coefficient as a function of the asymmetry parameter $\alpha$.](image)

**Conclusion.** In this work, we have analytically and numerically obtained the current and effective diffusion coefficient of a Brownian particle in a piecewise linear potential subject alternately to hot and cold baths. Good agreement is obtained between our numerical and analytical results. In some parameter regimes transport is enhanced.
Acknowledgments

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FIG. 4: (Color online) Effective diffusion coefficient as a function of the temperature of the hot bath.

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FIG. 5: (Color online) Current as a function of the asymmetry parameter $\alpha$. 

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FIG. 6: (Color online) Peclet number as a function of the asymmetry parameter $\alpha$. 

\[
\frac{velocity}{D_{eff}} = f(\alpha)
\]
