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Stochastic Resonance, Brownian Ratchets and the Fokker-Planck Equation

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Abstract. Our immediate aim is to arrive at quantitative realistic estimates of the optimum noise levels for a complete and feasible Brownian ratchet device. A number of difficult "Unsolved Problems of Noise" naturally arise in the course of this work. We pose a general philosophical question: "Is it is possible to relate stochastic resonance and Brownian ratchets in a formal way, through a consideration of the Fokker-Planck equation?" The evidence suggests that some forms of stochastic resonance can be formulated in terms of a Fokker-Planck equation and some cannot. Stochastic resonance may actually be a collection of similar but distinct phenomena.

We present a number of simulations which demonstrate stochastic resonance in a Brownian ratchet. We also show how current is dependent on a number of other parameters.

INTRODUCTION

When engineers design machines at the human scale they tend to regard inertial, elastic and gravitational forces as being the most significant. Even when dissipative forces are considered, these are usually regarded as small additions perturbations to the original theory. At the molecular end of the scale; if we try to design nano-machines then dissipative forces are the most significant forces and the effects of thermal motion of the surrounding medium are very evident. This gives rise to a chaotic agitated movement called Brownian motion. At this scale, it makes sense to attempt to *harness* the random thermal motion in the surrounding medium, rather than to try to resist it or to overpower it or to block it out. This idea can be traced at least as far back as Maxwell and on through Smoluchowski [1] and to Feynman [2]. It is a still topic of active research [3, 4, 5, 6]. Brownian ratchets work by directing particles locally using a potential field. They must operate in at least two modes. An example of a flashing ratchet is shown in Figure 1. A very surprising feature of Brownian ratchets is that in each of the modes, the probability current is "downhill" towards regions of lower potential and yet when the ratchet is switched between the modes, the steady state current can be "uphill" against the average potential gradient.

One of the main motivations for studying ratchets is to understand sub-cellular transport processes [7, 8, 9, 10, 11, 12, 13, 14]. There is considerable evidence that molecular motors in living cells use a ratchet mechanism.

Harmer *et al.* [15] have shown that a very simple discrete-time ratchet can demonstrate the same "uphill" current as the continuous time ratchet. This led to the notion that a combination of two "losing" games can be "winning."

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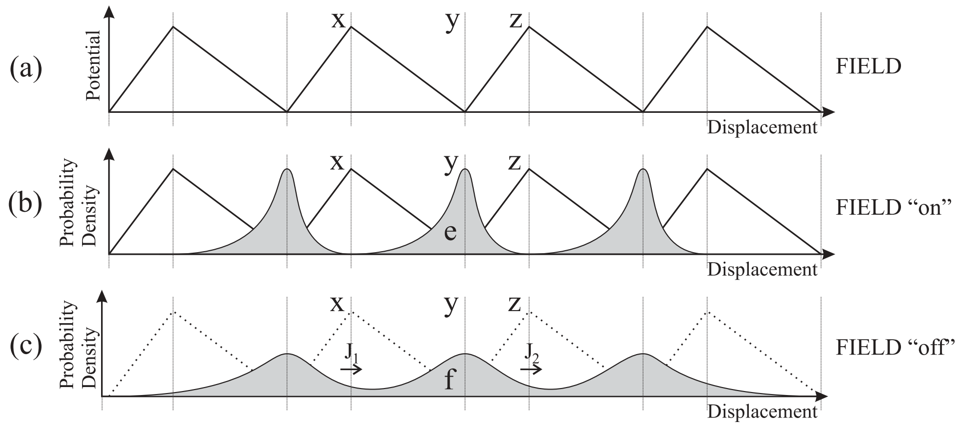

FIGURE 1. The Brownian ratchet requires a potential, Part (a) shows the ratchet shaped potential. The Brownian ratchet requires at least two modes of operation. Part (b) shows the effect when the field is asserted. The charged Brownian particles accumulate near points of lowest electrical potential, such as pont "y." Diffusion prevents the particles from all converging to the same point. This diffusion is the effect of numerous collisions with the particles that make up the surrounding medium. These collisions can also be regarded as noise. Brownian ratchets require the presence of noise. Part (c) shows the effect when the field is turned off and the system "relaxes" as the particles diffuse. The bulk of the distribution is near point "y" and the ratchet is asymmetrical so point "y" is closer to point "z" than it is to point "x." This means that the current density, J_2, past point "z" will be greater than the current density, J_1, past point "x." This inequality is the cause of the steady-state current in the ratchet.

Stochastic Resonance

Stochastic Resonance, SR, [16, 17, 18, 19, 20] is a phenomenon where we can obtain optimal output from a system by adding noise to the system. This idea has been applied to a great number of possible applications in physics, engineering and biology. Much of the early investigation required the use of thresholds or bi-modal potential wells and formulated the problem in terms of a Fokker-Planck equation. See, for example [16].

Stochastic resonance is believed to play a role in the normal operation of the nervous system and it is interesting to note that the Fokker-Planck plays a role in the operation of neural networks [21].

It should be admitted that not *all* forms of SR can be formulated in terms of a Fokker-Planck equation. For example, Bezrukov and Vodyanoy [22] have devised a time dependent Poisson process that has no activation barrier of any kind and is not formulated in terms of a Fokker-Planck equation. It seems that what we notionally call "Stochastic Resonance" is really a collection of several phenomena with similar appearance.

A possible connection between Brownian Ratchets and Stochastic Resonance

The earliest reference that we can find to a connection between Stochastic Resonance and Brownian ratchets is Gang *et al.* [23]. They expand the dynamics into independent subspaces according to the theory of Floquet. They make the equations tractable by only keeping a few important terms from an infinite expansion. Some approximation is involved. All the reasoning is algebraic. There are no experiments or simulations. Doering [24] gives clear analysis of some simple models. He computes the resulting current for both the "fast" flashing and "slow" flashing limits. The flashing is "slow" or "adiabatic" if the temporal period of the potential function in the ratchet is long compared with the characteristic relaxation time of the system. Doering includes graphs demonstrating a non-monotonic change in probability current density **J** with increasing mean particle energy, $k_B T$, but the final results are not quantitative. Berdichevsky and Gitterman [25] give a very complex and detailed analysis of SR and ratcheting in a Josephson junction with noise and also conclude that SR and ratchet effects exist in diffusive systems with oscillating barriers [26].

We have shown that Parrondo's discrete-time ratchet exhibits a Stochastic Resonance effect [27]. We have also shown that, with some modification, Parrondo's games can be used to model realistic Fokker-Planck equations and can be used to numerically simulate the dynamics of Brownian ratchets [28]. Our aim here is to simulate realistic Brownian ratchets using Parrondo's games as a numerical method. The aim is to optimize designs for possible ratchets.

Our interest in SR is that we must ensure that the optimum level of noise applies, in order to achieve optimum current in the ratchet device.

OUTLINE OF APPROACH

It is possible to derive a Partial Differential Equation for the probability density of finding a particle at a certain place and time [29, 6]. This is called the "master" equation or "Fokker-Planck" equation:

$$\frac{\partial^2}{\partial z^2}\left(D(z,t)\,p(z,t)\right) - \frac{\partial}{\partial z}\left(\alpha(z,t)\,p(z,t)\right) - \frac{\partial}{\partial t}p(z,t) \quad = \quad 0\,. \tag{1}$$

In this approach we solve for $p = p(z,t)$ which is the probability density of finding a particle near the point z, in space, at time t. We then apply other operators to p in order to calculate any macroscopic parameters of interest, such as probability current density, J, or mean position $E[z]$. We apply finite-difference techniques to Equation 1 to convert it to an equivalent set of difference equations which have the form of Parrondo's games [28]. These difference equations can be evaluated numerically.

Definition of "Noise"

The natural definition of noise would be to use a standardized model of white noise, dB as a reference. This is summarized in the term $g(z,t)\,dB$, in the Langevin equation: $dz(z,t) = \alpha(z,t)\,dt + g(z,t)\,dB$. In this paper we use $D^{(2)} = D = g^2$ as the operational macroscopic definition of "noise." This definition of noise increases monotonically with increasing mean energy of the molecules in the surrounding medium, $\frac{3}{2}kT$. Reif [30] gives an expression for an ideal gas, $D =$constant$\times(kT)^{3/2}$. The choice of different definitions of noise, g, $D = g^2$ or kT would not alter the basic phenomena; it would only re-scale the axes.

Definition of "Probability Current"

We must apply a law of total probability in the form of a continuity law $\nabla J + \frac{\partial p}{\partial t} = 0$. We define the probability current density as $J = -\nabla(D\cdot p) + (\alpha\cdot p)$ which is a form of Fick's law and is consistent with Risken [29] . In this context we require that $\alpha(z,t) = u\underline{E} = u(-\nabla V(z,t))$ where u is the mobility of the Brownian particle, V is the applied voltage and $\underline{E}$ is the resulting electric field [1]. In three dimensions, we can combine the continuity equation and Fick's law to get the Fokker-Planck equation: $\nabla^2(D\cdot p) - \nabla(\alpha\cdot p) - \frac{\partial p}{\partial t} = 0$. For the one dimensional case, with constant diffusivity, we get

$$D\frac{\partial^2 p}{\partial z^2} - \frac{\partial(\alpha p)}{\partial z} - \frac{\partial p}{\partial t} = 0\ . \tag{2}$$

Risken [29] and Parrondo [6] affirm that the Fokker-Planck equation does describe the fundamental dynamics of the physical process in a Brownian ratchet. This is the physical model that we use. Our aim is to make it realistic and to calculate the effects of our choices.

Boundary Conditions and Initial Conditions

We require the probability current density at infinity to be zero, i.e. $\lim_{z\to+\infty} J(z) = \lim_{z\to-\infty} J(z) = 0$. If we integrate the Continuity Equation together with the boundary conditions the we get a law of total probability: $\int_{-\infty}^{+\infty} p(z,t)dz = 1$ for all values of t. This

[1] If charge becomes crowded then space-charge effects will be significant and the effective electric field will be altered, $\underline{E} = \underline{E_1} + \underline{E_2}$. The first component, $\underline{E_1} = -\nabla V(z,t)$, is due to the applied voltage. The second term is due to space charge and corresponds to Poisson's equation (with zero boundary conditions), $\nabla\underline{E_2} = \frac{(pq)}{\varepsilon}$, where q is the charge per Brownian particle and consequently (pq) is the expected value of the charge density. The constant, ε, is the permittivity of the surrounding medium. In these simulations we have assumed that the sample of Brownian particles is sparse and that $\underline{E_2}$ is not significant, compared with $\underline{E_1}$.

is an important normalization condition. All solutions and simulations must satisfy this condition.

An important consequence of these boundary conditions is that we can define the mean drift velocity in terms of probability density, p, or current density, J:

$$v = \frac{\partial}{\partial t} E\left[z\right] = \frac{\partial}{\partial t} \int_{-\infty}^{+\infty} z p(z,t) dz = \int_{-\infty}^{+\infty} J(z,t) dz \ . \tag{3}$$

We imagine that the particles are injected into a single slot between the teeth of the ratchet at $t = 0$. A reasonable abstraction is $p(z,0) = \delta(z)$. In the numerical simulations, we spread the initial probability across the width of a single slot of the ratchet. This would correspond to the injection of a small sample into a single slot of the ratchet.

Asymptotic Solution

We are interested in the behavior of the ratchet as the distribution spreads out, for large time $t \to +\infty$. The initial conditions do not have a great effect on the parameters of interest, including rates of increase in variance and probability currents, J, in the asymptotic limit. In the simulations this is achieved by running the simulations for a sufficient time, to eliminate the effect of the initial transients.

FINITE DIFFERENCE SIMULATIONS

We have previously shown that Parrondo's games are a particular way of sampling the Fokker-Planck equation [28]. Parrondo's games were originally conceived as a purely heuristic model or "*gedankenexperiment*" but we have shown that they can be generalized to make them realistic.

We have also previously shown that that Parrondo's original games demonstrated an effect which had the same form as Stochastic resonance [27, 31]. In this paper we use more realistic choices for the parameters (including: sampling time and sampling distance, diffusivity, particle mobility and charge) for our simulations of Brownian ratchets and show that these more realistic ratchets also exhibit an effect which has the same form as stochastic resonance. We made choices of the sampling times and distances for a finite element simulation of sodium ions, Na^+, diffusing in water, H_2O. We chose a feature size for the ratchet teeth of $l = 2\ \mu$m, which is well within the limits of existing MEMS technology. We have assumed that the effect of charge crowding is negligible. A typical instant in the numerical simulation is shown in Figure 2(a). The general shape of the distribution is Gaussian although it is clearly modulated by another function, the impression of the teeth of the ratchet. If the field is asserted for a long time then the profile within each slot of the ratchet closely resembles the steady state solution, which is a two sided exponential function.

The time evolution of the ratchet process consists of a series of these functions and is shown in Figure 3. It is possible to apply operators to the distributions in Figures 2 and 3 to calculate quantities of interest, such as probability current density J or mean

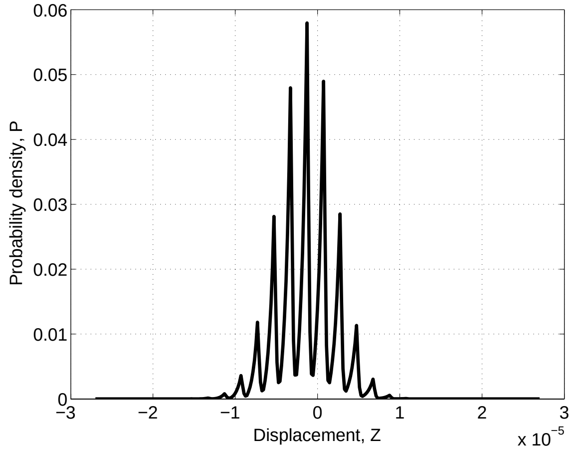

FIGURE 2. A typical time-slice, showing $p(z, t_0)$ for a fixed value of time t_0. The PDF is essentially Gaussian, multiplied by a modulating function, caused by the teeth of the ratchet.

position of the distribution $E[z]$, as shown in Figure 4. We can see how the mean position of the particle shifts in response to the modulation of the electric field of the ratchet. The time interval for which the field is "off" represents noise, since the particle simply undergoes Brownian motion in response to agitation of the surrounding particles. There is no constraint that limits the effect of the noise. This is equivalent to Game "A" in Parrondo's games. The time interval for which the field is "on" represents the action of the ratchet. It is during this time interval that the mean position of the particle moves. If this mode of operation persists for long enough though then the distribution of the particles reaches an equilibrium and detailed balance is achieved and the current of particles will stop. It is necessary to turn off the field and allow some diffusion in order for the current to be maintained.

The presence of noise is needed to maintain the current. More noise produces more current up to a certain point, after which the ratchet is overwhelmed by noise and the current diminishes and eventually stops. This has the form of the stochastic resonance curve, shown in Figure 5.

STOCHASTIC RESONANCE

We can create a parametric graph of the asymptotic rates of probability current in the ratchet as a function of increased diffusivity. This graph is shown in Figure 5 and clearly has the form of a stochastic resonance curve. The rate of probability current in the ratchet can be regarded as a rate of change in the first moment, $\partial E[z]/\partial t$ The operation of the ratchet affects all of the moments. The second central moment or variance, σ^2, contains information about the spread of the distribution. Spread has to be regarded as an undesirable feature of ratchets. Lindler *et al.* have raised the

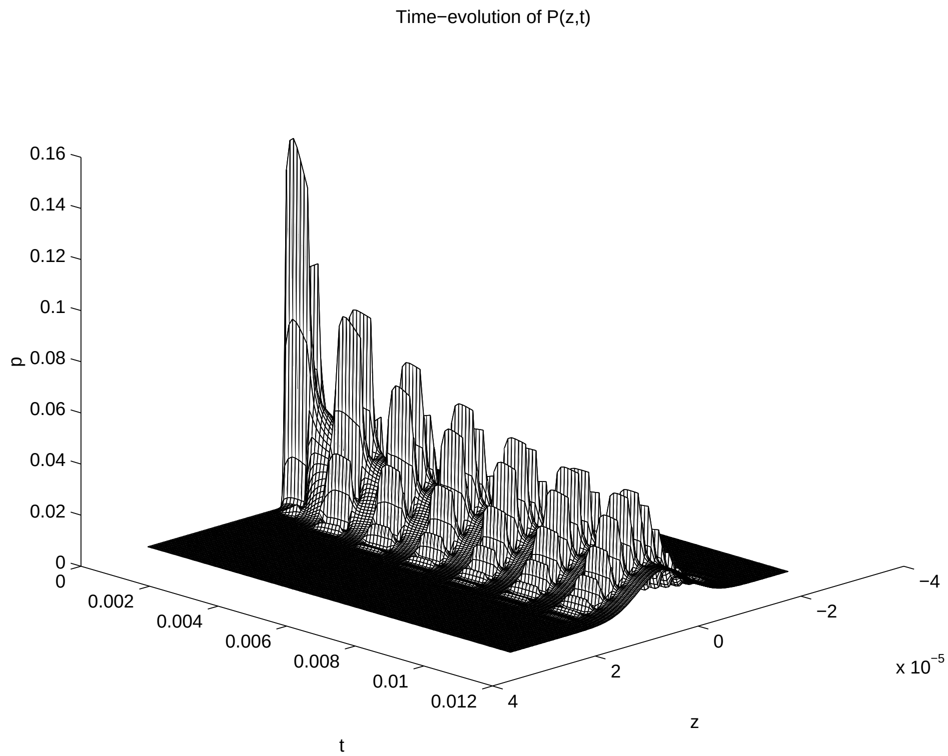

FIGURE 3. A finite-difference simulation of a Brownian ratchet, based on Parrondo's games. z is space, t is time and p is probability density. The spatial period of this ratchet is $L_z = 2\ \mu$m. The temporal period of this ratchet is $T_0 = 1.5$ ms. The physical constants are scaled for the diffusion of hydrated sodium ions in water.

issue of transport coherence [32]. They use a normalized measure of transport and include scaling factors of the spatial period of the ratchet and the effective diffusion coefficient. Einstein's solution to the diffusion equation is a spreading Gaussian curve with variance $\sigma^2 = 2Dt$ and we can use this to define an effective diffusion coefficient for any time varying distribution $p(z,t)$. We can define the effective diffusion coefficient as: $\lim_{t\to\infty}\left(\sigma^2(t)/(2t)\right)$ where $\sigma^2(t)$ is the variance at time t. We can then define the Péclet number [32] as $P_e = vL_z/D_{eff}$ where v is the mean drift velocity of the Brownian particles and L_z is the spatial period of the ratchet. The results for our ratchet are shown in Figure 6 we can see that this ratchet, as constructed is not very coherent. Lindler *et al.* have achieved Péclet number of the order of $P_e = 20$ with some designs. There is a clear Stochastic resonance peak in the graph of the Péclet numbers.

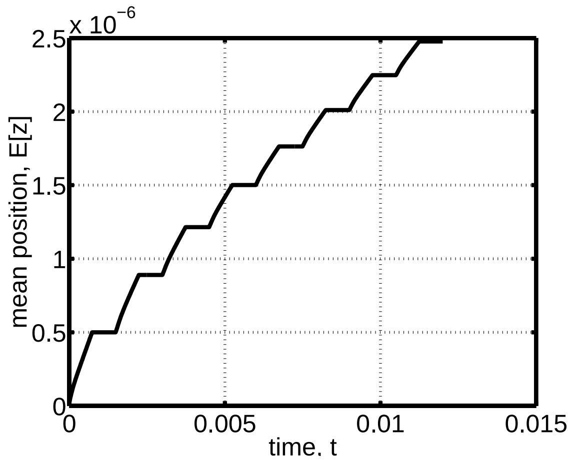

FIGURE 4. Time-evolution of the mean of the distribution $P(z,t)$, called $E[z]$. When the field is asserted, the mean position of the particles moves in a generally "upward" direction. When the field is turned off, the mean remains constant although diffusion causes the field to spread. The total shift in mean position of this ratchet is very modest. Part of the motivation of this work is to optimise the transport effect of the Brownian ratchet, subject to constraints.

CONCLUSIONS AND OPEN QUESTIONS

The conclusions of the present work are: **(***i***)** that Parrondo's games are not just a heuristic model. They can be made quantitative and can be used as a numerical method and **(***ii***)** we confirm that the one dimensional Brownian flashing ratchet exhibits stochastic resonance and **(***iii***)** we can use Parrondo's games as a numerical method which could be used to optimise the performance of a ratchet design.

There are a couple of open questions that naturally arise: **(***i***)** "Does the Fokker-Planck equation unify some types of Stochastic Resonance?" and **(***ii***)** "Do other "Fokker-Planck" systems, such as neural-networks have the same *type* of stochastic resonance as Brownian ratchets?"

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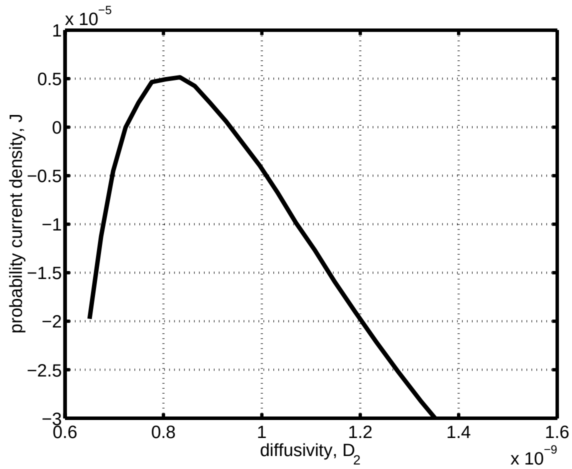

FIGURE 5. Parametric relationship between the Diffusivity, or Fick's law constant, $D = D^{(2)}$ and the probability current density, J. All other parameters are held constant; the feature size of the teeth was 2um, The temporal period of the ratchet was 1.5 ms, the voltage across each 2 μm tooth was 60 mV. This gives electric field strengths in a similar range to those used in commercial gel electrophoresis. The potential across each tooth is easily small enough to avoid electrolysis since the standard reduction potential of Na is much larger in magnitude, $E^0 = -2.71$ V [33]. The temporal duty cycle was held at a symmetrical 50%:50% and the spatial duty cycle was held at an asymmetrical 80%:20%. This breaking of symmetry is necessary to generate current in the ratchet. The only independent variable here is the diffusivity of the particle, D. The ratchet selects preferentially for particles with a certain range of diffusivity.

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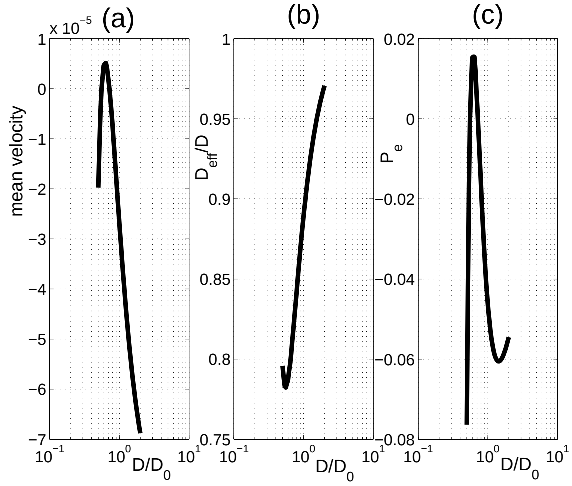

FIGURE 6. In plot (a) we see how the mean drift velocity varies as we vary the diffusion coefficient around a nominal value, $D_0 = 1.3 \times 10^{-9} \mathrm{m}^2\mathrm{s}^{-1}$, in (b) we show the effective diffusion coefficient of the whole device and in (c) we see the normalized drift coefficient or "Péclet" numbers.

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