Brownian motors thermally coupled to the environment

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1 Introduction

Brownian motors are devices that can use stored energy to create directed motion on a microscopic scale. As well as being able to crank a rotor in the in the fashion of a traditional motor, they are also able to pump ions against a gradient and translocate molecules. Brownian motors have been implemented in the laboratory, for example Ref [1] created a stochastic heat engine by placing a single colloidal particle in a time dependent optical trap. Likewise, Ref [2] placed a colloidal particle in an optical tweezer and drove the particle with explosive vaporization of the surrounding liquid, thus demonstrating a thermal mechanism for Brownian motors. Brownian motors also include devices that can transport molecules over a long distance, for example Ref [3] placed DNA molecules in a time dependent potential to transport the molecules. A very important class of Brownian motors are those where the energy is supplied by a chemical reaction. None of the above experiments fit this criteria, however these types of motors are ubiquitous in biology [4, 5]. Recently, thanks to improvements in imaging techniques, researchers have been able to make highly detailed images of these motors and their working components [6].

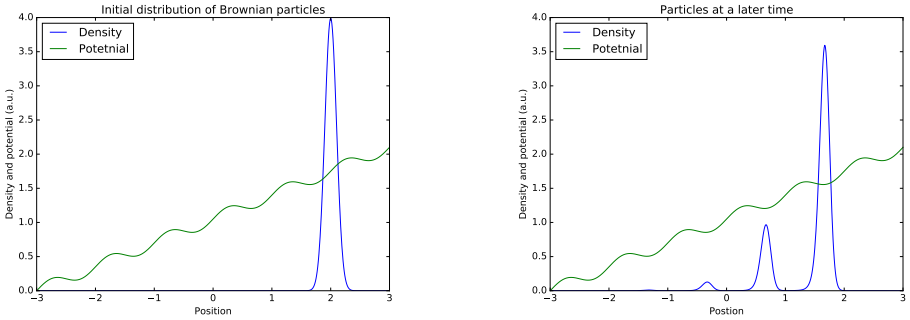

Figure 1: Schematic showing the probability density of particles diffusing in a one dimensional periodic potential at a fixed temperature. We see that the particles tend to drift down the potential as they diffuse, this drift will be called the current J which we will quantify in section 1.1.

In this project, we will model Brownian motors using concepts from statistical mechanics. In particular, a Brownian motor will be modeled by a Brownian particle diffusing over its free energy landscape [7], which in one dimension will be denoted by x. In the case of Brownian motion, it is natural to think of x as a spatial coordinate, however in the case of Brownian motors this is not always the case. Often we will think of x as a reaction coordinate for a chemical reaction, or in the case of a rotary motor, it could be the angle of the motor. We will think of a Brownian particle moving in titled periodic potential of the form $V(x) = fx + v_0(x)$ for some external forcing f and some periodic function $v_0(x)$ with period L. This is shown schematically in figure 1, in this figure we have a particle with a certain known probability density. The particle is agitated by thermal vibrations in a random diffusive manner, however there is also a forcing on the particles that we describe using the potential. Different types of Brownian motors have been explored in the literature, including the Feynman ratchet [8], the Landauer blowtorch [9], thermal ratchets [2], time dependent potentials [3, 1] and tilted periodic potentials [10, 5].

The tilted periodic potential (Figure 1) is of particular interest for this project because it can be used to model biological motors [10, 5]. One way to model Brownian motors of this class is to think of a reaction coordinate x that describes the conformation of a molecule in a chemical reaction. An example of this is the reaction ATP $\rightleftharpoons$ ADP + P, where ATP is adenosine tri-phosphate, ADP is adenosine di-phosphate and P is a lone phosphate molecule. This reaction coordinate is then coupled to a mechanical coordinate y so that each time that a reaction takes place, the motor will move in some way. Since this is a chemical reaction, the free energy will be decreased as time moves forwards. So a system that has a potential that is periodic in x is not sufficient to describe this situation, we will need to "tilt" the potential by adding a forcing f. The value of f will depend on the ΔG of the reaction (i.e. how far out of equilibrium the reaction is). It is shown in [5] that this can be modeled by the two dimensional Smoluchowski equation. In this project we will only be modeling the one

dimensional Somluchowski equation, so we will have to consider the case where x and y are tightly coupled. An example of tight coupling is the kinesin motor [10] that is used in cells to transport molecules. The kinesin motor is strongly bound to a track that it "walks" along, on each step the motor will hydrolyze an ATP molecule using the reaction shown above. This reaction liberates about $12k_BT$ Joules of energy that the motor uses to move forward. Kinesin motors are able to take many steps forward while taking few steps backwards all while falling off their track very infrequently [11].

1.1 The Smoluchowski equation coupled to the environment

As we will see, the diffusion is increased by increasing the temperature and the drift is increased by increasing f. In some cases such as the Landauer blowtorch, the environment has a non uniform temperature held fixed by an external heat source [9]. With this in mind, we interpret Figure 1 as follows: Brownian particles are subject to a given potential and are agitated by thermal noise, these agitations can give the particles the energy to move over barriers created by the potential. As one could imagine, these thermal interactions draw energy from the environment causing the temperature of the environment to change. Normally two simplifying assumptions are made at this point [7], (i) that the thermal fluctuations created by the motor are very small compared to the thermal energy of the surrounding environment which is assumed to be effectively infinite, (ii) that when these temperature fluctuations occur, they diffuse away so rapidly that they do not need to be accounted for. In this project, we will question the second assumption in the case of Brownian motors. Assumption (ii) has also been questioned previously by Streater in the context of Brownian motion [12, 13]. In these articles, Streater investigates Brownian motion from a microscopic view and then comes up with a mathematical model to describe Brownian particles that are thermally coupled to the environment, he then goes on to prove that the model is thermostatistically consistent in the sense that energy is conserved and that entropy increases. We will explore a similar set of equations in the context of Brownian motors and we will try to determine the length scales at which the thermal coupling is important.

The main part of this project will be trying to understand the behavior of the coupled partial differential equations given by:

$$J(x,t) = \gamma^{-1}\frac{\partial}{\partial x}\left(\frac{\partial V(x,t)}{\partial x}P(x,t) + k_B\frac{\partial}{\partial x}\left[T(x,t)P(x,t)\right]\right) \tag{1}$$

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial J}{\partial x} \tag{2}$$

$$\frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(-\kappa q(x,t) + D\frac{\partial T(x,t)}{\partial x}\right) \tag{3}$$

Where

- $P(x,t)$ is the probability density as a function of reaction coordinate x and time t

- $J(x,t)$ is called the current
- γ is the friction coefficient
- $V(x,t)$ is the potential for the motor
- k_B is the Boltzmann constant
- $q(x,t) = \partial_x V(x,t) J(x,t)$ is the heat from the motor
- κ is the thermal conductivity
- D is the thermal diffusivity

Equation (2) is called the Smoluschowski equation [14] and equation 3 is the heat equation. These equations make our intuitive notions more precise, we see that the first term on the right hand side of the Smoluchowski equation (equation 2) is a drift term that is forced by our potential and that the second term contains a diffusion term that is scaled by our temperature. In fact, Figure 1 was made by solving equation (2)numerically. Likewise, equation (3) also appeals to how our intuition of how the motor should effect its environment. The first term represents the heat flux being produced by the motor [15], while the second term represents the diffusion of temperature into the environment.

2 Preliminary results

In order to see how these equations behave with time, we have to resort to numerical methods (see section 2.2). However we note that for a given potential there will be a stationary solution that we will refer to as the "steady state", given periodic boundary conditions, we will give an analytical form for this steady state.

2.1 Steady state solution

In the steady state, we have:

$$\frac{\partial P(x,t)}{\partial t} = 0 = \frac{\partial J}{\partial x} \tag{4}$$

$$\frac{\partial T(x,t)}{\partial t} = 0 = \frac{\partial}{\partial x}\left(-\kappa q(x,t) + D\frac{\partial T(x,t)}{\partial x}\right) \tag{5}$$

Suppose that we have periodic boundary conditions such that $P(x=0) = P(x=L)$, $J(x=0) = J(x=L)$ and $T(x=0) = T_0 = T(x=L)$ where L is the size of one period and T_0 is the temperature of the bath (room temperature). Section 5.2 of [16] gives the steady state current as:

$$J_s = \left[\frac{2k_B T(L)}{\psi(L)} - \frac{2k_B T(0)}{\psi(0)}\right] P_s(0) \left[\int_0^L dx'/\psi(x')\right]^{-1} \tag{6}$$

with $\psi(x) \equiv \exp[-\int_0^x dx' \frac{\partial_x V(x')}{2k_B T(x')}]$. Meanwhile, the density is:

$$P_s(x) = P_s(0) \left[\frac{\int_0^x \frac{dx'}{\psi(x')} \frac{T(L)}{\psi(L)} + \int_x^L \frac{dx'}{\psi(x')} \frac{T(0)}{\psi(0)}}{\frac{T(x)}{\psi(x)} \int_0^L \frac{dx'}{\psi(x')}} \right] \tag{7}$$

In this case, J_s is a constant and $P_s(0)$ is also a constant. Assuming that we know these constants it is now possible to find the steady state temperature. We have:

$$\frac{\partial T}{\partial t} = 0 = \partial_x S_s = \kappa \partial_x V J_s - D \frac{\partial T}{\partial x} \tag{8}$$

Rearranging, we find

$$\frac{\partial T}{\partial x} = \frac{\kappa \partial_x V J_s - \partial_x S_s}{D} \tag{9}$$

Integrating both sides:

$$\int_0^L \frac{\partial T}{\partial x} dx = T(L) - T(0) = 0 = \frac{\kappa J_s}{D} \int_0^L \partial_x V dx - \frac{S_s}{D} L \tag{10}$$

Noticing that $V(x) = v_0(x) + fx$, where $v_0(0) = v_0(L)$, we get $\int_0^L \partial_x V dx = fL$, so

$$S_s = \kappa J_s f \tag{11}$$

and

$$T(x) = T(0) + \frac{\kappa J_s}{D} \int_0^x \partial_x V dx - \frac{S_s}{D} x = T(0) + \frac{\kappa J_s}{D} (v_0(x) - v_0(0)) \tag{12}$$

It would seem that one should be able to calculate the steady state current and density directly from the equations shown above. However, we notice that the constants J_s and $P_s(0)$ have to satisfy equations (6), (7) and (12) while also satisfying the normalization condition $\int_0^L P(x) dx = 1$. To do this we define an objective function given by

$$obj(J_s, P_s(0)) = \left(J_s - \left[\frac{2k_B T(L)}{\psi(L)} - \frac{2k_B T(0)}{\psi(0)} \right] P_s(0) \left[\int_0^L dx' / \psi(x') \right]^{-1} \right)^2 \tag{13}$$

And we minimize this objective function with respect to J_s and $P_s(0)$ under the constraint $\int_0^L P(x) dx = 1$. Another way to do this is to guess a steady state density and temperature and use finite differencing to simulate forward in time until the transients die out.

2.2 Numerical simulation

2.2.1 Finite differences

The one dimensional equation can be solved on a discrete grid by using the finite differences method, the main idea behind this strategy is to approximate derivatives with equations of the form:

$$\frac{df}{dx} \approx \frac{f(x-h) - f(x+h)}{2h} \tag{14}$$

for some small h. The first thing to notice here is that our equation is "flux conservative", i.e. it can be written in the form

$$\frac{\partial P}{\partial t} = \frac{\partial J(x)}{\partial x}$$

In our case, $J(x) = \gamma^{-1}\left(\frac{\partial V}{\partial x}P + k_B\frac{\partial}{\partial x}[TP]\right)$. Now we will discretize space and time, we will split time into N discrete times $T_1, T_2, ..., T_n, ..., T_N$ and space into K discrete points $x_1, x_2, ..., x_k, ..., x_K$. With this, we can approximate the partial derivatives that occur in our equation, first we can approximate $\frac{\partial J}{\partial x}$ with.

$$\left.\frac{\partial J}{\partial x}\right|_{k,n} = \frac{J^n_{k+1} - J^n_{k-1}}{2\Delta x} + O(\Delta x^2) \tag{15}$$

And we can approximate $\frac{\partial P}{\partial t}$ with

$$\left.\frac{\partial P}{\partial t}\right|_{k,n} = \frac{P^{n+1}_k - P^n_k}{\Delta t} + O(\Delta t) \tag{16}$$

We would like to have the equation involving J written in terms of P, by propagating these derivatives through the definition for J we get.

$$P^{n+1}_k \approx P^n_{k-1}\left[\frac{k_B\Delta t}{2\Delta^2}T_{k-1} - \frac{\Delta t}{2\Delta}\partial_x V_{k-1}\right] + P^n_k\left[1 - \frac{k_B\Delta t}{\Delta^2}T_k\right] + P^n_{k+1}\left[\frac{k_B\Delta t}{2\Delta^2}T_{k+1} + \frac{\Delta t}{2\Delta}\partial_x V_{k+1}\right] \tag{17}$$

Using this equation we make a matrix that has the terms multiplying P^n_{k-1} as its lower off diagonal, the terms multiplying P^n_k as its main diagonal and the terms multiplying P^n_{k+1} as the upper diagonal. From now on we will call this matrix A, in order to step the distribution $P(x,t)$ forward one step (i.e. to $P(x, t+\Delta t)$), we need to use the implicit equation

$$\left(I - \frac{1}{2}A\right)P_{dis}(x, t+\Delta t) \approx \left(I + \frac{1}{2}A\right)P_{dis}(x,t) \tag{18}$$

where P_{dis} acknowledges that P has been discretized. Likewise, equation (3) can be discretized to give

$$T_j^{n+1} \approx T_{j-1}^n \frac{\Delta t D}{2\Delta^2} - T_j^n \left[1 + \frac{\Delta t \kappa k_B}{4\Delta^2}(V_{j+1} - V_{j-1})(P_{j+1}^n - P_{j-1}^n) + \frac{\Delta t D}{\Delta^2}\right] + T_{j+1}^n \left[\frac{\Delta t D}{2\Delta^2}\right] - \Delta t \kappa \left(\frac{V_{j+1} - V_{j-1}}{2\Delta}\right)^2 P_j^n \quad (19)$$

and we can form a similar implicit equation to simulate this forward in time. If we know $P(x,t)$ and $T(x,t)$ at time t, then we can use these methods to simulate forward in time and obtain $T(x, t+\Delta t)$ and $P(x, t+\Delta t)$.

Fortunately the matrices that we are dealing with are very sparse, so the program used to solve this equation can save on memory by calling sparse matrix libraries.

2.2.2 Stochastic methods

We can simulate the path of a single particle by using stochastic methods to solve the Langevin equation. By simulating many times we should be able to recover the distributions that were found through finite differencing. When simulating the system at the microscopic level, equation (2) becomes [7]

$$\gamma \dot{x}(t) = -V'(x(t)) + \xi(t) \quad (20)$$

Where $\xi(t)$ is called Gaussian white noise of zero mean and has the essential properties that: $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(s) \rangle = 2\gamma k_B T \delta(t-s)$. We can also consider the stochastic equation with time discretized, in which case we get:

$$x(t_{n+1}) = x(t_n) - \Delta t[V'(x(t_n)) + \xi_n]/\gamma \quad (21)$$

This equation can be simulated numerically, or can be used to derive Equation (2) by taking the limit $\Delta t \to 0$ as is done in Appendix B of [7]. In the results section, we will show some results of these numerical simulations.

2.2.3 Numerical results

Here we will show some results of finite differencing and of the stochastic methods. Figure 2 shows a simulation of a particle density for a certain amount of time. In this figure we see that the density tends to accumulate into the wells and that wherever the density has a sharp peak, it will interact with the environment thermally. The strength of these thermal interactions depends on κ and for a non vanishing D they tend to diffuse away into a smoother shape. If we allow these simulations to run for long enough, then eventually we will reach the predicted steady state.

Meanwhile, figure 3 shows a similar situation that has been simulated stochastically. In this case, we are able to deal with a temperature that is non constant in space, however we are not able to quantify the particles interaction with the environment. This means that κ vanishes in our stochastic model. In the future, we aim to be able to deal with these thermal interactions by using the microscopic equations given by Streater [12, 13].

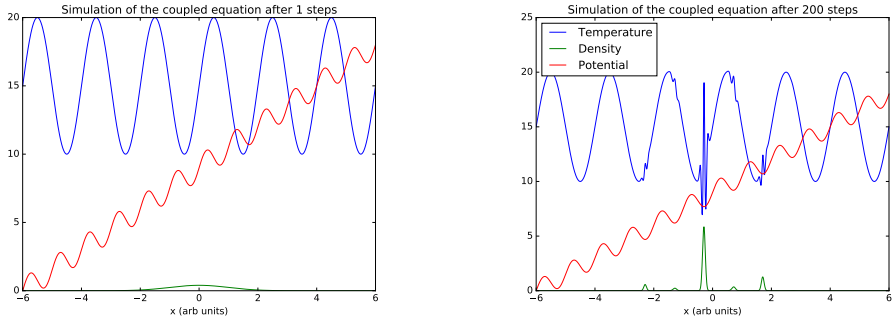

Figure 2: Finite differencing simulation of a distribution of particles, we see that the particles are locally interacting with the environment thermally.

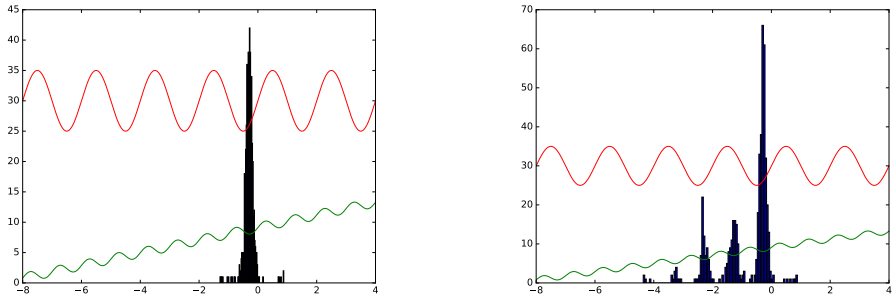

Figure 3: Stochastic simulation of a distribution of particles, In this simulation I have coupled the equations so that the diffusion of the particles is dependent on the temperature, however the temperature is not affected by the particles (i.e. in the case where $\kappa \to 0$).

3 Outlook

The main goal of this project is to see how thermal interactions with the environment effect the properties of Brownian motors. To do this we will create a program that can find the probability current J_s in the steady state as discussed in section 2.1. As mentioned, this involves solving a constrained optimization problem, this program has already been implemented in Julia [17] while using JuMP [18] to call out to an external solver. We also want to be able to solve this problem by simulating the system forward in time until it reaches its steady state, this is only partially implemented. As well as this we would like to be explore the dynamical properties of the system numerically and stochastically, the code for this exploration is only partially implemented. Finally, we would like to be able to determine at what length scales the thermal coupling becomes important for the operation of the motor.

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