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. 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 [1], 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 an ensemble of particles with a certain known density. These particles are being pushed around by thermal vibrations in a random diffusive manner, however there is also a forcing on the particles that we describe using a potential.

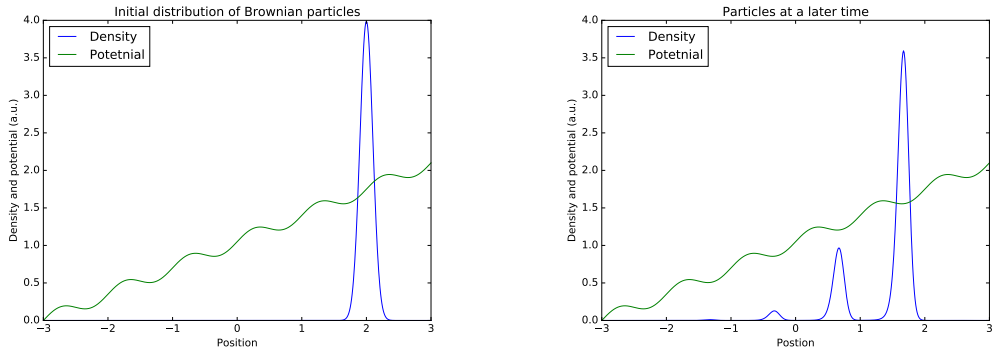

Figure 1: Schematic showing particles diffusing in a one dimensional periodic potential at a fixed temperature. We see that the particles tend to drift down the potential as they diffuse, this drift will be called the current J which we will quantify in section 1.1.

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 [2]. 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 as they move down the slope of 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 [1], (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. It is important to note that assumption (ii) has been questioned by Streater in the context of Brownian motion [3, 4]. 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 and we will try to determine the length scales at which the thermal coupling is important.

1.1 The Smoluchowski equation coupled to the environment

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 time t and reaction coordinate x
- $J(x,t)$ 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 [5] 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 [6], 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 now impose periodic boundary conditions such that $P(0,t) = P(L,t)$, $J(0,t) = J(L,t)$ and $T(0,t) = T_0 = T(L,t)$ where L is the size of one period and T_0 is the temperature of the bath (room temperature). Section 5.2 of [7] gives the steady state current as:

$$J_s = \left[\frac{2k_BT(L)}{\psi(L)} - \frac{2k_BT(0)}{\psi(0)}\right] P_s(0) \left[\int_0^L dx'/\psi(x')\right]^{-1} \tag{6}$$

with $\psi(x) \equiv \exp[-\int_0^x dx' \frac{\partial_x V(x')}{2k_BT(x')}]$. 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_{k-1}^n as its lower off diagonal, the terms multiplying P_k^n as its main diagonal and the terms multiplying P_{k+1}^n 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

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

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 [1]

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

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:

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

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 [1]. In the results section, we will show some results of these numerical simulations.

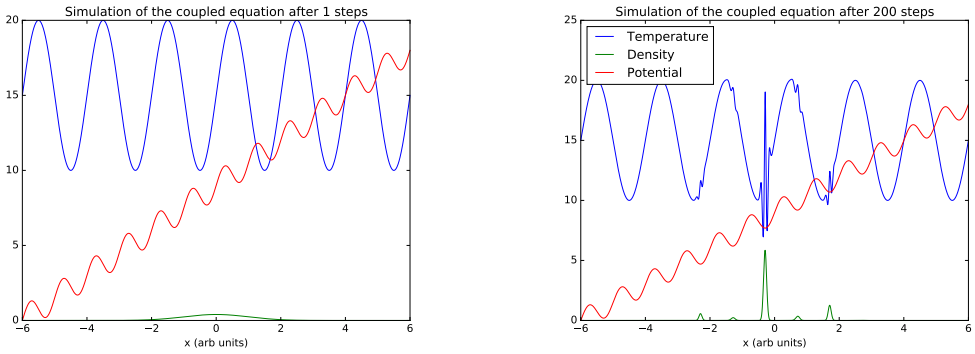

Figure 2: Finite differencing simulation of a distribution of particles, we see that the particles are locally interacting with the environment thermally.

3 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.

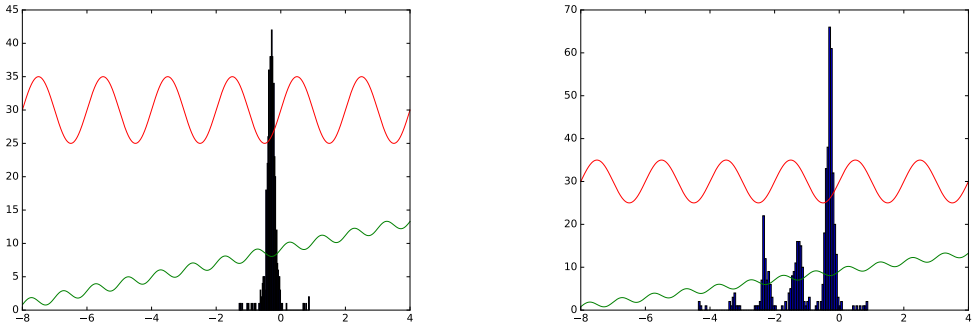

Figure 3: Stochastic simulation of a distribution of particles, In this simulation I have coupled the equations so that the diffusion of the particles is dependent on the temperature, however the temperature is not affected by the particles (i.e. in the case where $\kappa \to 0$).

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