Negative conductance in two finite-size coupled Brownian motor models *

Ryoichi Kawai† Adam Marcus‡

August, 2000

Abstract

We examine two different models of interactive Brownian particles immersed in a symmetric, periodic potential. The first model extends the coupled Brownian motor examined in Hänggi et al. [3], differing by its consideration of non-homogeneous noise-strength coefficients. The second model contrasts the first in its use of an inversely proportional interaction between particles. The observed properties include true negative conductance appearing in each of the two models with the objective of finding the smallest system size exhibiting this property.

1 Introduction

With the contemporary push in miniaturization, a new level of importance has been placed on the study of nanosystems and their potential roles in technology. The concept of negative conductance, while still fairly new, has already found its way into various scientific disciplines: biomolecular research in the form of active transport [2], molecular chemistry as a tool in particle separation [1], and theoretical physics accompanying the theory of Brownian motors [3]. In this paper, we examine two models of coupled Brownian particles, utilizing Monte Carlo simulation techniques on a periodic Langevin equation. We study the effects of a position-dependent multiplicative noise source used in previous experiments [4], a constant torque-induced velocity ω, and an interaction between particles. Furthermore, since the stochastic and interactive forces are symmetric in both models, ω represents the only cumulative force on the system. Thus the flow of motion is initiated by a force moving in the *opposite direction*, making the system both counterintuitive and worthy of investigation.

*Research supported by the National Science Foundation (NSF) Research Experiences for Undergraduate (REU) site award, Grant No. DMR-9987872

†Department of Physics, University of Alabama at Birmingham, Birmingham, AL 35294. Email: kawai@uab.edu

‡College of Arts and Sciences, Washington University in St Louis, St Louis, MO 63105. Email: adam@math.gatech.edu

2 Classical Model

The first model is an extension of Kuramoto's model for N-particle coupled phase oscillators (see [5] for details)

$$\dot{\theta}_i = \omega - \frac{K}{N}\sum_{j=1}^{N}\sin(\theta_i - \theta_j) + \xi_i$$

with K acting as a spring constant and $R_i(t)$ a Gaussian random number. Kuaramoto's choice of forces is fairly popular due to its proportional interactive term and constant external force term. Due to its proven success, we begin by adapting this classical model.

2.1 Developing an Extension

Previous investigations [4] considered the case

$$\xi_i = \left|\sin(\theta_i/2)\right| R_i(t)\sqrt{\frac{2Q}{dt}}, \tag{1}$$

and established results for the noise-strength coefficient $Q = 1$. In an attempt to decrease the number of necessary particles, as well as to provide a more realistic basis for the system, we consider a non-homogeneous noise-strength coefficient. Taking ξ in terms of its component values as in [6], we have

$$\xi_i = R_i(t)\sqrt{\frac{k_B T(\theta_i)}{\gamma_i dt}} \tag{2}$$

with k_B equal to Boltzmann's constant, T the temperature, and γ the frictional force. Assuming the particles are sufficiently small, thus having negligible mass, we can define the frictional force in terms of a constant α (which depends on the radius) and the coefficient of friction η, leading to the following:

$$\xi_i = R_i(t)\sqrt{\frac{k_B T(\theta_i)}{6\pi\eta\alpha_i dt}} \tag{3}$$

$$= \left|\sin(\theta_i/2)\right| R_i(t)\sqrt{\frac{2C}{\alpha_i dt}} \tag{4}$$

where $T(\theta_i) = \sin^2(\theta_i/2)$ as in the previous model, and $C = \frac{k_B}{12\pi\eta}$. Hence we are justified in merely substituting $Q = C/\alpha_i$ into Eq. (1) to convert the constant into a non-homogeneous, inversely proportional term.

2.2 Results

The non-homogeneous noise-strength coefficient model

$$d\theta_i = \omega dt + \left|\sin(\theta_i/2)\right| R_i(t)\sqrt{\frac{2C}{\alpha_i}}dt - \frac{K}{N}\sum_{j=1}^{N}\sin(\theta_i - \theta_j)dt \tag{5}$$

underwent 2×10^8 iterations at a time step $dt = 5\times10^{-6}$ using the second order Heun method to approximate the continuity of time.

The results of the computation were fitting for the type of situation defined above. As Figure 1 shows, there was a fairly robust negative conductance displayed in the 7-particle system, far fewer than the homogeneous model would allow [4].

One interesting occurrence is that, while the lone particle with radius $\alpha = 1$ was moving against the applied force, the other six particles, radius $\alpha = 2$, moved *with* the system's torque. Even as late as $t = 1000$, the average particle displacement remained almost constant, as can be seen in Figure 5. This fairs well with our chosen scenario, especially considering our assumption of negligible mass. The properties of this system make it almost ideal for nanoscale particle separations [2], especially considering the low number of particles involved in the system. By applying a constant velocity, the particles moved off in separate directions with respect to their sizes. Thus by applying a random noise source, our system has actually *lowered* its own randomness!

3 Inverse Model

We now break away from the classical extension and introduce an experimentally new model of coupled Brownian motion. Before we are able to accomplish this, though, some computational hazards must be dealt with due to the unwanted explosions of inversely proportional forces as particles near each other. The difference between these models is shown in Figure 2.

3.1 Inversely Proportional Interactive Term

In order to investigate the properties of the inverse model, we define the function

$$g(x) = \frac{2x - xk^2 + k\sqrt{k^2x^2 - 4x^2 + 4}}{2} \tag{6}$$

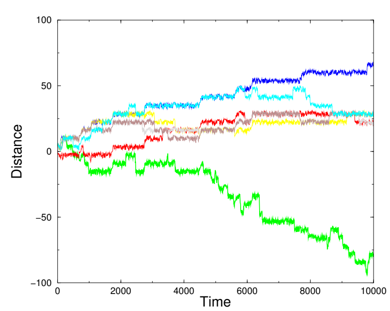

Figure 1: A 7-particle system modeling Eq. (5) [$K = 1.5$, $\omega = 0.035$, $C = 1$, $\alpha_1 = 1$, $\alpha_2 \ldots \alpha_6 = 2$].

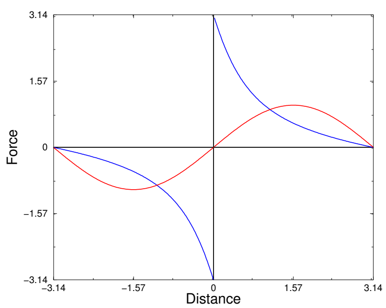

Figure 2: Comparison of interactive forces

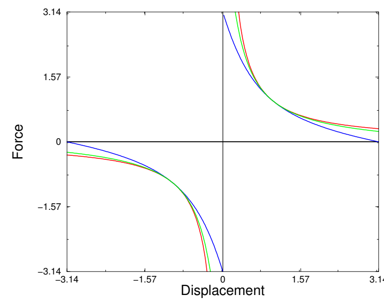

Figure 3: Increasing levels of accuracy for $k = \pi,\ 2\pi$

for some scaling constant k to approximate the behavior of the inverse function $1/x$, with x corresponding to the distance between particles. Eq. (6) is chosen primarily so that

1. $\lim_{k\to\infty} g(x) \Rightarrow \frac{1}{x}$
2. $\lim_{k\to\infty} g'(x) \Rightarrow \frac{-1}{x^2}$

making it a suitable approximation for a gravitation-like potential.

Figure 3 shows that even for relatively small values of k, the accuracy of the approximation is quite good. The value used in the computations, $k = 4\pi$, is already too close to the line $y = 1/x$ to be able to distinguish.

The other properties that make $g(x)$ a desirable approximation for this system lie in the symmetry about the lines $y = x$ and $y = -x$. Furthermore, g possesses both $x-$ and $y-$intercepts, keeping the force from exploding as particles approach each other and causing the force to disappear as particles approach diametrically opposite positions on the circle.

Most importantly, the parameter k can be chosen so that an arbitrarily accurate approximation for can be made. Since the greatest error naturally occurs as $x \to 0$, Eq. (6) can be solved for a given maximum error ϵ,

$$k \geq \frac{1}{\epsilon^2} \;\Rightarrow\; \frac{1}{x} - g(x) \leq \epsilon \qquad \forall x \geq \epsilon \tag{7}$$

thereby providing the necessary value for k to achieve such an accuracy.

3.2 Development of the Equation

Consider a variance of the general Ginzburg-Landau equation on a periodic system, with the interactive potential distributed over all of the particles in the system, specifically:

$$\dot{\theta}_i = f(\theta) + h(\theta)\xi_i(t) - \frac{1}{N}\sum_{i=1}^{N} \frac{\partial V(\theta)}{\partial \theta_i} \tag{8}$$

For the purpose of isolating the system from any outside fluctuations, we again define $f(x)$ to be a constant ω. For the purpose of imitating some inversely proportional force, we choose gravity as a natural candidate, making

$$V(\theta) = \frac{Gm_1m_2}{(\theta_1 - \theta_2)^2} \tag{9}$$

and thus

$$\frac{1}{N}\sum_{i=1}^{N}\frac{-\partial V(\theta)}{\partial\theta_i} = G\sum_{j\neq i}\frac{m_im_j}{(\theta_j - \theta_i)} \tag{10}$$

For the stochastic term, we turn again to Eq. (2), only this time using a different approach. We shall still use the Stratovich interpretation of a multiplicative noise, only this time defining the friction force $\gamma_i = \mu m_i$ where μ is the (homogeneous) coefficient of friction. Making a substitution similar to the one in Section 2.1, we obtain the following stochastic differential equation:

$$\theta_i = \omega dt + \big|\sin(\theta_i/2)\big|R_i(t)\sqrt{\frac{2C}{m_i}dt} - \frac{G}{N}\sum_{j\neq i}m_im_jg\big(u(\theta_j - \theta_i)\big)dt \tag{11}$$

where $u(\theta)$ is defined to be the unique real number in $(-\pi, \pi]$ such that $u(\theta) = \theta + 2\pi n$ for some $n \in \mathbf{Z}$.

3.3 Results

The model only underwent 2×10^7 iterations since the attractive forces caused the particles to converge much more quickly than in the previous model. Again a time step of $dt = 5 \times 10^{-6}$ and the second order Heun method were used to approximate the continuity of time. For the purpose of computation, G was scaled to 3.0. In a true gravitational system, the gravitational constant $G \approx 6.67 \times 10^{-11}$ would need to be used, but for computational purposes this has been scaled to a more reasonable value. Since C and m_i are each scalable in their own rights, the system is still theoretically realizable.

The inversely proportional model gave some surprising results, which are clearly shown in Figure 4. The negatice conductance displayed by the five particles with $m = 0.1$ was extremely robust, dominating the overall displacement of the system, evident in Figure 5. Even when the system reset, as can be seen by the upward sloping in the smaller particles, the particles quickly realligned and resumed Brownian motor behavior. The system, with as few as 15 particles, formed a negative conductance that required over 50 particles in the classical model [4].

4 Conclusions and Discussion

In regards to the effectiveness of each model, it was clear that both had potential in their own rights. The gravitational system is extremely robust even for low

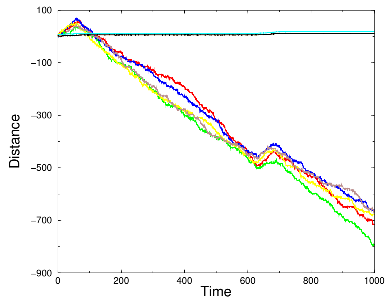

Figure 4: A 15-particle system modeling Eq. (11) [$\omega = 0.080$, $C = 2$, $m_1 \ldots m_5 = 0.1$, $m_6 \ldots m_{15} = 5$].

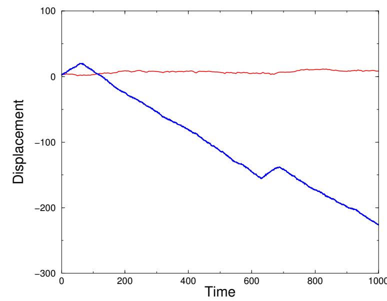

Figure 5: The downward sloping average of the new model vs. the stable average of the classical model

numbers of particles and still holds much to be explored. The non-homogeneous classical model, on the other hand, has shown negative conductance for an extremely small system of particles. Perhaps the only down side lies in the inability to instantiate such systems in the physical world. The classical model's interactive force has no true parallel in nature, making it a purely theoretical phenomenon. While the inversely proportional model mimics the effects of gravity, the absurdly low value of G requires the masses and temperature to be scaled more than 10^5 to obtain a large enough force to balance out any substantial torque induced velocity. The scaling could be reduced by increasing the radius of the system, but this in turn would cause a decrease in the system speed. Thus a realization of this model would require a macroscale system with a fairly substantial temperature gradient and it would still take ages to produce a noticeable effect. As far as Brownian motors go, anything large enough to benefit technology is purely theoretical, and yet these systems are known to appear in nature [2], making them worthy of further research.

5 Acknowledgments

We would like to thank Dr. Vohra and the rest of the UAB Physics department for establishing a research program for interested undergraduate students.

References

[1] R. D. Astumian and M. Bier, *Biasing Brownian motion in different directions in a 3-state fluctuation potential and an application for the separation of small particles*, Phys. Rev. Lett. **76** (1996), 4277–4280.

[2] I. Derényi, P. Tegzes, and T. Vicsek, *Collective transport in locally asymmetric periodic structures*, Chaos **8** (1998), 657–664.

[3] P. Hänggi, R. Kawai, P. Reimann, and C. Van den Broeck, *Coupled Brownian motors*, Springer Verlag, New York, 1999.

[4] M. Kambon and R. Kawai, *Finite-size effects on noise-induced negative mobility in coupled phase oscillators*, manuscript (1999).

[5] R. Kawai, P. Reimann, and C. Van den Broeck, *Nonequilibrium noise in coupled phase oscillators*, manuscript (1999).

[6] M. Miguel and R. Toral, Instabilities and Nonequilibrium Structures, VI (E. Tirapegui and W. Zeller, eds.), Kluwer Academic Pubs., 1997.