SELF INDUCED TEMPERATURES IN BROWNIAN MOTORS

JACK DEVINE

April 27, 2016

CONTENTS

1 Introduction 2
1.1 The Smoluchowski equation coupled to the environment . . . 2
2 Methods 2
2.1 Finite differences 2
2.2 Stochastic methods 3
3 Results 3

ABSTRACT

Brownian motors are capable of converting chemical energy directly into work and are crucial for many biological processes. The purpose of this project is to consider the motors thermal interaction with the environment, we want to know whether these thermal interactions will change the efficiency of the Brownian motors as compared to calculations made without considering coupling to the environment.

1 INTRODUCTION

Brownian motors are devices that can use stored energy to create directed motion, 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.

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:

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

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

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

Where $P(x,t)$ is the probability density as a function of time t and reaction coordinate x, γ is the friction coefficient, V is the potential for the motor, k_B is the Boltzmann constant, T is the temperature, κ is the thermal conductivity, $q(x,t) = \partial_x V(x,t) J(x,t)$ and D is the diffusion coefficient for the temperature. Equation 2 is called the Smoluschowski equation (need a citation here) and equation 3 is the equation that governs the evolution of the temperature.

2 METHODS

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:

$$\frac{df}{dx} \approx \frac{f(x-h) - f(x+h)}{2h} \tag{4}$$

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, $J(x) = \gamma\left(\frac{\partial V}{\partial x}P + k_B T\frac{\partial P}{\partial x}\right)$. 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.

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

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

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

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

$$\frac{P_k^{n+1} - P_k^n}{\Delta t} = \frac{1}{2\Delta x^2}\left(P_{k+1}^n(V_{k+2} - V_{k+1}) + k_B T(P_{k+2}^n - P_{k-1}^n + P_k^n - P_{k-1}^n) - P_{k-1}(V_k - V_{k-1})\right)$$

Solving for P_k^{n+1} gives

$$P_k^{n+1} = \frac{\Delta t}{2\Delta x}\left(P_{k+1}^n(V_{k+2} - V_{j+1}) + k_B T(P_{k+2}^n - 2P_{k-1}^n + P_k^n) - P_{k-1}^n(V_j - V_{k-1})\right) + P_k^n$$

If we write

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

$$dX_t = \mu(x,t)X_t + \frac{1}{2}\sigma(x,t)^2 dW_t \tag{5}$$

Where W_t is called a Wiener process.

3 RESULTS

Here we will show some results of finite differencing and of the stochastic methods. Figure 1 shows a simulation of a particle density for a certain amount of time.

[1]

REFERENCES

[1] Valentin Blickle and Clemens Bechinger. Realization of a micrometre-sized stochastic heat engine. *Nature Physics*, 2011.

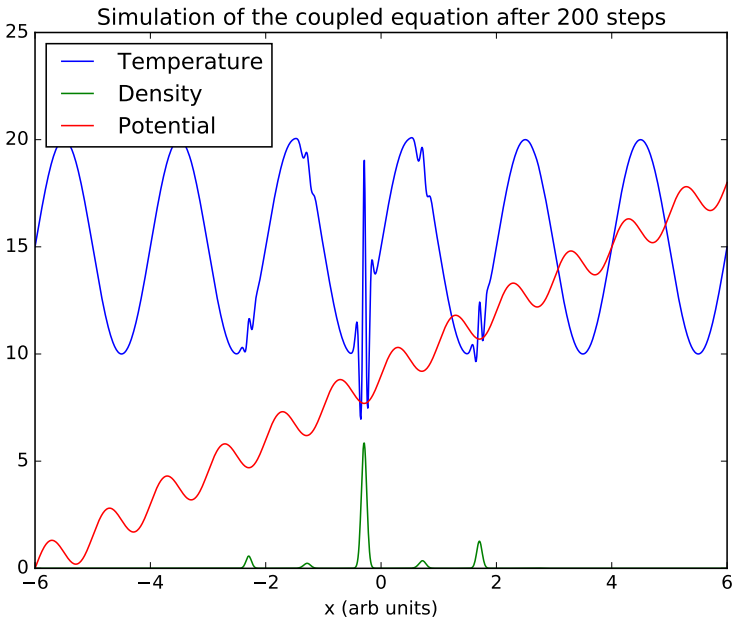

Figure 1: Finite differencing simulation of a distribution of particles, we see that the particles are locally interacting with the environment thermally.