Microscopic models of Brownian ratchets

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ABSTRACT

A hard disk microscopic ratchet is introduced and studied with molecular dynamics. The properties of the systematic motion that appears when its two compartments are at different temperature are documented.

Keywords: Brownian motors, Maxwell demons, nonequilibrium, hard disk molecular dynamics

1. INTRODUCTION

A Maxwell demon is a non-macroscopic object that violates the second law. In the original construction proposed by Maxwell, it was represented as a microscopic being that would, in a container with two compartments, preferentially let pass fast particles from one side and cold particles from the other side, thereby "spontaneously" creating a temperature gradient. While Maxwell was under the impression that such a construction might be possible, provided one would be able to operate and manipulate at the atomic level, Smoluchowsky argued a few decades later that the demon would not operate basically because it would eventually "heat-up". The fact that this thermal motion of the demon restores the agreement with the second law was illustrated in more detail by Feynman through the ratchet and pawl construction in his famous lectures[1] in the late 1950's. In the meantime, Szilard focused on the innocuous reference by Maxwell to the demon as an intelligent being, a point that was not discussed by Smoluchowsky. He introduced the concept of one bit as the unit of information and used an argument based on an ingenious construction to derive a relation between information and entropy. More precisely, the Szilard machine seems to violate the second law, except if one assumes that information is somehow related to negative entropy, namely $-k_BT\ln 2$ per bit. Over the next several decades, physicists tried to clarify the Szilard statement. Brillouin and Gabor were apparently convinced that there is a minimum energy cost of $k_BT\ln 2$ in any experimental observation that would generate 1 bit of information. Landauer however argued that the essence of the hand-waving arguments of Szilard should be reduced to the less surprising observation that the erasure of one bit of memory corresponds to the doubling of the phase space of the physical entity that stores this information, hence to an increase of the entropy by $k_BT\ln 2$. This was further confirmed by Bennett who showed that calculations (and presumably measurements) can in principle be done reversibly, at no cost in entropy. In the end, the original Szilard construction appears to have been just another Maxwell demon, whose life had utterly confused several generations of physicists. A detailed discussion of the history of the subject and a copy of the original papers can be found in Ref. [2], see also [3].

The study of Maxwell demons is treacherous. Yet they are for several reasons much more relevant today than at the time of Maxwell. First, advances in nanotechnology and of corresponding experimental techniques make it possible to trap, observe, manipulate and manufacture objects at a very small scale. Second, as the 21st century announces itself as the age of biology, the small scale structures that control essential features of biological life are at the forefront of scientific investigations. Physicists can contribute by providing better tools to describe and understand the behavior (and in particular the limitations) of small scale nonequilibrium systems. Third, statistical mechanics is still struggling to unravel the relation between dynamical, probabilistic and thermodynamic concepts, as promising new avenues of research have appeared (dynamical chaos,[4] fluctuation theorem[5]). Finally, while we may not yet be able to carry out precise experiments on the likes of Maxwell demons, we can perform numerical experiments.[6,7] In this context, hard disk molecular dynamics are of particular interest. A first major advantage is that both the dynamics between the collisions (free motion) and the collisional rules are known analytically, hence the only error is due to computer round-off. A second advantage is the speed as compared to usual molecular dynamics where small time steps are needed for high accuracy. The main contribution of this paper is to present a hard disk molecular ratchet and to study in detail its properties, with special

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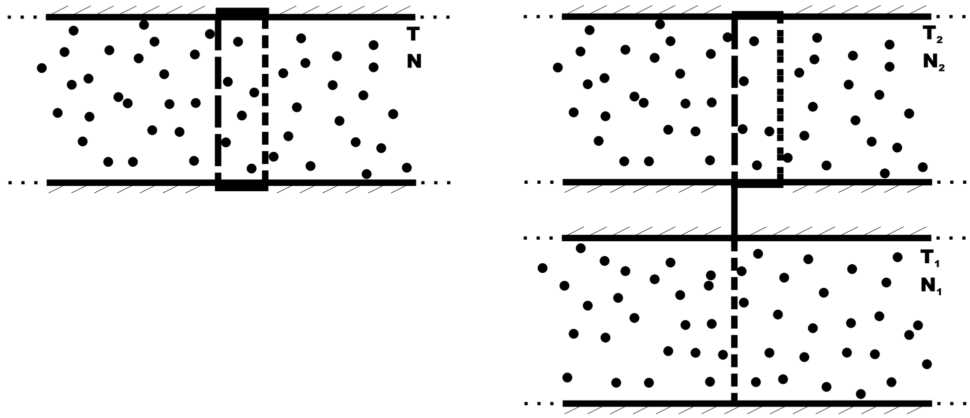

Figure 1. *a* (left): Schematic representation of Lucifera. *b* (right): A second cylinder at a different temperature and a rigid arm is added to Lucifera.

emphasis on the rectification of thermal fluctuations when the set-up operates away from equilibrium. We also give an example of how a Maxwell demon arises when the physics is not done correctly.

The organization of this paper is as follows. We start with the presentation of the hard disk Maxwell demon called Lucifera and discuss some details of the simulation technique that allows to restore agreement with the second law in section 2. The hard disk molecular ratchet is introduced as a nonequilibrium variant of Lucifera in section 3. We close with a final discussion in section 4.

2. LUCIFERA

Lucifera is a Maxwell demon. She is schematically represented in Fig. 1.a. She consists of two parallel semi-transparent sheets (total mass M) at a fixed distance of each other, which can freely move in a cylinder along the horizontal x-axis. Their motion is induced by collisions with a gas of hard disks (mass m=1, total number = N), which is enclosed in the same cylinder at equilibrium at temperature $T = 1$ (the Boltzmann constant is $k_B = 1$ by an appropriate choice of the energy unit). Boundary conditions are periodic at left and right ends, and perfectly reflecting on top and bottom. The sheets of Lucifera undergo perfectly reflecting collisions with the hard disk when the relative velocity of sheet and particle is below a specific energy hold, while the particles move unhampered through the sheets when the relative velocity is higher than this threshold. Furthermore, a spatial asymmetry is introduced by assuming that the thresholds are different for both sheets. In Fig. 2, we show the average over 2000 trajectories of Lucifera's motion. One clearly notices a systematic net displacement of Lucifera to the left. This motion however is in violation of the second law. Indeed the system considered here is an isolated equilibrium system and rectification of thermal fluctuations is excluded. If one were to attach a small load to Lucifera, she would be able to pull it up while cooling down the Enskog gas in which she lives. Another more appropriate way to state the inconsistency here is that Lucifera is violating detailed balance. When the latter condition is satisfied any transition between two states is equally likely to occur in both directions, excluding the possibility of systematic biased motion.

Lucifera's motion originates from an erroneous description of the collision process when the relative speeds of particle versus sheets exceeds the corresponding threshold. Indeed the hard disks have a finite radius, hence they do not cross the sheet instantaneously, even when the sheets are infinitesimally small. The fact that an elastic collision occurs below the threshold implies that their is a potential interaction between the sheet and the outer core of the disk. This potential has a finite maximum so that it can be crossed when the relative speed is above the corresponding threshold. The error is that during this crossing, both the sheet and the hard disk will slow down since part of their kinetic energy is transformed into potential energy, see appendix for more details.

The unfortunate aspect of the error is that it cannot at first sight be corrected within the framework of hard core interactions. We have however found an ingenious way around the problem. We assume that the interaction

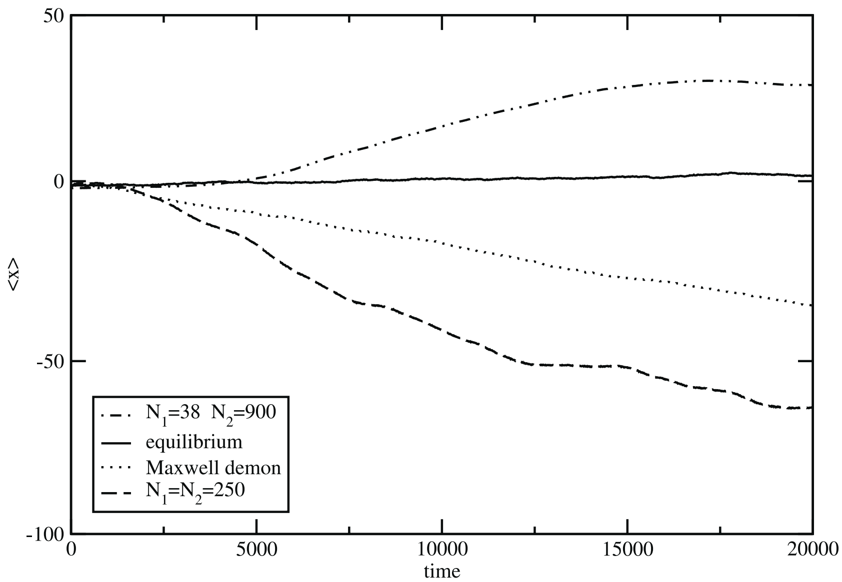

Figure 2. The dotted line corresponds to the Maxwell demon discussed in the main text, cf. Fig. 1.a. The parameter values are $M/m = 25$, $T = 1$, $N = 250$ and energy thresholds 1.0 and 0.5 for the left and right sheet respectively. The full line is the (unbiased) motion that appears when the collision rule between disks and sheets are corrected. Both results are averages over 2000 runs. The lower and upper curves correspond to the nonequilibrium version of Lucifera, cf. Fig. 1.b. The parameter values of the lower curve are $N_1 = N_2 = 250$, $M/m = 5$, $T_1 = 1.9$, $T_2 = 0.1$ and thresholds 10.0, 0.1 in the upper and 0.1 in the lower cylinder. For the upper curve we have $N_1 = 38$, $N_2 = 900$, $M/m = 20$, $T_1 = 20.8$, $T_2 = 0.078$ and thresholds 10.0, 0.05 in the upper and 0.05 in the lower cylinder. Both results are averages over 500 runs.

of the sheet is only with the center of the hard disk. So particles either bounce back from the sheet, which is instantaneous, or they cross the sheet, which is now also an instantaneous event, dependent on whether the relative speed when the center hits the sheet is below or above the threshold respectively. This interaction offers two bonuses. First everything is again reduced to hard core collisions. Second, it is now obvious how to write a hard disk molecular dynamics program in the presence of corners. Writing such a program with hard disks is notoriously difficult. For one a collision of the disks with the corner would make the particles spin, hence rotational degrees of freedom should be included. In our collision rule, the hard disks are in fact reduced to point particles (located at their centers) in their interaction with *other* objects, hence collisions with the corners of these other objects now have zero probability.

We can now return to the study of Lucifera in her “exorcised” form. With the thus modified correct collision rules, one verifies that Lucifera performs an unbiased motion, cf. Fig. 2. On a large time scale her motion converges to Brownian motion. In Fig. 3, we represent the probability density for her displacement after a long time interval (1000 and 4000 time steps) which is clearly Gaussian within the numerical accuracy. This Gaussian spreads out further as time goes on, cf. inset in Fig. 3, where we plot the root mean square displacement as a function of time. One clearly identifies a behavior of the form $\sqrt{2Dt}$ with D the diffusion coefficient.

3. LUCIFERA IN NONEQUILIBRIUM

Lucifera is clearly an asymmetric object when her two thresholds are not equal. In other words, she could perform the function of the ratchet in a Brownian motor, like for example the ratchet and pawl referred to before from

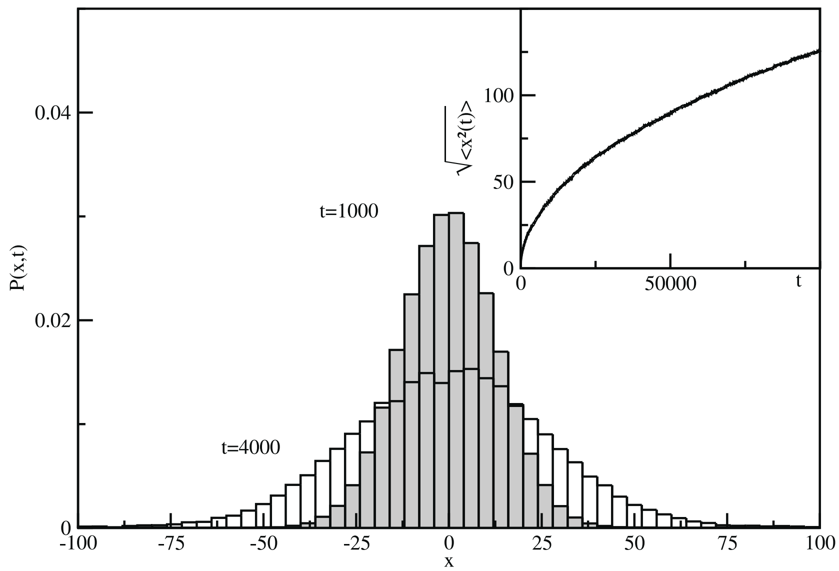

Figure 3. Probability density $P(x,t)$ for the position x of Lucifera at time $t = 1000$ and $t = 4000$. Inset: root mean square displacement versus time. The thresholds are 1.0 and 0.5, the particle number is $N = 250$ and the mass ratio is $M/m = 25$ (averages over 1500 runs).

the Feynman Lectures.[1] In order to proceed, we need to include a nonequilibrium component and we do it in a way very similar to Feynman: we introduce a second reservoir at a different temperature and add a rigid arm to Lucifera that sits in this other reservoir, see Fig. 1.b. Lucifera is now ready to move: she breaks, by construction, spatial left-right symmetry while the simultaneous contact with two reservoirs at different temperature implies that the more stringent symmetry of detailed balance, characteristic for an equilibrium system, is also broken. This is precisely what is observed. The resulting systematic speeds are typically rather small, so we have focused on a choice of thresholds that more or less optimizes the average speed, see Fig. 2 for a typical result. Note two important differences with the Feynman construction. First, Lucifera operates purely on the basis of hard disk collisions with the advantages mentioned before. Second, the momentum of the Feynman ratchet is not conserved along its direction of motion, while it is conserved in Lucifera.

Lucifera is, in her exorcised nonequilibrium form, an example of a microscopic Brownian motor that is able to rectify thermal fluctuations. A natural question arises as to the efficiency of this process. In his discussion of the ratchet and pawl construction, Feynman argues that one should in principle be able to reach Carnot efficiency. However, as first noted in Refs. [8, 9], he oversaw the fact that a small scale object, that is at the same time in contact with two heat reservoirs at different temperature, will conduct heat. The presence of this irreversible process implies that one cannot reach Carnot efficiency. Furthermore Parrondo and Espanol[8, 9] also give a simple phenomenological theory that allows to quantify the conductivity. Lucifera offers a non-trivial and interesting test case for this theory, see also [10]. It is assumed that the speed u of the object, in our case Lucifera, obeys a simple linear Langevin equation[11]:

$$M\partial_t u = -(\gamma_1 + \gamma_2)u + \zeta_1(t) + \zeta_2(t), \qquad \langle \zeta_i(t)\zeta_j(t')\rangle = 2\gamma_i k_B T_i \delta(t-t')\delta_{i,j} \tag{1}$$

where γ_1 and γ_2 are the friction coefficients in cylinders 1 and 2, respectively. $\zeta_1(t)$ and $\zeta_2(t)$ are the Gaussian white fluctuating forces associated to the friction processes. Note that we have assumed that the combined effect

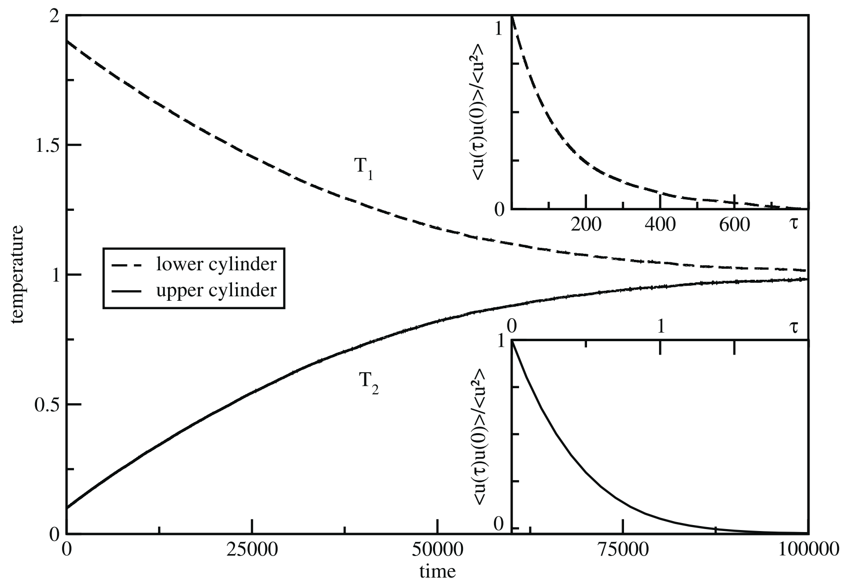

Figure 4. Temperature relaxation in both reservoirs as a result of the thermal contact generated by Lucifera. Parameter values: $M/m = 5$, $N_1 = N_2 = 250$ and thresholds 10.0, 0.1 in the upper and 0.1 in the lower cylinder. Inset: decay of the velocity correlations at equilibrium ($T = 1$) in the upper and lower cylinder respectively. Important deviations from an exponential fit are observed at high threshold values (like in the upper cylinder).

of both cylinders to the motion of Lucifera can be obtained by adding the separate contributions which are moreover taken to be linear and of the equilibrium form. The rate of heat transfer $Q_{1\to 2}$ (the heat flux) from cylinder 1 to cylinder 2 can now be calculated as follows. From (1) one finds that the heat fluxes between the different constituents of the system are given by the following expressions at the steady state :

$$\begin{aligned} Q_{1\to piston} &= \frac{\gamma_1}{M}[k_B T_1 - M\langle u^2\rangle] = \\ Q_{piston\to 2} &= -\frac{\gamma_2}{M}[k_B T_2 - M\langle u^2\rangle] = Q_{1\to 2} \end{aligned} \tag{2}$$

implying that the piston thermalizes at the effective temperature $(\gamma_1 T_1 + \gamma_2 T_2)/(\gamma_1 + \gamma_2)$ and that:

$$Q_{1\to 2} = \frac{k_B}{M}\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}(T_1 - T_2). \tag{3}$$

To check the validity of this description we turn back to our hard disk simulations. We start by considering an equilibrium system ($T_1 = T_2 = T_{eq} = 1$), focusing on the behavior of the piston velocity correlation function $\langle u(t)u(0)\rangle$. Note that the friction in a single reservoir can be measured by putting the threshold(s) for the crossing of Lucifera equal to zero in the other reservoir. We observe, to a reasonable approximation that the velocity correlations decay exponentially with a relaxation time proportional to the piston mass M if the thresholds of the sheets are small, but non-exponential features become apparent at high threshold value (see inset Fig. 4). We thus conclude that the motion of the piston can only in first approximation be described as damped Brownian motion. The application of the above theory to nonequilibrium generates additional inaccuracies. First, as one would expect due to the presence of specific thresholds, the friction coefficients are strongly dependent on the temperature. Second, the larger speeds of Lucifera are realized in highly asymmetric cases. The timescales are then very different in both cylinders and memory effects that are neglected in Eq. (1) could play a significant role. Third, the full story is obviously much more complicated and hydrodynamic effects, to cite just one point that has been investigated in some detail,[12] can not be neglected. To illustrate the kind of results that are obtained, we show an example of the observed temperature relaxation in Fig. 4. We find in agreement with Eq. (3) that the heat flux between both cylinders is to first approximation proportional to the applied temperature difference. The coefficient of conductivity is of the same order of magnitude as the theoretical prediction from Eq. (3). For example, as can be seen from Fig. 4, the decay time for the velocity correlations $(\gamma_1/M)^{-1}$ and $(\gamma_2/M)^{-1}$ are of the order of 100 and 1/2 respectively (cf. insets), hence $(M = 5)$ $\gamma_1 \approx 1/20 \ll \gamma_2 \approx 10$. The predicted heat conductivity is then $\kappa = (k_B/M)(\gamma_1\gamma_2/\gamma_1 + \gamma_2) \approx (\gamma_1/M) \approx 10^{-2}$. The temperature decay is described by

$$\frac{d}{dt}(N_1 k_B T_1) = -\frac{d}{dt}(N_2 k_B T_2) = -\kappa(T_1 - T_2) \tag{4}$$

implying $(N_1 = N_2 = 250,\ k_B = 1)$ an exponentional decay of $T_1 - T_2$ with time constant $N/(2\kappa) \approx 10000$, in rough agreement with the observed profile. The quantitative difference is presumably due to a combination of the above cited complications.

4. DISCUSSION

We have presented a microscopic model of a ratchet that can be fully simulated, with the known advantages of speed and accuracy, within the context of hard disk dynamics. This allows unprecedented access to detailed information on such systems. Apart from its clear pedagogical interest, as illustrated by Lucifera as a Maxwell demon, the obtained insights are hardly a luxury, when one realizes that there is presently no theory predicting the amplitude or even the direction of the resulting ratchet motion. As an illustration we have included in Fig. 2 the results for a second case with a temperature gradient in the same direction, but resulting in a systematic motion in the opposite direction. While we have a crude and approximate description of the heat conductivity of Lucifera, it remains an open challenge to formulate a simple theory that describes her systematic motion. This is in stark contrast with the theory for overdamped Brownian motors, which is by now well developed.[13]

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APPENDIX A. HARD DISK MOLECULAR DYNAMICS SIMULATION

The collision of a hard disk (mass m) with a plane infinitely thin sheet (mass M) that is free to move in a direction x orthogonal to its orientation, is described by conservation of momentum and energy along the x-axis:

$$\begin{aligned} &m v_x + M V_x = m v_x' + M V_x' \\ &\tfrac{1}{2} m v_x^2 + \tfrac{1}{2} M V_x^2 = \tfrac{1}{2} m {v_x'}^2 + \tfrac{1}{2} M {V_x'}^2 \end{aligned} \tag{5}$$

v_x, V_x and v_x', V_x' are the pre and post-collisional x components of the speed of particle and sheet respectively. This equation, which is quadratic in the speeds, always has two solutions. One is the "trivial" solution

$$\begin{aligned} v_x' &= v_x \\ V_x' &= V_x \end{aligned} \tag{6}$$

The other solution is given by

$$\begin{aligned} v_x' &= \frac{m - M}{M + m} v_x + \frac{2M}{M + m} V_x \\ V_x' &= \frac{M - m}{M + m} V_x + \frac{2m}{M + m} v_x \end{aligned} \tag{7}$$

Usually, it is argued that the trivial solution is unphysical, having in mind the existence of an infinitely high repulsion between sheet and particle at contact. We are however interested in a sheet that is semi-transparent, i.e., sheet and particle can cross through each other when the relative velocity is above a certain threshold. This can be physically realized by assuming a potential of interaction $U(x)$ of the following form:

$$U(x) = \begin{cases} U_0 & |x| < d \\ 0 & |x| > d \end{cases} \tag{8}$$

where x is the relative distance between sheet and particle. Clearly, when the relative kinetic energy is smaller than U_0, particle and sheet cannot cross and the post-collisional velocities are given by (7). When the kinetic energy is above U_0, crossing will occur and both the sheet and particle will resume their original velocities, cf. (6), after the encounter is finished. The problem we face is that the collision process is not instantaneous, even if we take the limit $d \to 0$, because the particle is a hard disk with a finite spatial extension. Furthermore, conservation of energy during the crossing implies that the kinetic energy is reduced by an amount U_0. This slowdown was not taken into account in the first version of Lucifera, and lies at the origin of its Maxwell demon behavior. The error can be removed while staying entirely in the context of hard core dynamics by assuming that the interaction (8) is with the center of the hard disk. Both the repulsive and crossing collision (when $d \to 0$) are thus instantaneous with post-collisional speeds given by (6) or (7) respectively. For a very fast algorithm to manage a large number of particles, see Ref. [14].

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