Maxwell’s Demon, Rectifiers, and the Second Law: Computer Simulation of Smoluchowski’s Trapdoor

P. A. Skordos  
Santa Fe Institute, Santa Fe, NM and  
Massachusetts Institute of Technology, 545 Technology Square, Cambridge, MA 02139

W. H. Zurek  
Theoretical Division, MS B213, Los Alamos National Laboratory, Los Alamos, NM 87545  
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We have simulated numerically an automated version of Maxwell’s demon inspired by Smoluchowski’s ideas of 1912. Two gas chambers of equal volume are connected via an opening that is covered by a trapdoor. The trapdoor can open to the left but not to the right, and is intended to rectify naturally occurring fluctuations in density between the two chambers. Our results confirm that though the trapdoor behaves as a rectifier when large density differences are imposed by external means, it can not extract useful work from the thermal motion of the molecules when left on its own.

I. INTRODUCTION

The second law of thermodynamics has been a subject of debate ever since it was formulated. It says that the entropy of a closed system can only increase with time, and thus natural phenomena are irreversible. In other words a system left on its own can only evolve in one direction, towards equilibrium. This is in contrast to time-reversible dynamics and raises the question of how reversible dynamics can lead to macroscopic irreversibility. An answer can be furnished using probabilistic arguments in statistical mechanics, but the arguments are difficult to translate into a rigorous proof without postulating a new axiom about nature, the stosszahlansatz, also called the assumption of molecular chaos [1, 2], which is at odds with dynamic reversibility. As a result, the origin of the second law of thermodynamics remains elusive and provides a source of interesting discussions on the foundations of physics.

A popular way of challenging the second law is the idea of “perpetual machine of the second kind”, which is supposed to extract useful work in a closed cycle from the perpetual thermal motion of gas molecules. This is prohibited by the second law because if it were possible to convert thermal energy into useful work in a closed, equilibrated system, then the entropy of an isolated system could be made to decrease. However, it remains puzzling why a microscopic device can not be constructed to take advantage of spontaneous variations in density between microdomains of gas, to bring a system from a state of maximum disorder (equilibrium) into an ordered state, and eventually to convert thermal energy into useful work.

The history of microengines that convert thermal energy into useful work began when J.C. Maxwell proposed such a microengine at the end of his book Theory of Heat [3], which he named a “demon”. Since then the term “demon” has become a standard. Maxwell’s demon works by opening and closing a tiny door between two gas chambers, based on the information that the demon has about individual molecules. The method used to obtain information is not specified. The demon allows only fast molecules to pass from left to right, and only slow ones to pass from right to left. This leads to a temperature difference between the two gas chambers, which can be used to convert thermal energy into useful work. It is currently believed, however, that Maxwell’s demon can not violate the second law [4, 5, 6, 7, 8] because the information needed to operate the demon’s door does not come without a price. As Bennett explains in [5] following an idea that goes back to [9] and [10], the demon must dissipate energy into a heat bath in order to erase the information that it obtains by examining molecules. The heat bath may be the molecules that the demon examines or it may be another system that is colder than the demon and the gas molecules. The energy lost in the heat bath is always greater than or equal to the energy that can be extracted after the demon has finished its operations. Thus, the second law of thermodynamics is not violated even when the demon is “intelligent” — that is, capable of universal computing ability — as it was pointed out by one of us [10, 11].

There is an alternative approach, however, to designing microengines that convert thermal energy into useful work; and that is to focus on purely mechanical devices, and to avoid the issues of measurement and information that haunt the original Maxwell’s demon. Purely mechanical, automated Maxwell’s demons are completely described within a theoretical framework such as newtonian physics. In particular, there is no measurement mechanism outside of such mechanical model. An example is the trapdoor mechanism discussed by Smoluchowski in [12, 13]. A well-known and similar in the spirit to Smoluchowski’s trapdoor is the ratchet and pawl mechanism discussed by Feynman in [14].

Our paper describes the computer simulation of a trapdoor mechanism inspired by Smoluchowski’s ideas. Our results confirm Smoluchowski’s insight that though the trapdoor acts as a rectifier when large density differences
are imposed by external means, it can not extract useful work from the thermal motion of the molecules when left on its own. The next section describes our trapdoor mechanism and the simulation program. Following that, we discuss how the trapdoor succeeds at rectifying large density differences that are imposed by external means. Then, we show how our trapdoor system fails to work when left to operate on its own. Finally, we discuss how the trapdoor can be modified to work successfully as a pump and create density differences in the system initially in equilibrium. This requires, however, dissipation of its random motions which can be accomplished only by “opening” the system, that is, for example, by keeping the trapdoor at a lower temperature than the molecules. Such a pump, of course, is no more a threat to the second law than is a refrigerator.

II. DESCRIPTION OF THE MODEL

The system that has been simulated is shown in Figure 1. It consists of two gas chambers of equal area, connected via an opening that is covered by a trapdoor. The simulation is two-dimensional and the gas molecules are billiard balls moving on the plane and colliding with each other. All the collisions conserve energy and momentum, except for particle-wall collisions that reflect a particle’s momentum like light rays reflect off mirrors. The collision forces are derived from infinite hard core momentum, except for particle-wall collisions that reflect a particle in a similar manner. As we shall see in the next section. The trapdoor is a line segment of zero width, impenetrable by the molecules, which moves horizontally at constant speed, and reverses its direction when it comes in contact with the door stops. During its motion, the trapdoor slides along ideal rails and thus remains vertical at all times. Accordingly, collisions between the trapdoor and the molecules conserve energy and momentum except for collisions at the edges of the trapdoor which do not conserve the y-component of momentum (that is, the trapdoor does not move at all in that direction — it can be thought of as moving on rails which are attached to the infinitely massive box containing the gas). The collision equations are discussed in detail below.

To evolve the system of molecules and the trapdoor we use the following algorithm: Given the positions and velocities at time \( t_0 \), we find all the collisions that are about to occur. We select the shortest collision time \( \Delta t \), and move all the particles and the door freely during \( \Delta t \). At time \( t_0 + \Delta t \) we perform the collision that occurs at this time, and then repeat the cycle looking for the next shortest collision time. The algorithm works because collisions in our system are instantaneous. The types of collisions that can occur are of four types: particle against particle, particle against wall, particle against door, and door against door stop.

The evolution algorithm can be implemented efficiently on a computer if we are careful to avoid unnecessary computations. For example, we do not need to examine all pairs of particles at every time step. If we see that two particles are far from each other, then we need not examine them again until a number of time steps have elapsed. Only then these two particles will have another chance of being near each other and being able to collide. Also, if we compute the collision time for a pair of particles that are near each other, and another pair of particles collides before them, we need not discard the first collision time. We simply decrement the first collision time by the time interval by which the whole system is evolved. A word of caution, however, is necessary. The process of decrementing collision times should not be repeated more than a few times because the roundoff error in subtracting small intervals of time becomes significant very quickly. Also, a collision involving some particle must invalidate all pre-computed collision times involving that particle.

Two kinds of elementary formulas are used in the evolution algorithm: collision equations give the new velocities in terms of the old velocities, and timing equations give the time interval until an upcoming collision. The timing equations are the simpler of the two. They are derived from geometrical constraints and the fact that the particles and the door move at constant velocity between collisions. For example, to compute the collision time between two particles, we “draw a straight line” from the current position of the particles to the point where the particles are tangential to each other. The geometrical constraint of tangency allows two possibilities, and we have to choose the one that occurs first and is the physical one. Algebraically we have to solve a quadratic equation, and to pick the smallest positive solution. The timing equations for the other types of collisions in our system are derived in a similar manner.

The collision equations are a little more complicated than the timing equations. As usual the collision equations are derived from conservation of kinetic energy, conservation of linear momentum, and the condition that forces act radially. The last condition means that the force vector must pass through the center of the particle disk that is colliding, and hence momentum is exchanged along this direction. For nearly all collisions the radial force condition is satisfied automatically in setting up the geometry of the problem. However, there is one type of collision in our system that requires explicit use of the radial condition. This occurs when a particle disk collides with the edges of the moving trapdoor. Since it is not discussed in most textbooks, we review briefly the equations.

The radial action condition requires that the change
in y-momentum divided by the change in x-momentum equals the tangent of the angle \( \theta \) formed by the center of the colliding disk, the point of contact, and the x-axis. The point of contact is the edge of the moving trapdoor. If \( v_x, v_y \) are the old velocities and \( v'_x, v'_y \) are the new velocities of the colliding disk, we have the equation

\[
(v_x - v'_x) = \frac{\cos \theta}{\sin \theta} (v_y - v'_y) .
\]  

(1)

To find the velocities following a collision in terms of the velocities before the collision, we use equation (1) together with kinetic energy and x-momentum conservation. The y-momentum is not conserved because the collision equations for all other types of collisions in our system can be found in standard textbooks [15].

\[
v'_x = \frac{-2csv_y + 2c^2V_x + (s^2 - \delta c^2)v_x}{(\gamma c^2 + s^2)}
\]  

(2)

\[
v'_y = \frac{-2csv_x + 2cVs_y + (\gamma c^2 - s^2)v_y}{(\gamma c^2 + s^2)}
\]  

(3)

\[
V'_x = V_x + \frac{m}{M}(v_x - v'_x)
\]  

(4)

where

\[
c = \cos \theta \\
s = \sin \theta \\
\gamma = (1 + m/M) \\
\delta = (1 - m/M)
\]

and where \( M, V_x \) are the mass and x-velocity of the trapdoor; \( m, v_x, v_y \) are the mass and velocities of the particle; and \( \theta \) is the angle formed by the center of the particle, the colliding edge of the trapdoor, and the x-axis. The collision equations for all other types of collisions in our system can be found in standard textbooks [15].

The numbers we used in our simulations were chosen to correspond to a standard gas like nitrogen. We experimented with different masses for the trapdoor, and in the results reported below the mass of the trapdoor is of the order of three to four times the mass of one particle, unless otherwise indicated. Using a trapdoor mass which is comparable to the molecular mass leads to an average speed for the trapdoor that is comparable to that of the molecules, and facilitates numerical simulation. A very light trapdoor moves too fast and increases the numerical roundoff error; while an excessively heavy trapdoor (orders of magnitude heavier than a molecule) can delay the approach to equilibrium and requires longer time averaging. It should be emphasized that our qualitative conclusions are expected to be independent of the mass of the trapdoor, and we certainly do not have any indications in our numerical results to question this expectation. Thus, the choice of the mass of the door was dictated primarily by the above considerations of numerical convenience. Our simulations took typically several days using standard Unix workstations, and the relative error in the total energy of the system was kept less than \( 10^{-10} \) using double precision arithmetic. The running times were dictated primarily by the desire to gather good statistics. By contrast, the rectifying behavior described in the next section can be seen on a much less imposing timescale of a few minutes, depending of course on the efficiency of the algorithm and on the number of particles used.

### III. THE TRAPDOOR AS A RECTIFIER

This section discusses the behavior of the trapdoor when large density differences between the two chambers are imposed by external means. It is found that under these circumstances the trapdoor acts as a diode, and prolongs the duration of states of higher density in the left chamber. There are a number of ways to exhibit this rectifying behavior. We shall describe here three of them.

The first way is to measure the equilibration time or transient response to an initial density difference, for example when all molecules start in the left chamber. To be precise we place all molecules along the outermost wall of one chamber with the trapdoor set motionless in the closed position, and measure the density in each chamber until the populations in the two chambers equalize. Figure 2 shows the absolute value of the difference in the number of molecules between the two chambers plotted against time. The difference in the number of molecules is normalized by the total number of molecules, which is 500 in this experiment. Two curves are shown, one for the case when all molecules start in the left chamber, and one for the case when all molecules start in the right chamber. We see that in the latter case the populations equalize “immediately”. In other words the density difference vanishes much more quickly when the molecules
start in the right chamber than when the molecules start in the left chamber.

The second way of observing the rectifying behavior of the trapdoor is shown in Figure 3. The data comes from the same kind of equilibration experiment as Figure 2 where all the particles are positioned initially along the outermost wall of one chamber. Now, we look at the time interval it takes 25 molecules to pass from one chamber to the other as a function of the density difference. If $T$ is this time interval, then the ratio $25/T$ measures the current of particles — the rate — at which they pass through the middle wall opening in response to the density difference during that time. Figure 3 plots the particle current against the density difference between the two chambers for a system of 500 particles. The resulting curve resembles qualitatively the voltage-current characteristic of an electrical diode, and indicates that the trapdoor acts as a rectifier when large density differences are imposed by external means.

The precise quantities plotted in Figure 3 are the rates — inverse time intervals $(1/(T_{i+1} - T_i))$ — as a function of the average number of particles difference between the two chambers $(\Delta N_{i+1} + \Delta N_i)/2$ which exists during the interval $(T_{i+1} - T_i)$. $\Delta N_i$ is the number of particles difference at the starting time $T_i$, and $\Delta N_{i+1}$ is the number of particles difference at the finishing time $T_{i+1}$ when 25 molecules have moved from the source chamber (high density) to the sink chamber (low density). The y-axis is in units of $25 \times 10^9$ particles/sec. The x-axis is in units of the normalized difference in the number of particles, so that an interval of size 0.1 corresponds to 25 particles moving from one chamber to the other $(0.1 \times 500 \times \frac{1}{T} = 25)$. The intervals $(-1,-0.9)$ and $(0.9,1.0)$ are not included in the plot because the times immediately after the release of the system from our initial conditions do not correspond to smooth flow.

The third and last method of exhibiting the rectifying behavior of the trapdoor focuses on steady state behavior. In contrast to the equilibration experiments above, this method measures the time averaged flow of molecules through the middle wall opening when a large density difference is maintained artificially. In particular, we continually “reverse bias” the system by removing the molecules that hit the rightmost wall of the right chamber and reinserting them in the left side of the left chamber. This results in a density difference that pushes the trapdoor towards the closed position. In an opposite experiment we forward bias the system by reinserting molecules from the leftmost wall into the right chamber.

Table 1 lists the flow of molecules (number of particles per second) passing through the middle wall opening under reverse and forward bias conditions. Molecules passing left to right are counted positive and molecules passing right to left are counted negative. We list the results for two different systems, a system of 500 particles and a system of 100 particles. The time intervals used to time averaged are about $10^{-5}/$sec for the 100 particle system and $10^{-4}$/sec for the 500 particle system, which are both large enough to guarantee convergence; that is the average values will not change over longer time intervals. We have checked this by plotting the time averages against time, and seeing that the curves approach a horizontal slope and a constant value. The values in Table 1 show that the flow allowed by the trapdoor in the forward bias condition is 22 times as large as the flow allowed in the reverse bias condition for 500 particles, and 17 times as large in the case of 100 particles. In other words, the trapdoor acts as a rectifier.

It is worth pointing out that the rectifying behavior of the trapdoor depends greatly on the geometry of the system. Experimentally we have found that our trapdoor becomes a better rectifier the longer the trapdoor is, and the more molecules there are near the trapdoor. When many collisions take place exclusively on one side of the trapdoor during the time interval it takes the trapdoor to move significantly, the trapdoor is pushed and kept near one door stop. The probability of moving significantly away from that door stop is very small. For example, if many collisions take place exclusively on the left side of the trapdoor, the trapdoor will be kept near the middle wall opening, bouncing between the middle wall door stop and the large number of particles on its left side. The trapdoor performance can be improved further by placing one door stop slightly inside the right chamber. This centers the jittering of the door exactly on the middle wall and decreases the chance of a molecule leaking from the high density left chamber into the low density right chamber. For similar reasons we expect that making the trapdoor have finite width, that is using a two dimensional trapdoor in the shape of a rectangle will result in even better rectifying behavior for large density differences.

|                   | $N = 500$     | $N = 100$     |
|-------------------|---------------|---------------|
| Reverse Bias      | $4.26 \times 10^9$ | $1.05 \times 10^9$ |
| Forward Bias      | $-9.31 \times 10^{10}$ | $-1.81 \times 10^{10}$ |
| ratio             | $1 : 22$      | $1 : 17$      |

**Table I:** The flow of molecules through the middle wall opening in forward and reverse bias conditions, for systems of 100 and 500 molecules. The molecules crossing from left to right are counted positive, and those crossing from right to left are counted negative.

**IV. VERIFICATION OF THE SECOND LAW**

Having seen that the trapdoor acts as a rectifier under external bias, we now consider what happens when the trapdoor and molecules are left to evolve on their own in an isolated container. The asymmetry of the trapdoor’s location, opening to the left but not to the right, intends to hinder the passage of molecules from left to right while providing an easy access from right to left. In this way,
the trapdoor attempts to exploit the naturally occurring fluctuations in density between the two chambers and to make states of high density in the left chamber last longer than corresponding states of high density in the right chamber. Ultimately, the trapdoor attempts to keep a higher average number of molecules in the left chamber than in the right chamber.

However, our simulations show that the trapdoor does not succeed. When the trapdoor and molecules are left to evolve on their own, the time average number of molecules in the left chamber is actually smaller than the time averaged number of molecules in the right chamber. Moreover, this imbalance is not a true density difference and does not violate the second law. The reason for the unequal number of molecules is that the presence of the trapdoor in the left chamber occupies space, which makes the available area in the left chamber slightly smaller than the available area in the right chamber.

The effect of the excluded area by the trapdoor has been measured by performing an experiment of 20 particles where each chamber measured $13.5 \times 10^{-7} \text{cm}$ horizontally and $18 \times 10^{-7} \text{cm}$ vertically. The particle radius was $R = 6 \times 10^{-8} \text{cm}$ giving a mean free path in the order of $20 \times 10^{-7} \text{cm}$. The length of the trapdoor (vertical direction) was $10 \times 10^{-7} \text{cm}$. Given these numbers we can estimate the average number of particles in the left chamber by assuming uniform density (equilibrium) in a time average sense. If $N_L$ is the time averaged number of particles in the left chamber and $A_L$ the available area in the left chamber, we have

\[
\frac{N_L}{A_L} = \frac{N_R}{A_R} = \frac{1 - N_L}{A_R}
\]

which gives $N_L = A_L/(A_L + A_R)$. To estimate the available area in each chamber, $A_L$ and $A_R$, we consider the area in which the centers of the particles can travel. Thus $A_R = [(13.5 \times 18) - (13.5 + 13.5 + 18) \times 0.06] \times 10^{-14} \text{cm}^2$ for the right chamber, and for the left chamber we subtract from the above $A_L$ the area excluded by the trapdoor $[(10 \times 0.06) + \pi (0.06)^2] \times 10^{-14} \text{cm}^2$. Putting these together we find $N_L = 0.484$. In simulating this experiment we found the time averaged number of particles in the left chamber to be 0.486 in excellent agreement with the theoretical estimate $0.484$.

There is also an alternative way of checking that the observed particle number difference between the two chambers is not a true density difference, and it can not lead to a violation of the second law. The idea is to open a second hole in the middle wall, in addition to the opening covered by the trapdoor. If the trapdoor could lead to a true density difference, pumping molecules from one chamber to the other through the opening covered by the trapdoor, then the second free opening should exhibit the return flux of molecules and lead to perpetual flow between the two chambers. Our simulations of this experiment did not show any flow.

Our simulations show that the operation of the trapdoor is consistent with the second law of thermodynamics in the sense that the particles are distributed uniformly in the available area on the average, and the entropy of the system is maximized. Our simulations have also shown that the time averaged temperature is the same in each chamber and equal to the temperature of the trapdoor (average kinetic energy divided by the number of degrees of freedom, two for the particles, and one for the trapdoor). Finally, we have confirmed that the time averaged velocities in each chamber are distributed as Gaussian distributions in $v_x$ and $v_y$. The two Gaussian distributions are identical to each other and identical between the two chambers, which is consistent with the Maxwell-Boltzmann distribution law and equipartition of energy.

An intuitive explanation of why our trapdoor system fails to work when operating in an isolated container of gas molecules is that the trapdoor gets thermalized — its temperature equals the temperature of the particles — and the trapdoor’s thermal motion prevents the rectifying behavior. To contrast, a macroscopic trapdoor works successfully as a rectifier because it can get rid of excess energy through dissipation. Following this analogy a little further, we may expect that our trapdoor would work successfully if a reservoir of lower temperature than the particles were used to dissipate its motion. The trapdoor would then act as a pump, letting the molecules through from one chamber to the other more easily in one direction than the other, on the average. We have tested this idea in simulations, and we report the results in the next section.

V. THE TRAPDOOR AS A PUMP

To convert our trapdoor system into an effective pump, we modify the evolution algorithm to cool the trapdoor by removing energy in small increments. In particular, we scale the trapdoor’s velocity by 0.5 every $\Delta t$ time interval with $\Delta t$ sufficiently small. The lost energy is reinserted in equal amounts to all the particles by scaling their velocities, conserving the total energy of the system. Moreover, the cooling of the trapdoor is performed only when the trapdoor is near the closed position, which makes the trapdoor tend to remain closed. The goal of the cooled trapdoor is to pump molecules from the right chamber into the left chamber.

Our experiments show that this design works successfully. Further, they show that the mass of the trapdoor in relation to the mass of each particle is crucial for efficient operation. If the trapdoor mass is much smaller than the mass of one particle, then the action of a single particle coming from the right chamber is enough to open the trapdoor and let the particle through, even though some energy is lost by interacting with the trapdoor. Easy access from the right chamber is desirable. On the other hand, if the trapdoor mass is much larger than the mass of one particle, many particles must collide with the trapdoor in a short period of time in order to open the trapdoor. Clearly, this situation does not pose an inefficiency, but it leads to a smaller and smaller velocity difference, which again leads to a violation of the second law.
occur very frequently, and so a heavy trapdoor does not work very well. Our simulations show that a very light trapdoor with dissipation can act effectively as a one-way door, opening to particles from the right, and remaining closed to particles from the left. A heavier trapdoor with dissipation works also, but not as well.

In Figure 4 we report results for a trapdoor system with dissipation, where the mass of the trapdoor is $4.7 \times 10^{-2} g m$, or one tenth of the mass of one particle. The time interval which controls the rate of energy dissipation is $2.5 \times 10^{-13} s e c$, while the mean free path and mean collision time in the left chamber are of the order of $20 \times 10^{-7} c m$ and $5 \times 10^{-11} s e c$. The length of the trapdoor is $6 \times 10^{-7} c m$ and each chamber measures $13.5 \times 10^{-7} c m$ horizontally and $18 \times 10^{-7} c m$ vertically. In this experiment we have also included a second hole in the middle wall, of size $1 \times 10^{-7} c m$, in addition to the hole covered by the trapdoor. The purpose of the additional hole is to verify that the trapdoor indeed acts as a pump of molecules from right to left, by exhibiting the return flux of molecules left to right. Graph (a) of Figure 4 shows how the normalized number of molecules in the left chamber builds up as soon as the system is released from a state of equal number of molecules in each chamber. Similar simulations that were run much longer than Figure 4 show that the time averaged of the number of molecules in the left chamber stabilizes around 0.76 (over $10^{-5} s e c$). Graph (b) of Figure 4 shows the accumulated flux of particles through the trapdoor covered opening, and the accumulated flux of particles through the second opening that allows free passage. The slope of the accumulated flux (measured by averaging over $10^{-5} s e c$) is approximately $2 \times 10^{9} p a r t i c l e s / s e c$. The time averaged temperature of the trapdoor is 11 degrees Kelvin, compared to 270 degrees Kelvin for the particles. These results show that the trapdoor can operate successfully as a rectifier when a reservoir of lower temperature is available. However, as discussed previously it can not operate successfully when run at the same temperature as the gas molecules, in accordance with the second law of thermodynamics.

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FIG. 1: The automated Maxwell’s demon we simulated numerically was inspired by Smoluchowski’s trapdoor. The dashed lines show the region where the trapdoor can move.

FIG. 2: The normalized absolute value of the difference between the number of particles in the two chambers is plotted against time, as the system approaches equilibrium. Two curves are shown, one for the case when the particles start in the left chamber, and one for the case when the particles start in the right chamber.

FIG. 3: The flux of particles from one chamber to the other is plotted against the density difference that initiates the flux. \(N_1\) is the number of particles in the left chamber, \(N_2\) the right chamber, and \(N\) the total number of particles. The y-axis is in units of \(25 \times 10^9\) particles/sec.
FIG. 4: A trapdoor with a cooling mechanism acts as a pump. The graph on the top (a) shows how the fraction of the total number of molecules in the left chamber builds up after the system is released from an initial state with an equal number of molecules in each chamber. The graph on the bottom (b) shows the accumulated flux of molecules through the trapdoor opening (negative slope) and the accumulated flux of molecules through an additional opening that allows free passage (positive slope).