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A MEMS Brownian ratchet

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Abstract

A Brownian ratchet is a device that can rectify the random Brownian motion of particles to yield a directed steady-state flow. We can imagine a thermofluid field of particles, which interact with the ratchet. The laws of thermodynamics imply that the ratchet must use energy from some other source.

The dynamics of continuous-time Brownian ratchets are determined by a stochastic partial differential equation. We have used a simplified discrete-time model of a Brownian ratchet called 'Parrondo's games', which are governed by a difference equation. In their original form, Parrondo's games are a finite set of simple games of chance. An indefinite pure sequence of any single game is neutral or even losing. A periodic or randomised sequence of mixed games can be winning. There is a steady state flow of probability in the preferred direction.

We have been able to design a feasible and consistent device, by mapping the conservation law of total probability onto the law of conservation of charge. This device can absorb energy from a mechanical field to produce a directed flow of charge. The fundamental architecture is based on a 'bucket-brigade' device. The capacitors are 2-port MEMS devices. We use CMOS transmission gates to connect the capacitors in the required topology.

We present an analysis and simulation of the MEMS Brownian ratchet and suggest some possible applications.

Keywords: Brownian ratchet; MEMS; Re-parameterisation

1. Brownian ratchets

Brownian motion was first observed by the Scottish botanist, Robert Brown, in the summer of 1827, following his voyage to Australia in 1822. He noticed that grains of pollen were subject to perpetual random agitated movements when they were suspended in water. A typical sample path is shown in Fig. 1. The phenomenon was studied experimentally for the remainder of the 19th century and was not completely understood until the work of Marian Smoluchowski and Albert Einstein [1].

In 1871, James Clerk Maxwell published a thought experiment [2] involving 'a being whose faculties are so sharpened that he can follow every molecule in its course.' A slightly fanciful illustration of a Maxwell's demon is shown in Fig. 2. The Demon may appear to be hard at work but, given access to suitable energy storage elements, his net mechanical effort is zero. Maxwell came to the shocking conclusion that such a being, now known as a 'Maxwell's demon,' might harness the microscopic movements of molecules to perform useful macroscopic work in a way that would violate the second law of Thermodynamics. Later works by Szilard, Brillouin, Landauer and Bennett have shown that the decisions made by the 'demon' supply information (or 'negative-entropy') to the system and that this information cannot be supplied without continually resetting the mental state of the demon. This entails an energy cost. Maxwell's demon is therefore really a heat engine. It is an unusual and exotic heat engine but it does not violate the second law.

In 1912 Marian Smoluchowski [3] examined a similar thought experiment where the molecules interacted with the machinery through a paddle wheel and the selective role of the demon was taken by ratchet and pawl mechanism. A schematic diagram of the ratchet and pawl is shown in Fig. 3. Smoluchowski's ratchet appeared to harness the random Brownian motion of the paddle wheel in order to perform useful macroscopic work. Marian Smoluchowski, and later Richard Feynman [4], concluded that such a machine would work but that it would require a constant input of energy in order to prevent the pawl from reaching thermodynamic equilibrium with its surroundings. Smoluchowski's ratchet is also seen to be an unusual heat engine, which does not violate the second law. A machine based on these principles is called a Brownian ratchet.

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Fig. 1. A sample path of a Brownian motion.

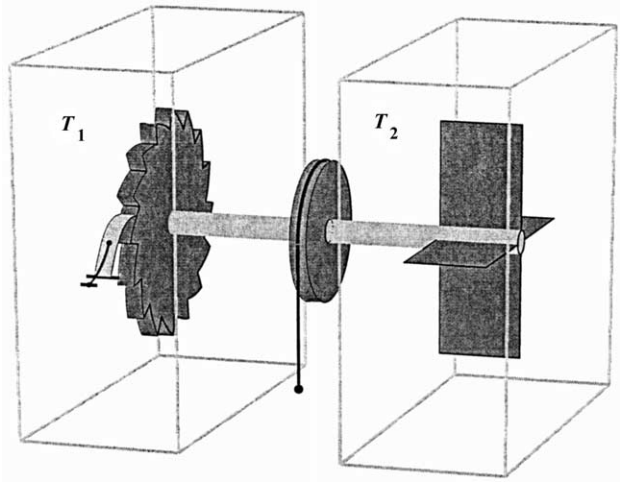

Fig. 3. The ratchet and pawl machine.

There is quite an extensive literature on Brownian ratchets [5–13] and it is still a subject of active research. The contemporary model for a Brownian ratchet does not have the same physical appearance as the rotary 'ratchet and pawl' machine of Smoluchowski. A more modern paradigm is that of a 'flashing ratchet' where an asymmetrical field is 'flashed' on and off [9]. This is illustrated in Fig. 4(a)–(c).

In part (a), we see the asymmetrical form of a potential field. Potential is considered to be energy per unit material in the working substance. This could be Voltage (electrical potential) or it could be any potential associated with a conservative field. This potential is cycled 'on' and 'off' periodically. We imagine particles in the ratchet moving in response to the field and to gradients of particle concentration (or probability density).

In part (b), we see the steady-state distribution of particles in the field. They are confined most strongly to the regions of least potential, such as points near reference plane 'y'. We assume that the potential is strong enough to prevent significant barrier penetration through planes 'x' and 'z'. The entire distribution of particles is divided into a number of sub-distributions.

In part (c), we see the effect of removing the field. The non-steady-sate, non-equilibrium diffusion of particles causes the sub-distribution at 'y' to spread out. The concentration of particles at reference plane 'y' is reduced and there are fluxes of particles, Φ_1 and Φ_2, passing through reference planes 'z' and 'x' respectively. The forward flux, Φ_1, is larger than the reverse flux, Φ_2, because most of the particles were initially located closer to reference plane 'z' than to reference plane 'x' so $\Phi_1 > \Phi_2$.

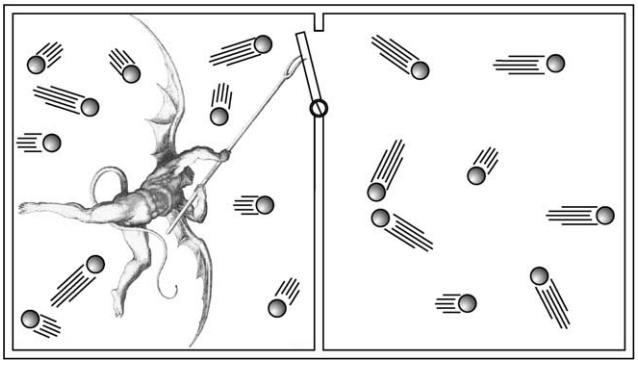

Fig. 2. Maxwell's demon 'hard at work'.

The effect over the entire ratchet is a superposition of the effects from each of the local sub-distributions. The precise rule for this combination is determined by a stochastic partial differential equation called the Fokker-Planck equation [14–16]:

$$\frac{\partial p}{\partial t} = -\frac{\partial(\alpha p)}{\partial y} + \frac{1}{2}\frac{\partial^2(\beta p)}{\partial y^2} \tag{1}$$

where $p(y, t/x, t)$ is the transition probability density, $\alpha(x, t)$ is the infinitesimal first moment and $\beta(x, t)$ is the infinitesimal second moment. Eq. (1) is also known as the Kolmogorov equation or the 'master' equation. The functions $\alpha(x, t)$ and $\beta(x, t)$ are related to the potential function and to the laws of diffusion, such as Fick's law. The result of this ratchet process is that there is a net flow of particles to the right. This flow is paid for by the energy cost of asserting the field after diffusion has occurred.

When the field is re-asserted, particles that have crossed reference plane 'z' are now pushed to the right and form part of the next sub-distribution. Particles that have crossed reference plane 'x' are pushed to the left and form part of the previous sub-distribution. The ratchet then settles down again towards the steady-state distribution shown in part (b).

Given the technical complexity of the Fokker–Planck equation, it is expedient to use a simplified model that captures the essential features of the original complex system. We can aggregate the probability densities of the various sub-distributions into single point probabilities, $V_{t,k}$, and we can aggregate the various fluxes between these sub-distributions into transition probabilities, $A_{i,j}$. We can

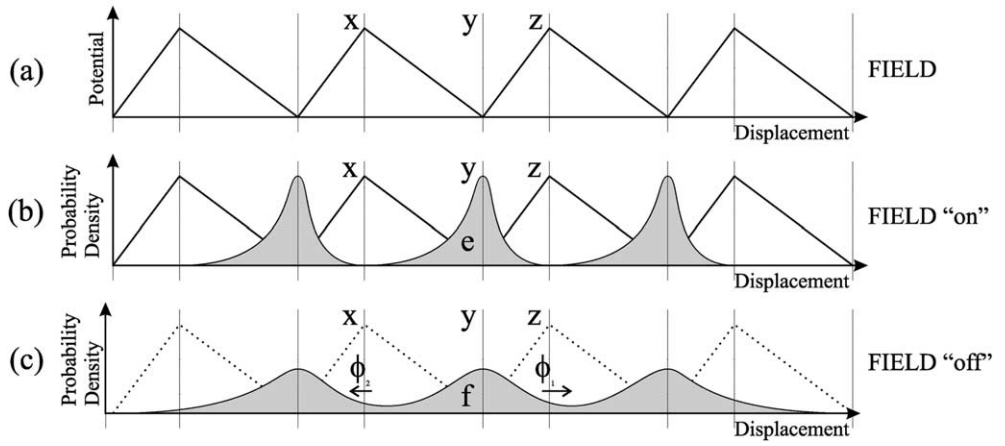

Fig. 4. A flashing ratchet.

aggregate each of the phases (b) and (c) in Fig. 4 into single time 'ticks' of a discrete time system. The earliest known model of this type was proposed by Juan Parrondo [17].

2. Parrondo's discrete time ratchet

Discrete models contain just a few variables which can be easily optimised. A discrete model can be converted into a design for a 'cell'. Large numbers of identical cells could then be assembled to create an entire machine.

Parrondo's games are a simplified discrete-time model of a flashing ratchet [17–20]. They are formulated as a set of state-dependent games of chance. We could think of them as a generalised version of the Bernoulli trials where the coins are possibly biased and the coin that will be tossed next is determined by the present amount of capital, k. The process for these games can be represented by a decision tree which is shown in Fig. 5. The results of these decisions, and the subsequent trials, affect the state of the player, k.

It is possible to define similar discrete-time games with various spatial periods, other than three. If we use a periodic potential of the type shown in Fig. 4 then the pattern of rewards must be a function of the state, k. Given this constraint, the smallest period that allows us to generate the required transport effect is a period of three.

Parrondo's "game A" is intended to model pure diffusion:

$$\frac{\partial p}{\partial t} = \left(\frac{1}{2}\right)\beta\frac{\partial^2 p}{\partial y^2}. \tag{2}$$

We can use the symbol D to denote the Fick's law constant $D = 1/2\beta$ and replace the continuous probability variable p with a discrete probability V. There are many possible finite-element models for a diffusion operator. Lapidus [21] describes how some of these can be derived. If we locally approximate the solution the PDE with a finite-order Taylor polynomial then we can estimate the partial derivatives in terms of the function values at the sample points. This converts a partial differential equation into a partial difference equation. The simplest explicit formula involves the use of three sample points:

$$V(k,t) = \rho V(k-1,t-1) + (1-2\rho)V(k,t-1) + \rho V(k+1,t-1) \tag{3}$$

where $\rho = D\tau/\lambda^2$, D is the Fick's law constant, τ is the sampling time and λ is the sampling distance. Courant et al. [22] have shown that this method converges to the true solution in the limit as the mesh size becomes very small provided $0 < \rho \leq 1/2$. At one extreme, $\rho \rightarrow 0$, is an operator where nearly all particles remain in the same well. This

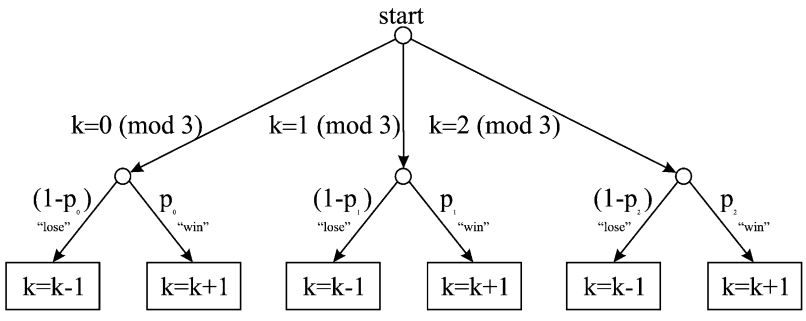

Fig. 5. Structure of a single trial of a Parrondo's game.

is very accurate but computationally intensive. The operator used in Parrondo's game A is at the other extreme, $\rho = 1/2$. Every particle moves to a new state. This operator is known in the finite difference literature as the Schmidt formula:

$$V(k,t) = (1/2)V(k-1,t-1) + (1/2)V(k+1,t-1). \quad (4)$$

This operator is not ideal for simulation of diffusion because, in the short term, it entails less increase in entropy per unit of real-time than the other operators. This is not really consistent with the second law of thermodynamics. In the longer term, the variance of the whole distribution of $V(k,t)$, for fixed t is $\sigma^2 = 2\rho\lambda^2 = 2Dt$, which is consistent with the analytical solution to the diffusion equation, regardless of the choice of ρ.

The Parrondo process is equivalent to the operation of an indefinitely large non-deterministic state machine. Part of this machine is represented in Fig. 6. In Parrondo's games, the state-variable, the capital, k and the spatial 'displacement' are considered to be equivalent. The asymmetrical potential function is represented indirectly through the state dependent probabilities $[p_0, p_1, p_2]$. Exact information about potential and energy has been lost in the transformation to discrete time. The (Newtonian) law of conservation of matter has been replaced by the law of total probability. The probability functions shown in Fig. 4 are replaced by a time dependent probability vector:

$$\underline{V_t} = [\ldots, V_{t,-2}, V_{t,-1}, V_{t,0}, V_{t,+1}, V_{t,+2}, \ldots] \quad (5)$$

It can be shown that the time evolution of Parrondo's games can be represented as a non-homogeneous Markov chain. We can represent the time evolution of the system using simple algebraic notation. For the effect of one trial of game A, we could write

$$\underline{V_{(t+1)}} = \underline{V_t}[A_{i,j}] \quad (6)$$

For a single play of "Game B", we could also write

$$\underline{V_{(t+1)}} = \underline{V_t}[B_{i,j}] \quad (7)$$

It is understood that games A and B and possibly other games could be included in the sequence. In general, the sequence is mixed, with different games being played at different times. The matrices all have the form:

$$[A_{i,j}] = \begin{bmatrix} \ddots & \ddots & & & & & & & & & \\ \ddots & 0 & a_0 & & & & & & & & \\ & (1-a_1) & 0 & a_1 & & & & & & & \\ & & (1-a_2) & 0 & a_2 & & & & & & \\ & & & (1-a_0) & 0 & a_0 & & & & & \\ & & & & (1-a_1) & 0 & a_1 & & & & \\ & & & & & (1-a_2) & 0 & a_2 & & & \\ & & & & & & (1-a_0) & 0 & a_0 & & \\ & & & & & & & (1-a_1) & 0 & \ddots & \\ & & & & & & & & \ddots & \ddots & \end{bmatrix} \quad (8)$$

All of the elements which are not explicitly represented are zero. The variation along the diagonals has a period of 3. Parrondo's original specification for the games was

$$\text{Game A}: \ [a_0, a_1, a_2] = \left[\frac{99}{200}, \frac{99}{200}, \frac{99}{200}\right]$$

$$\text{Game B}'': \ [b_0, b_1, b_2] = \left[\frac{19}{200}, \frac{149}{200}, \frac{149}{200}\right]$$

Game A corresponds approximately to the process in Fig. 4(c) and game B corresponds approximately to the process in Fig. 4(b).

The natural way to measure flow within Parrondo's games is to estimate asymptotic rates of increase in the expected value of the capital, k as a function of time. Simulations of Parrondo's original games yield a rate of return $Y \approx +0.0166$. That is, for every dollar that we invest we expect to make a long term profit of \$0.0166 per time tick. The rate of flow is modest but positive, in contrast to the pure sequences, which are negative.

The fact that Parrondo's games use discrete-time means that they could be implemented within a clocked architecture using silicon, as long as we could find a rigorous way to re-parameterise the equations.

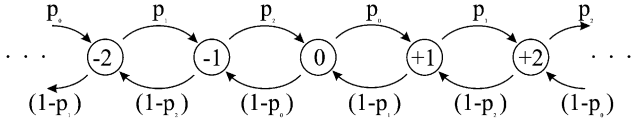

Fig. 6. State transitions of a Parrondo's game.

3. Asymptotic rate of transport from Parrondo's ratchet

If we were designing a ratchet, or a set of games, then we might have some free choice of the conditional probabilities,

$[a_0, a_1, a_2]$ and $[b_0, b_1, b_2]$, and we would need to know how the rate of return, Y, depended on these conditional probabilities. It is possible to apply the theory of Markov chains with rewards [23] to this problem and it can be shown that

$$Y = Y_0\left(\frac{1-\Gamma}{1+\Gamma}\right) \tag{9}$$

where $Y_0 = 3$ and Γ is given by

$$\Gamma = \frac{1 + ((1-a_0)(1-a_1)(1-a_2))}{1 + (a_0 a_1 a_2)} \tag{10}$$

Eq. (9) only strictly applies to a homogeneous sequence of games A but these formulae can be applied to the more general mixed case by applying the formulae in the appropriate sequence. There must be a rule to specify the sequence of games, {A, B, B, A, B,…}, and this must be taken into account when calculating the asymptotic rate of return.

4. Optimum form of the ratchet

Simulations reveal that periodic sequences yield the greatest return. Further investigation by the authors, using genetic algorithms, reveal that the most effective form of the games is a set of three games that are played in a strict periodic sequence $\{G_0, G_1, G_2, G_0, G_1, G_2,\ldots\}$. The transition probabilities are as follows:

Game G_0 : $[\mu, (1-\mu), (1-\mu)]$

Game G_1 : $[(1-\mu), \mu, (1-\mu)]$

Game G_2 : $[(1-\mu), (1-\mu), \mu]$

where μ is a very small probability, $0 < \mu < 1$. We can think of μ as being a very small, ideally 'microscopic', positive number. The games are most effective as $\mu \to 0$ where the return is $Y \to 1$. Each game has two conditional probabilities that are close to 1.0 and are almost certainly winning. Each game has one conditional probability that is close to 0.0 and is almost certainly losing. The losing part of the game represents a barrier. The reason for including the parameter, $\mu \neq 0$, is that the ideal case, $\mu = 0$, is not feasible in practice. We must be content with an approximation. The rate of return form any pure sequence of these games is approximately

$$Y \approx (1/2)\mu \tag{11}$$

which is very close to zero and yet the return from the cyclic combination of these games is approximately

$$Y \approx 1 - 3\mu \tag{12}$$

which is very close to a certain win. We can engineer a situation where we achieve an almost certain win every time out of games that, on their own, deliver almost no benefit at all. These games work better as a team than on their own.

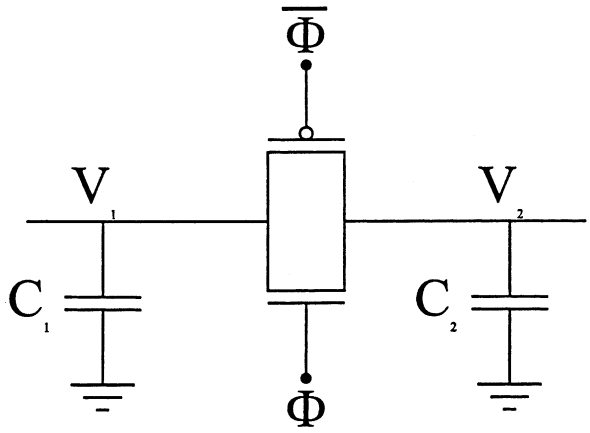

Fig. 7. A transmission gate structure with charge sharing.

5. Re-parameterisation of equations for the ratchet

If we examine Fig. 6 or consider a single row from Eqs. (6) or (7), then we can write

$$V_{(t+1),n} = V_{t,(n-1)p_t,((n-1)(\mathrm{mod}\ 3))} + V_{t,(n+1)p_t,((n+1)(\mathrm{mod}\ 3))} \tag{13}$$

where $p_{t,k}$ are the particular conditional transition probabilities that apply at time $t + 1$. The conserved quantity (probability) at time $t + 1$ is a weighted sum of the neighbouring conserved quantities at an earlier time t. If we wish to map the law of conservation of charge onto the law of total probability, then we need a discrete mechanism for creating weighted sums of charge. One very simple mechanism for achieving this is to use the (normally undesirable) effect of charge sharing [24,25].

5.1. Probabilistic interpretation of charge sharing

In Fig. 7, we see two capacitors separated by a CMOS transmission gate [26] which is driven by complementary clock signals, Φ and $\bar{\Phi}$. Suppose that Φ is initially low and C_1 and C_2 are at initial voltages V_1 and V_2, respectively. The stored charges in C_1 and C_2 are given by

$$Q_1 = C_1 V_1 \Leftrightarrow V_1 = \frac{Q_1}{C_1} \tag{14}$$

and

$$Q_2 = C_2 V_2 \Leftrightarrow V_2 = \frac{Q_2}{C_2} \tag{15}$$

The transmission gate is now closed as Φ goes high. We assume that the time constant of the resulting circuit is small compared with the period of the clock. Both capacitors now move to an equilibrium distribution of charge and a new voltage V_3. Eqs. (14) and (15) together with the conservation of charge now imply that

$$V_3 = \left(\frac{C_1}{C_1 + C_2}\right)V_1 + \left(\frac{C_2}{C_1 + C_2}\right)V_2 \tag{16}$$

The equations for charge sharing now become

$$Q_1' = \left(\frac{C_1}{C_1 + C_2}\right)(Q_1 + Q_2) \tag{17}$$

and

$$Q_2' = \left(\frac{C_2}{C_1 + C_2}\right)(Q_1 + Q_2) \tag{18}$$

where Q_1' and Q_2' are the new amounts of charge stored in the capacitors. This is consistent with conservation of charge and $(Q_1' + Q_2') = (Q_1 + Q_2)$. If we think of the charge as being like an 'electron gas' that occupies the two capacitors then the fractions $\mu = C_2/(C_1 + C_2)$ and $(1 - \mu) = C_1/(C_1 + C_2)$ are the probabilities that any given electron will be found in one or other of the two capacitors. Probability and charge map linearly onto one another. The scaling factor is simply the number of unit electron charges in the system. We know, from Eqs. (11) and (12) that we would like μ to be very close to 0, or possibly to 1, but this is not completely feasible since C_1 and C_2 must be finite positive numbers. The formal expressions for μ are

$$\mu = \left(\frac{Q_2'}{Q_1' + Q_2'}\right) = \left(\frac{C_2}{C_1 + C_2}\right) \tag{19}$$

and

$$1 - \mu = \left(\frac{Q_1'}{Q_1' + Q_2'}\right) = \left(\frac{C_1}{C_1 + C_2}\right) \tag{20}$$

5.2. MEMS variable capacitors

If the capacitors could not vary, then every cycle of this machine would contribute to charge sharing in such a way that all capacitors would tend towards the same potential. This is shown in the simulation in Figs. 10 and 11. This is analogous to Parrondo's games where we toss a completely fair coin, or to unconstrained diffusion. We cannot achieve the ratcheting effect without the ability to vary the conditional probabilities in Eq. (13) or the proportion of charge sharing in Eqs. (17) and (18). This means that we must be able to vary C_1 and C_2 and every other capacitor in the ratchet. This will requite mechanical work that must be provided by an actuator. We propose the use of comb drive actuators [27] as both variable capacitors and actuators. These should be arranged in pairs and be connected mechanically but remain electrically isolated. A schematic diagram of a comb drive actuator is shown in Fig. 8. One actuator can be driven to vary the capacitance of the other. The pair of actuators can be regarded, from a mechatronic point of view, as an electrical 2-port device. This lends itself to analysis using the method of bond-graphs [28]. We can think of a pair of 'back to back' comb drives as an energy-storing transducers.

If we allow C_1 and C_2 to vary then we can think of the ratio of change of μ, i.e. μ_{t2}/μ_{t1}, as being like a compression ratio in mechanics. It is very difficult to make this large because of leakage in the storage elements or breakdown of the switching elements.

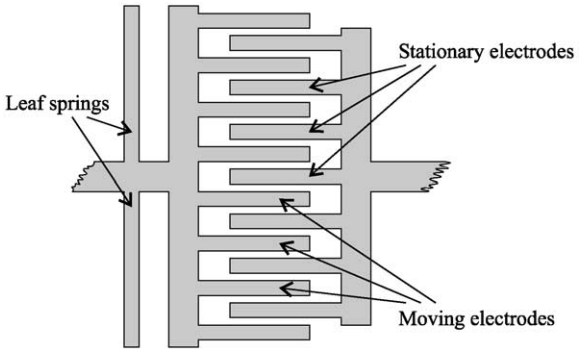

Fig. 8. Comb drive actuator.

6. A four stroke sequence of operation

In Fig. 4, we consider the ratchet to have two phases or 'strokes'. We can use the word 'stroke' in reference to classical thermodynamic cycles such as the Carnot, Diesel, Otto and Stirling cycles. The word 'phase' is a reference to non-overlapping clock phases in a clocked digital circuit. In the MEMS ratchet, the concepts of 'stroke' and 'phase' converge.

The laws of Parrondo's games require that the probability of remaining in the same state for two successive time ticks is zero. This is clear from the graphical definitions in Figs. 5 and 6. The problem is that if we use the charge sharing method, described in Eqs. (17) and (18), then we cannot entirely exclude all charge from a capacitor, no matter how forceful our actuator may be. The easiest way around this is to simply switch the capacitor electronically to some other location. When we perform our accountancy to check for conservation of charge we will not find *any* charge at that location. Some of the charge can then be switched back to the original location in the next part of the cycle. We can avoid the use of a large amount of complicated controlling circuitry if we settle for two asymmetrical cycles of two phases rather than one symmetrical cycle of two phases. This is indicated in Fig. 9. The sequence in time is a cyclic repetition of {(a), (b), (c), (d)}. Phases (a) and (c) are diffusion phases where the carriers spread out to an equilibrium distribution. These are analogous to the process in Fig. 4(c). Phases (b) and (d) are compression phases where the capacitors are changed in value because they are driven by the comb actuators. Charge is actively 'compressed' into one or other of the capacitors in accordance with Eqs. (17) and (18). These compression phases are analogous to the process in Fig. 4(b).

The aim is always to move as much charge as possible to the right, in the 'positive' direction. This means that in

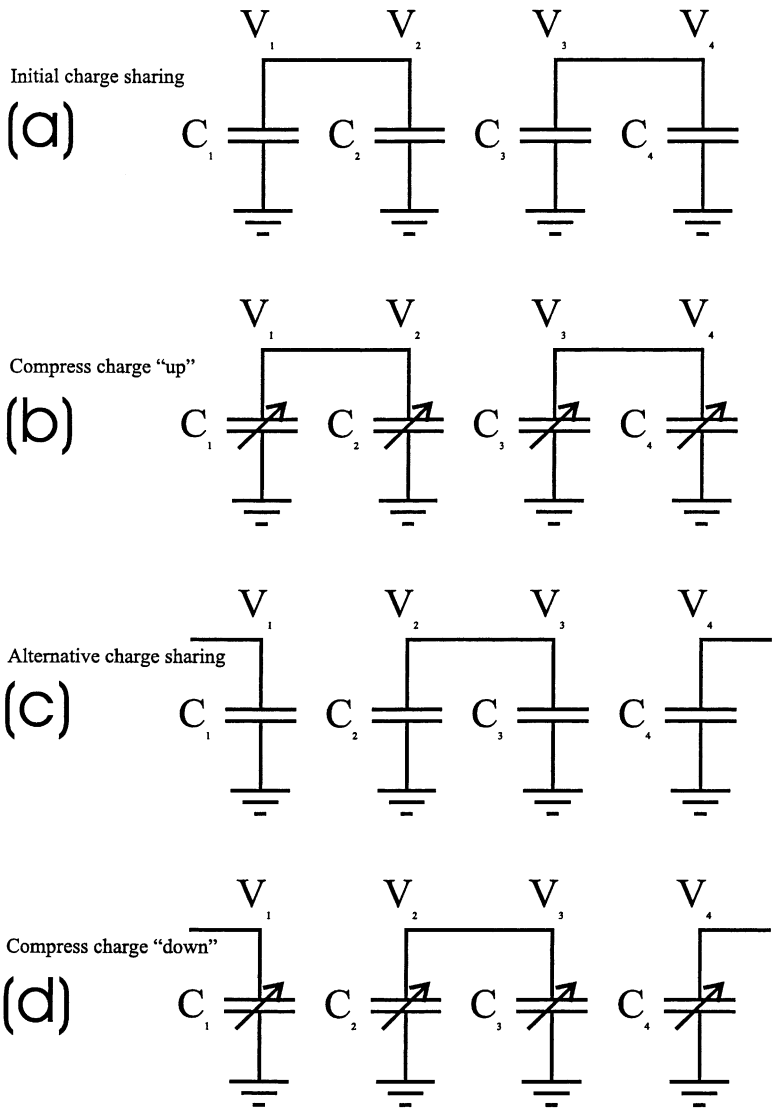

Fig. 9. A four stroke plan for swapping charge between capacitors.

Fig. 9(b) we need to increase C_2 and C_4 and decrease C_1 and C_3. In Fig. 9(d) we need to decrease C_2 and C_4 and increase C_1 and C_3. These should be done using the maximum possible compression ratio. It should be noted that the voltages V_1 to V_4 vary with time.

7. Simulation of the electrical circuit

We tested the electrical part of the system using P-SPICE. The results are shown in Figs. 10 and 11. We have used a split power supply to allow signals of either sign. This is not a necessary feature for a MEMS ratchet. The source V_0 is connected to capacitor C_1 through a diode. This is to allow the initial charge of C_1. No further charge is injected onto the system after this. The simulation shows the effect of charge sharing. The charge from C_1 gradually propagates down the ratchet, as the transmission gates are switched. This is quite analogous to the diffusion of charge in a conductive dielectric, which is governed by Poisson's equation.

As charge is shared, all the capacitors acquire the same voltage. In order to investigate the charge pumping effect of the ratchet, we would have to write our own simulator in a mathematical language, such as MATLAB. This is clearly the next stage of the work.

8. Analogies to other machines

Machines that use mechanical energy to change the value of a capacitive system to generate large potentials are not new. The classical examples are Volta's Electrophorus and the Wimshurst machine. The idea of using MEMS technology to implement ratchets has already been proposed by Abbott et al.[29]. A MEMS electrostatic ratchet could be

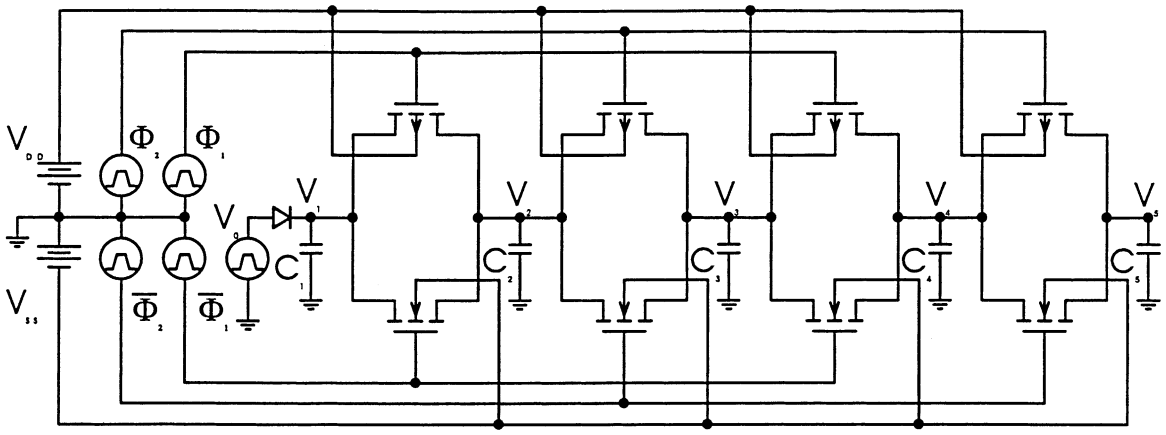

Fig. 10. SPICE model for the transmission gates.

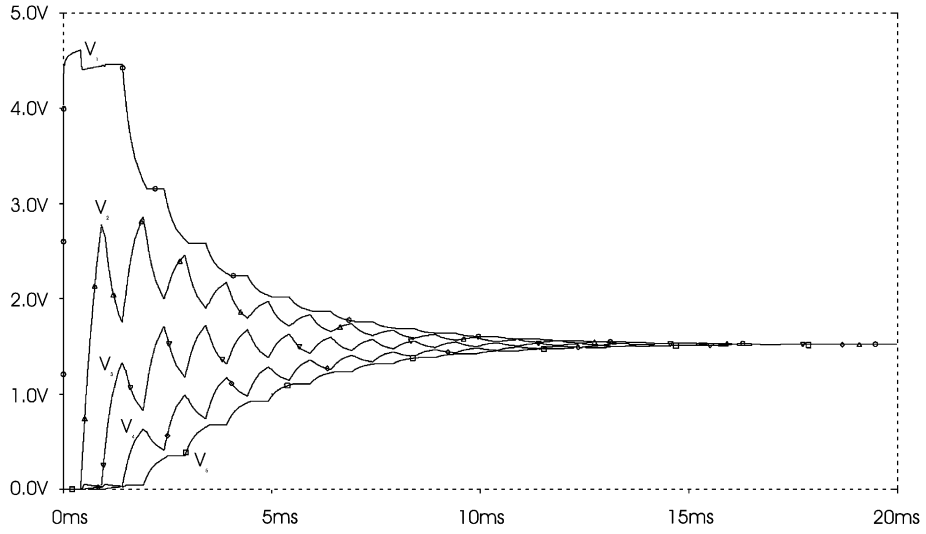

Fig. 11. Result from SPICE simulation, showing charge sharing.

a method of generating large potentials in a small space on a chip.

In their optimal form, the action of Parrondo's games is very much like a peristaltic pump or a stepper motor. The system is driven in a tightly controlled manner from one state to the next. The emphasis is on accurate control or measure. The peristaltic pump can deliver an accurate amount of a substance at a required moment in time. The stepper motor can produce an accurate rotation or translation. The MEMS ratchet could be used to accurately deliver a known amount of charge at a specified time. This could have application in instrumentation.

9. Summary

We have indicated how Parrondo's games could be re-parameterised in a form that could be constructed using MEMS technology. The main aim of this work is to carry out a 'thought experiment' to bring physical principles, such as energy, back into the study of discrete time ratchets. There are also some possible applications

- to induce large electrical potentials
- to deliver controlled amounts of charge

although more detailed and qualitative analyses are required. The authors agree that the key issue to be resolved is the efficiency of the proposed ratchet.

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