Brownian ratchets with distributed charge

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ABSTRACT

The rectification of thermal motion can give rise to a steady state flow of particles. This process is believed to occur in nature and to be of central importance for intra-cellular transport. Ajdari and Prost have proposed an "on-off" or "flashing" ratchet and Magnasco has proposed a similar "tilting" or "rocking" ratchet mechanism. These developments led to new and active fields of research in statistical physics and physical chemistry. Recent work by Gillespie and Eisenberg suggests that the effectiveness of the natural transport process, in biological ion channels, depends strongly on how we model the effect of ion to ion interactions. At high local ion concentrations the effect of the crowding of charge is significant. It is necessary to include this effect in the models. If we are interested in average ion currents then we can replace the complicated many-body problem with a time-average mean-field for the distribution of charge.

To date, all analyses of artificial, human-made, ratchets require us to neglect the effect of distributed charge. This means that the analysis is only strictly valid for dilute solutions. The purpose of our present paper is to include the effect of distributed charge in the analysis of artificial Brownian ratchets.

We formulate the Brownian ratchet problem for the case where distributed charge is significant. We investigate methods of solution and find that the finite difference approach is not adequate because the governing equations are very "stiff." We propose an alternative approach based on Fourier series.

Keywords: Brownian ratchet, diffusive transport, distributed charge, Poisson's equation, Fokker-Planck equation

1. DISTRIBUTED CHARGE

If charged particles are free to move then they will naturally migrate to positions of least energy, subject to the fact that they are still in a state of constant thermal agitation called Brownian motion. If the applied fields are varied with time then the system may be operating far from equilibrium. One important aspect of this non-equilibrium behaviour is that it is possible for variations in the applied field to cause transport of charged particles. Devices that make use of this effect are called "Brownian ratchets."^{1,2}

In 1992 Ajdari and Prost^3 proposed the "flashing" ratchet as a possible mechanism for intra cellular transport and in 1993 Magnasco⁴ proposed the "rocking" ratchet mechanism. Several authors^{1, 2, 5, 6} have analysed Brownian ratchets mathematically and the basic mechanism is now well understood. A number of researchers have built and tested physical devices.^{7–12}

The simple analysis assumes that the applied field overwhelms any induced field due to local concentration of charge. This means that the simple analysis only applies to dilute solutions. Some research on ion-channels¹³ suggests that local concentrations of charge are important in cellular processes. We examine the effects of local concentration of charge on man-made or "artificial" Brownian ratchets.

Of course, isolated charge is very difficult to maintain in aqueous solution. Pure water contains positive and negative ions but these are always mixed together very finely, in solution, so they do not produce any net electric field. The plasma in our bodies contains many more charged ions, molecules and other particles. For example, isotonic saline contains about 6.5mg of NaCl per millilitre, which corresponds to about $n_0 = 67 \times 10^{24}$ Na⁺ ions

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302

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per cubic metre and the same concentration of Cl^- ions, which represents over 10×10^6 C of charge per cubic metre. It would be extremely difficult to separate this much charge without expending great energy. However, we can cause local separation of charge by applying strong electric fields. If we could separate even a *tiny* fraction of the ions then it would be possible to induce strong electric fields that could have a significant effect on the operation of Brownian ratchets

Most analyses of Brownian ratchets only consider one species of charged particle and do not consider the contribution to the electric field presented by local concentrations of charge. These are the two issues that we specifically address here.

2. THE GEOMETRY OF A PRACTICAL BROWNIAN RATCHET DEVICE

We consider a Brownian ratchet device with interleaving fingers or "digits" as shown in Figure 1(a). Successful devices of this type have been built and tested by Bader et al..^{11, 12} The fingers in a Brownian ratchet should be

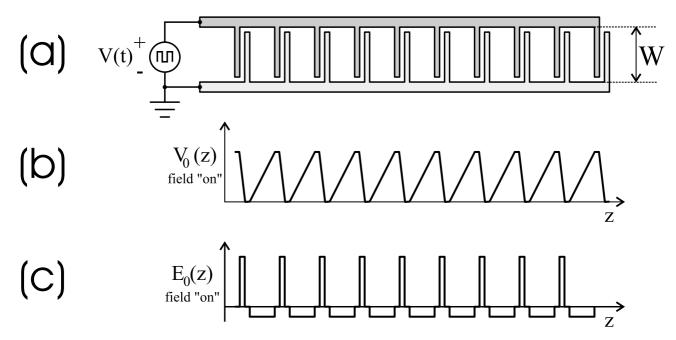


Figure 1. In the top figure (a), we see a schematic diagram of a top view of an inter-digitated Brownian ratchet. The width of the device is W. The fingers or "digits" are connected to power rails. All points connected to the nominally positive rail are shown in dark-grey. All points connected to the nominally negative rail are shown in light grey. These rails are driven by a time varying voltage source, V(t), which is assumed to be powerful in relation to the unpaired charge in the ratchet. The voltage source can be regarded as ideal. In the middle figure (b), we see the applied potential field in the ratchet, $V_0(z,t)$, due to the voltage source, V(t), at a time, t, when the field is fully on. In the bottom figure(c), we see the corresponding applied electric field, $E_0(z)$, due to the applied voltage, $V_0(z,t)$.

distinguished from electrodes since, ideally, they should not make ohmic contact with the channel. They should only influence the mobile charges in the channel through the electric field. In this regard, they are more like the gates in field effect transistors or the plates in thermionic valves.

If there were no free charges in the channel of the ratchet then we could apply Laplace's equation, $\nabla^2 V_0 = 0$, and obtain a simple result for the electric field, $\mathbf{E_0} = -\nabla V_0(z) = \text{constant}$. The voltage profile is piecewise linear and the electric field is piecewise constant, as shown in Figure 1 (b) and (c).

Strictly speaking, moving charges do generate magnetic fields and we should ask whether the magnetic field stores significant energy and whether gradients in this stored magnetic energy could produce forces, which would significantly affect the current of the Brownian particles in the ratchet. We argue that the individual particles in

the ratchet have random velocities and that these do not contribute to any macroscopically detectable magnetic field. The expected value of the sum is always zero, even when separation of charge has occurred.

The longitudinal current of particles in the channel, due to the ratchet action, would appear as an electric current, which would produce a magnetic field but this field would always be orthogonal to the drift velocity so the resulting Lorentz force $d\mathbf{F} = Id\mathbf{l} \times \mathbf{B}$ would be radially inwards to the channel. This radial movement would not affect the longitudinal flow of Brownian particles. In summary; the magnetic field should not affect the current and we believe that we are justified in using the quasi-electrostatic laws, Laplace's equation and Poisson's equation, to calculate the electric potential, given the volume charge density.

The device constructed by Bader et al.¹¹ had a single layer of fingers. It is important to prevent unwanted diffusion in the vertical direction. The channel of the Brownian ratchet was contained from above by a cover slip * and the tagged molecules in the channel were observed using a microscope. This would be the ideal situation if we wished to observe the progress of molecules through the ratchet. On the other hand, if the feature size of the fingers is small then the electric field near the close electrodes will only penetrate a small distance into the channel and if the channel were too high then there would be no ratchet action in most of the channel. This would affect the efficiency of the device. If we were to make the channel too narrow then the current would be reduced, because the ratchet would have fewer molecules to act on. It may be desirable to exert the electric field from two sides (top and bottom) and to use two layers of fingers, as shown in Figure 2(a). The geometry could be chosen to make the field almost uniform, as in the magnetic case for Helmholtz coils. The use of two layers of fingers would increase the maximum current that would be available from the ratchet. Ideally one would want to protect the fingers from corrosion and prevent electrolysis by using an overglass or passivating layer, of SiO₂ for example. This is shown schematically in Figure 2. For the device made by Bader et al., ¹¹ the physical

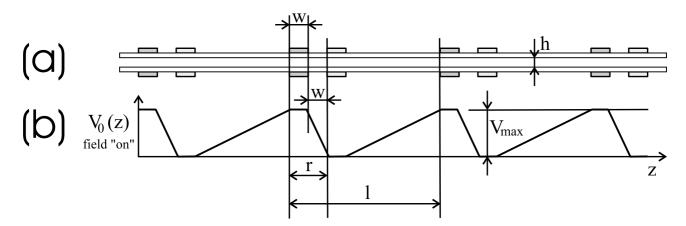


Figure 2. In the top figure (a), we see a schematic diagram of a side view of an inter-digitated Brownian ratchet. We see the fingers or "digits" in section. The colour coding is the same as for Figure 1(a). Ideally, we should place electrodes above and below the channel in which the ratchet action occurs. The fingers should be protected from the contents of the channel by a passivating layer, such as SiO_2 , to prevent corrosion and electrolysis. The entire structure could be built up using a planar VLSI process. In the bottom figure (b), we see the applied potential $V_0(z,t)$ at a time, t, when the field is fully on.

dimensions were $w=2~\mu\mathrm{m}$, $r=4~\mu\mathrm{m}$ and $l=20~\mu\mathrm{m}$. The height of the channel was $h=10~\mu\mathrm{m}$ and there was no upper row of fingers. The width of the device in Figure 1(a) is denoted by W. The maximum voltage applied to the ratchet was $V_{\mathrm{max}}=1.6~\mathrm{V}$. There was no passivating layer although inert electrodes of Pt were used and V_{max} was small enough to avoid electrolysis.

When voltage is applied to the fingers of the ratchet, electric fields will be generated and charged Brownian particles will move inside the channel of the ratchet. This is shown in Figure 3(a). The density of charged particles in the channel may be very large. For example, isotonic saline contains about $n_0 = 67 \times 10^{24}$ positive

^{*}A very thin slide of glass; used in microscopy to cover a preparation.

and negative charged ions per cubic metre. It is clearly not possible to show this many charges on the diagram. A small number of "little balls" have been shown to roughly illustrate the situation. Hydrated ions are surrounded by a little "ball" of polarised water molecules but they are actually extremely small in size. The diameters of the "balls" have been greatly exaggerated in order to make the illustration possible. The aggregate macroscopic effect of changes in concentration of these many billions of microscopic charges can accurately be modelled as a continuous charge-density function as shown in Figure 3(b). We can think of $\rho_v(z)$ as the intermediate-timeaverage mean-field for the distribution of charge. The units will be charge per unit volume and the total area under the curve must sum to zero for an un-charged ratchet.

We want to examine locally separated charge, which will induce changes in the electric field.

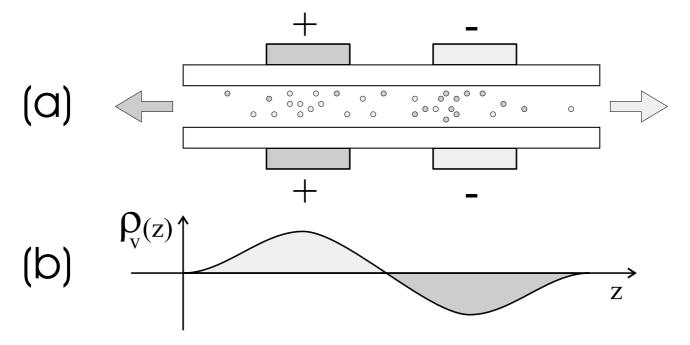


Figure 3. In the top figure (a), we see a greatly magnified schematic diagram of a side view of the channel and two pairs of fingers, which we see in section. The colour coding is the same as for Figure 1(a) and applies to the fingers and to the Brownian particles in the channel. These are greatly magnified since they cannot be shown at the natural scale or in sufficient numbers on a simple diagram. The negative particles accumulate preferentially near the positive fingers. The positive particles accumulate preferentially near the negative fingers. When the field is modulated, in time, there will be net current of negative particles to the right and positive particles to the left; this flow is the important "ratchet" action of the Brownian ratchet. The crowding of many numerous tiny particles give rise to an un-compensated volume charge density, ρ_v which is shown in the bottom figure (b). This distributed, and separated charge gives rise to and induced electric field which, at least in part, opposes the applied field.

3. APPLIED AND INDUCED ELECTRIC FIELDS

We assume that the particle densities of each species of Brownian particle are specified at an initial time, $t = T_0$. In the simple case of saline, NaCl, we would need two functions, $n_1(z,t)$ for the positive, Na⁺ ions, and $n_2(z,t)$ for the negative, Cl⁻ ions. The total charge density would then be $\rho_v(z,t) = +q_e \cdot n_1(z,t) - q_e \cdot n_2(z,t) = q_e (n_1 - n_2)$ where q_e is the electronic charge, $q_e \approx 1.602 \times 10^{-19}$ C. We can then apply Poisson's equation, ^{14–16} to determine the relationship between the particle densities and the induced potential:

$$\nabla^2 V_i = -\frac{\rho_v}{\epsilon} \tag{1}$$

$$\nabla^{2}V_{i} = -\frac{\rho_{v}}{\epsilon}$$

$$\nabla^{2}(V_{1} + V_{2}) = -\frac{q_{e}}{\epsilon} \cdot (n_{1} - n_{2})$$
(1)

where $V_i = V_1 + V_2$ is the induced potential due to charge crowding and ϵ is the electric permittivity of the solvent. For a vacuum the permittivity is defined as $\epsilon_0 = 1/(c^2\mu_0) \approx 8.854 \times 10^{-12} \text{ Fm}^{-1}$ and for other media it is defined in relative terms, $\epsilon = \epsilon_r \cdot \epsilon_0$. Water is composed of polarised molecules and the majority of the permittivity at frequencies below 1 GHz is due to orientation of these polarised molecules. The empirical value of ϵ_r for water at 20°C is $\epsilon_r \approx 80.37$; see Atkins¹⁷ for example. This value is sensitive to changes in temperature but does not vary much in relation to frequency^{18, 19} as long as the frequency is well below the value represented by the characteristic relaxation time, τ . We require $f \ll 1/(2\pi\tau) \approx 1 \text{ GHz}$, which is the case for signals of interest in Brownian ratchets.

We can divide V_i into positive and negative components, $V_i = V_1 + V_2$ and for linear dielectric materials we get: $\nabla^2 V_1 = -(q_e/\epsilon) \cdot n_1(z,t)$ and $\nabla^2 V_2 = +(q_e/\epsilon) \cdot n_2(z,t)$ and the total field experienced by the Brownian particles will be: $V_t = V_0 + V_1 + V_2$, which is the sum of the applied voltage, the induced voltage due to positive charge and the induced voltage due to negative charge. The total electric field will be

$$\mathbf{E_t} = -\nabla V_t = -\nabla (V_0 + V_1 + V_2) = -\nabla V_0 - \nabla (V_1 + V_2) = -\nabla V_0 - \nabla V_i . \tag{3}$$

4. PARTICLE CURRENT DENSITIES

Hydrated Ions and other Brownian particles are usually modelled as small spheres in a viscous fluid.¹⁷ Stokes' formula $F = 6\pi\eta r$ is assumed to apply and the result of this line of argument is that the drift velocities, α , should be proportional to the strength of the applied field, $\alpha = u\mathbf{E_t}$, where u is the mobility of the particle and and $\mathbf{E_t}$ is the total electric field.

If we have two species of Brownian particle, hydrated sodium and chloride ions, for example, then we would have two distinct particle mobilities, u_1 and u_2 and we would get two different expected values for the drift velocities of the different species:

$$\alpha_{\mathbf{1}} = +u_{1} \cdot \mathbf{E_{t}} \tag{4}$$

$$\alpha_2 = -u_2 \cdot \mathbf{E_t}. \tag{5}$$

The numerical values may be found in the literature.¹⁷ For the case of hydrated sodium ions we have $u_1 = 51.9 \times 10^{-9} \text{ m}^2 \text{s}^{-1} \text{V}^{-1}$ and for hydrated chloride ions we have $u_2 = 79.1 \times 10^{-9} \text{ m}^2 \text{s}^{-1} \text{V}^{-1}$. It also follows that the particle current density, **J**, will be linearly dependent on $\mathbf{E_t}$. We obtain

$$\mathbf{J} = -\nabla \left(D \cdot n\right) + \left(\alpha \cdot n\right),\tag{6}$$

which is a form of Fick's law.²⁰ The drift velocities are also known as the infinitesimal first moments and may be estimated in terms of the applied field: $\alpha(z,t) = u\mathbf{E_t} = u(-\nabla V(z,t))$. If we combine this with the law of continuity, $\nabla J + \frac{\partial p}{\partial t} = 0$, then we obtain the relevant form of the Fokker-Planck Equation:

$$\nabla^{2} (D \cdot n) - \nabla (\alpha \cdot n) - \frac{\partial n}{\partial t} = 0, \tag{7}$$

which describes the way in which the particle densities evolve over time. In general, there will be one Fokker-Planck equation for each species of Brownian particle, so we get

$$\nabla^{2} (D_{1} \cdot n_{1}) - \nabla (\alpha_{1} \cdot n_{1}) - \frac{\partial n_{1}}{\partial t} = 0$$
(8)

and

$$\nabla^{2} (D_{2} \cdot n_{2}) - \nabla (\alpha_{2} \cdot n_{2}) - \frac{\partial n_{2}}{\partial t} = 0$$

$$\tag{9}$$

where two mean drift velocities are given by: $\alpha_{\mathbf{1}}(\mathbf{z}, \mathbf{t}) = +u_1 \cdot \mathbf{E}_{\mathbf{t}}(\mathbf{z}, \mathbf{t}) = -u_1 \nabla V_t(z, t)$ and $\alpha_{\mathbf{2}}(\mathbf{z}, \mathbf{t}) = -u_2 \cdot \mathbf{E}_{\mathbf{t}}(\mathbf{z}, \mathbf{t}) = +u_2 \nabla V_t(z, t)$. Note that all different species of particle respond to the same field. The difference in sign is due to the different charges of the Brownian particles.

The two different infinitesimal second moments are effectively constant and are denoted by D_1 and D_2 . They represent the diffusivities of the two different species of Brownian particles. The numerical values may be found in the literature.¹⁷ For the case of hydrated sodium ions we have $D_1 = 1.33 \times 10^{-9} \text{ m}^2 \text{s}^{-1}$ and for hydrated chloride ions we have $D_2 = 2.03 \times 10^{-9} \text{ m}^2 \text{s}^{-1}$.

5. EVOLUTION OF THE RATCHET IN TIME

The analytic solution of Equations 8 and 9 is difficult. We propose that a numerical method should be used. The overall process would be as follows:

- Given the two particle density functions: $n_1(z,t)$ and $n_2(z,t)$ at time t=T,
- calculate the three components of the potential $V_t(z,t) = V_0(z,t) + V_1(z,t) + V_2(z,t)$,
- calculate the one electric field $\mathbf{E_t}(\mathbf{z}, \mathbf{t}) = -\nabla V_t(z, t)$,
- calculate the two infinitesimal moments, $\alpha_1(\mathbf{z}, \mathbf{t}) = +u_1 \cdot \mathbf{E_t}(\mathbf{z}, \mathbf{t})$ and $\alpha_2(\mathbf{z}, \mathbf{t}) = -u_2 \cdot \mathbf{E_t}(\mathbf{z}, \mathbf{t})$, and finally,
- numerically integrate the two Fokker-Planck equations over a time step of ΔT to obtain $n_1(z, t + \Delta T)$ and $n_2(z, t + \Delta T)$ at time $t = T + \Delta T$ for all values of z under consideration.

The process may be repeated many times, to obtain the solution for large intervals of time.

6. THE ONE DIMENSIONAL CASE

The device shown in Figure 1 is intended to have great symmetry in the two lateral directions, at right angles to the ion current. We make the approximation that fields and particle densities to not vary significantly in these directions. This allows us to greatly simplify the Fokker Planck equations to obtain:

$$D_{1} \cdot \frac{\partial^{2}}{\partial z^{2}} n_{1}(z, t) - \frac{\partial}{\partial z} \left(\alpha_{1}(z, t) \cdot n_{1}(z, t) \right) - \frac{\partial}{\partial t} n_{1}(z, t) = 0$$

$$(10)$$

and

$$D_{2} \cdot \frac{\partial^{2}}{\partial z^{2}} n_{2}(z,t) - \frac{\partial}{\partial z} \left(\alpha_{2}(z,t) \cdot n_{2}(z,t) \right) - \frac{\partial}{\partial t} n_{2}(z,t) = 0. \tag{11}$$

7. APPROPRIATE CHOICE OF SCALE

The average number of charges per unit volume, n_0 , is so enormous that very small perturbations in the particle densities, n_1 and n_2 can produce very large field strengths. We propose a change of variable to account for this. We define new variables ν_1 and ν_2 :

$$n_1(z,t) = n_0 \cdot (1 + \nu_1(z,t))$$
 (12)

$$n_2(z,t) = n_0 \cdot (1 + \nu_2(z,t)) \tag{13}$$

where n_0 is the mean number of ions per unit volume. We can substitute these new variables into Equations 2 and 3 to obtain an equation for the total electric field:

$$\mathbf{E_{t}} = -\frac{\partial V_{0}}{\partial z} + \left(\frac{n_{0} \ q_{e}}{\epsilon}\right) \cdot \int_{-\infty}^{+z} \nu_{1}\left(\zeta, t\right) - \nu_{2}\left(\zeta, t\right) \ d\zeta. \tag{14}$$

We expect the applied fields to be of the order $\frac{\partial V_0}{\partial z} \approx \frac{V_{\rm max}}{w} \approx 800 \times 10^3 \ {\rm Vm}^{-1}$. In contrast, we have $(n_0 \ q_e/\epsilon) \approx 15 \times 10^{15} \ {\rm Vm}^{-2}$ and if we integrate over a distance equal to the feature size, w, then we expect $\nu_1 - \nu_2 \approx 27 \times 10^{-6}$ which is a very small dimensionless ratio. This supports our original intuition that only small perturbations in n_1 and n_2 will be required.

If we substitute the change of scale in Equations 12 and 13 into Equations 10 and 11 then we obtain new forms of the Fokker-Planck equations, in the new variables ν_1 and ν_2 :

$$D_1 \cdot \frac{\partial^2 \nu_1}{\partial z^2} - \frac{\partial \alpha_1}{\partial z} \cdot (1 + \nu_1) - \alpha_1 \cdot \frac{\partial \nu_1}{\partial z} - \frac{\partial \nu_1}{\partial t} = 0$$
 (15)

and

$$D_2 \cdot \frac{\partial^2 \nu_2}{\partial z^2} - \frac{\partial \alpha_2}{\partial z} \cdot (1 + \nu_2) - \alpha_2 \cdot \frac{\partial \nu_2}{\partial z} - \frac{\partial \nu_2}{\partial t} = 0.$$
 (16)

It should be understood that ν_1 and α_1 are really functions of z and t and are shorthand for the more formal notation, $\nu_1(z,t)$ and $\alpha_1(z,t)$. The same applies to ν_2 and α_2 .

We have to solve the initial value problem for ν_1 and ν_2 , which means that we need to evaluate α_1 and α_2 using Equations 4, 5 and 14. We can rearrange these equations to obtain a simple and direct expressions for $\partial \alpha_1/\partial z$ and $\partial \alpha_2/\partial z$:

$$\frac{\partial \alpha_1}{\partial z} = +u_1 \cdot \left(\frac{n_0 q_e}{\epsilon}\right) \cdot \left(\nu_1(z, t) - \nu_2(z, t)\right) \tag{17}$$

$$\frac{\partial \alpha_{1}}{\partial z} = +u_{1} \cdot \left(\frac{n_{0}q_{e}}{\epsilon}\right) \cdot \left(\nu_{1}(z,t) - \nu_{2}(z,t)\right)$$

$$\frac{\partial \alpha_{2}}{\partial z} = -u_{2} \cdot \left(\frac{n_{0}q_{e}}{\epsilon}\right) \cdot \left(\nu_{1}(z,t) - \nu_{2}(z,t)\right).$$
(18)

Equations 15 and 16 need to be solved numerically together with the auxiliary conditions implied by Equations 4, 5, 14, 17 and 18.

8. THE PERIODIC CASE

The device shown in Figure 1 is periodic in the z dimension. If the ratchet reaches a steady state of operation then it is possible to simulate the entire ratchet by simply simulating all the activity within a single spatial period, L, of the device. The boundary conditions are periodic and all fields will be periodic and will derive from periodic potentials. This means that Equation 14 should be modified to take the boundary conditions into account. We have

$$\mathbf{E_{t}} = -\frac{\partial V_{0}}{\partial z} + \left(\frac{n_{0} \ q_{e}}{\epsilon}\right) \cdot \int_{-\frac{L}{\kappa}}^{+\frac{L}{2}} \nu_{1}\left(\zeta, t\right) - \nu_{2}\left(\zeta, t\right) \ d\zeta. \tag{19}$$

The choice of origin for the z axis is still arbitrary. The fact that all potentials are periodic implies that the periodic integral of all E fields must be zero:

$$\int_{-\frac{L}{2}}^{+\frac{L}{2}} E dz = -\int_{-\frac{L}{2}}^{+\frac{L}{2}} \frac{\partial V}{\partial z} dz = [V] - \int_{-\frac{L}{2}}^{+\frac{L}{2}} = 0.$$
 (20)

The law of continuity imposes the same normalisation condition on the peiodic particle density perturbation functions ν_1 and ν_2 :

$$\int_{-\frac{L}{2}}^{+\frac{L}{2}} \nu_1(z,t) dz = 0$$
 (21)

$$\int_{-\frac{L}{z}}^{+\frac{L}{2}} \nu_2(z,t) dz = 0.$$
 (22)

9. TWO APPROACHES TO THE SIMULATIONS

We have previously described finite difference methods for reducing these continuous Partial Differential Equations to sets of Partial Difference Equations, which could possibly be directly evaluated numerically.²¹ result from a typical finite-difference simulation is shown in Figure 4.

This was a simulation of a Brownian ratchet with very modest external applied fields and no crowding of charge.

We attempted to employ the finite difference method to numerically integrate the PDEs in Equations 15 and 16. We found that this method is intractably numerically unstable because of the very large range of scales involved. The PDEs are effectively very "stiff" equations and there are inherent stability problems in the näive finite difference approach to Equations 15 and 16. The typical numerical behaviour is shown in Figure 5.

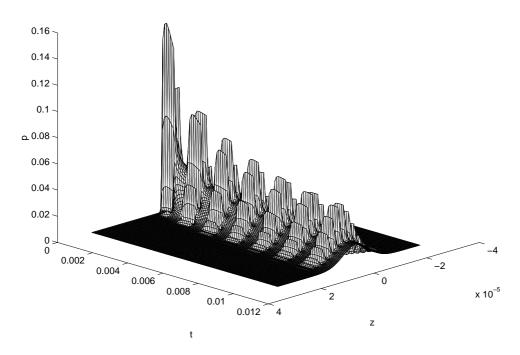


Figure 4. .

The behaviour prior to t = 0.05 demonstrates way in which very small numerical artifacts, such as round-off, can be magnified by the huge numbers involved, such as Avogadro's number. The output from the algorithm is obviously quite un-physical. This defect could not be removed by simply using ever larger mumbers of mesh points or simple re-scaling. It is a fundamental limit of the approach.

The applied field E_0 was turned off after t = 0.05 and all the quantities involved were then of the same order of magnitude. The simulation in this region produced much more plausible results, comparable with Figure 4.

Somewhat chastened by the experience of Figure 5 we are forced to propose an alternative numerical method to integrate Equations 15 and 16, together with all the auxiliary conditions. We believe that a good approach would be to use an alternative representation for the functions ν_1 and ν_2 . The natural basis functions would seem to be sines, cosines or complex exponential functions:

$$\nu\left(z,t\right) = \sum_{n=1}^{\infty} C_n e^{j\beta z} \tag{23}$$

where C_n are the complex Fourier coefficients of ν , β is the spatial wave-number, $\beta=2\pi/L$ and L is the spatial period or "wavelength" of the ratchet. Equation 23 can be integrated and differentiated directly and the results can be substituted into Equations 15 and 16. It should be noted that the complex coefficients are still functions of time, $C_n=C_n(t)$ which means that Equation 23 effectively transforms Equations 15 and 16 into coupled systems of Ordinary Differential Equations in the coefficients $C_n(t)$.

The Fourier approach would also automatically take care of the periodic boundary conditions and the normalisation constraints, Equation 20 and 22.

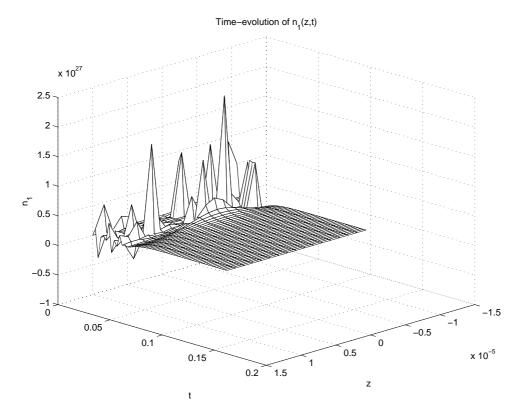


Figure 5. .

10. OPEN QUESTIONS

The key objective is clearly to identify how the crowding and separation of distributed charge can affect the performance of a ratchet device. On the road to this goal, we need to resolve a number of numerical issues. It is our opinion that the finite difference approach is not appropriate to the situation. It cannot handle very "stiff" systems of equations and has fundamental problems with stability.

We propose an alternative Fourier representation which should transform the Partial Differential Equations 15 and 16 into systems of ordinary differential equations in the Fourier coefficients. The key open question here is whether this representation can handle the radical contrasts of scale involved.

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