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

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Abstract

We have simulated numerically an automated Maxwell's demon inspired by Smoluchowski's ideas of 1912. Two gas chambers of equal area 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 variations 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.

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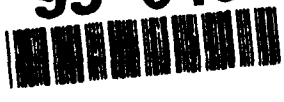

1 Introduction

The second law of thermodynamics has been a subject of debate ever since it was formulated. It says that the entropy of a closed macroscopic system can only increase with time, and thus macroscopic phenomena are irreversible. In other words a macroscopic 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 macroscopically irreversible phenomena. An explanation can be given 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* or assumption of molecular chaos [1, 2], which is at odds with dynamic reversibility. Thus, 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 motion of the second kind", to extract useful work in a closed cycle from the perpetual thermal motion of gas molecules. The second law prohibits this type of energy conversion because if it were possible to convert thermal energy into useful work, then the entropy of a closed isolated system could decrease, and this would violate the second law. On the other hand, it is not clear from first principles why a molecular size engine can not take advantage of spontaneous variations in density between microdomains of gas, to bring the 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 started when J.C. Maxwell introduced a microscopic engine at the end of his book *Theory of Heat* [4], which he named a "demon". Ever since the name 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 go from right to left. This results in a temperature difference between the two gas chambers, which can be used to extract useful work. However it has been argued that Maxwell's demon can not violate the second law [6, 7, 8, 9] because the information needed to operate the demon's door does not come without a price. As Bennett

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13. ABSTRACT *(Maximum 200 words)*

We have simulated numerically an automated Maxwell's demon inspired by Smoluchowski's ideas of 1912. Two gas chambers of equal area 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 variations 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.

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explains in [6] following an idea that goes back to [7] 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 dissipated in the heat bath is always greater than or equal to the energy that can be extracted after the demon has finished its operations. Hence the second law of thermodynamics is not violated [11, 12].

An alternative approach to designing microengines that convert thermal energy into mechanical work is to focus on purely mechanical devices, and to avoid the issues of measurement and information that have haunted the original Maxwell's demon. Purely mechanical demons are called automated Maxwell's demons, and they are described simply using a physical framework like newtonian mechanics. In particular, there is no measurement mechanism outside the mechanical model. An example of an automated Maxwell's demon is the trapdoor mechanism discussed by Smoluchowski in [13, 14], and also the ratchet and pawl mechanism discussed extensively in the Feynman Lectures on Physics [15].

We have performed numerical simulations to test whether the second law applies to the operation of a trapdoor mechanism inspired by Smoluchowski's ideas. Our experiments confirm Smoluchowski's insight that though the trapdoor can act 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. Our paper is organized as follows. First we describe our trapdoor system and the simulation program. Then we present results that show how the trapdoor succeeds at rectifying large density differences that are imposed by external means. Finally we discuss whether our trapdoor system can violate the second law of thermodynamics when left to operate on its own.

2 Description of the Model

The system we have 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 elastically. 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 potentials, and angular momentum (spin of the billiard balls) is not included in the model. All collision forces act radially through the center of the colliding balls.

The trapdoor moves between two *door stops*, one of which is located at the middle wall, and the other is located inside the left chamber. The location of the door stops allows the trapdoor to open to the left but not to the right. The trapdoor is a line segment of zero width, impenetrable by the molecules, which moves horizontally at constant speed, and reflects 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. Collisions between the trapdoor and the molecules conserve energy and linear momentum, except for collisions at the two edges of the trapdoor which do not conserve the y-component of momentum as we will see below.

To evolve the system of molecules and trapdoor we use the following algorithm: Given the system at time t_0, we find all the collisions that are about to occur. We select the shortest collision time Δt, and move all the particles and the door freely during the interval Δt. 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 above algorithm can be implemented efficiently on a computer if we are careful to avoid unnecessary computations. First 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 do not need to examine them again until a number of time steps have elapsed. Only then, these two particles have another chance of being near each other and being able to collide. Secondly 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 we evolve. These tricks can save a lot of computing time, but one should be careful in implementing them. For example the process of decrementing collision times should not be repeated more than a few times because the roundoff error in subtracting small time intervals becomes signif-

icant quickly. Also, any collision involving some particle P must invalidate all pre-computed collision times involving particle P.

Our simulation algorithm utilizes two kinds of mathematical formulas, *collision equations* giving the new velocities in terms of the old velocities, and *timing equations* giving the time interval until an upcoming collision. The timing equations are the simplest of the two, and 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 time until a collision between two particles, we draw straight lines from the current position of each particle to the point where the two particle disks are tangential to each other. By relating the lengths of the line segments to the velocities of the particles, we get a quadratic equation for the time elapsed. The solutions of the quadratic equation are examined to determine if the collision occurs physically, and to select the smallest solution if two solutions are possible. The timing equations for all the other types of collisions in our system can be 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 most problems the radial action 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 action 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 θ 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 get the equation

$$(v_x - v'_x) = \frac{\cos\theta}{\sin\theta}(v_y - v'_y) \tag{1}$$

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 trapdoor moves on ideal rails, and its y-velocity is always zero. After some algebra we get the following equations for the new velocities,

$$v_x' = \frac{-2csv_y + 2c^2V + (s^2 - \delta c^2)v_x}{(\gamma c^2 + s^2)} \tag{2}$$

$$v_y' = \frac{-2csv_x + 2csV + (\gamma c^2 - s^2)v_y}{(\gamma c^2 + s^2)} \tag{3}$$

$$V' = V + \frac{m}{M}(v_x - v_x') \tag{4}$$

where

$$\begin{aligned} c &= \cos\theta \\ s &= \sin\theta \\ \gamma &= (1 + m/M) \\ \delta &= (1 - m/M) \end{aligned}$$

and M, V are the mass and x-velocity of the trapdoor; m, v_x, v_y are the mass and velocities of the particle; and θ 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 [16].

The numbers we used in our simulations were chosen to correspond to a standard gas like nitrogen. We experimented with different values for the size of the gas chambers, molecular speeds, and other quantities, and the qualitative behavior of the gas was the same for all choices. For completeness we summarize some of the numbers. We looked at systems containing a number of molecules ranging from 20 to 500; these numbers being dictated by the computational power of our computers. We chose the radius of the molecules to be $3 \times 10^{-8} cm$, mass $4.7 \times 10^{-23} gm$, and velocities of the order $10^4 cm/sec$. We chose the size of the gas chambers to give a mean free path between collisions of the order of the size of the chambers. Specifically in the case of 500 molecules, the width of the each chamber was $13.5 \times 10^{-6} cm$ and the height was $18 \times 10^{-6} cm$. The mean free path at equilibrium in each chamber is estimated by the ratio,

$$\lambda = \frac{\text{Area}}{n\ 2\ R}$$

which gives $\lambda = (13.5 \times 18 \times 10^{-12})/(250 \times 2 \times 3 \times 10^{-8}) = 16.2 \times 10^{-6} cm$. 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.

3 The Trapdoor as a Rectifier

We now discuss the behavior of the trapdoor when large density differences between the two chambers are imposed by external means. We have 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 we can observe the rectifying behavior, and we look at three different methods.

The first method 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 we measure the density in each chamber until the populations in the two chambers become approximately equal. 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 above, where all the particles are positioned initially along the outermost wall of one chamber. The idea is to measure the time interval it takes for 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 $25/T$ gives the current of particles that pass through the middle wall opening in response to the density difference at that time. Figure 3 plots the particle current for a system of 500 particles against the density difference between the two

chambers. We see that the curve in figure 3 resembles very much the voltage-current characteristic of an electrical diode, indicating that the trapdoor acts as a rectifier when large density differences are imposed by external means.

Specifically figure 3 shows the values $1/(T2-T1)$ against the average density difference $(D2+D1)/2$ during the time interval $(T2-T1)$. $D1$ is the density difference at the starting time $T1$, and $D2$ is the density difference at the finishing time $T2$ when 25 molecules have moved from the source chamber (high density) to the sink chamber (low density). The y-axis is in units of 25×10^9particles/*sec*. The x-axis is in normalized number of particles difference, so that an interval of size 0.1 corresponds to 25 particles moving from one chamber to the other $(0.1\times500\times\frac{1}{2}=25)$. We have not included in our plot the intervals $(-1,-0.9)$ and $(0.9,1.0)$ because the times immediately after releasing the system from our initial conditions do not correspond to smooth flow from one chamber to the other.

The third and last method of observing the rectifying behavior of the trapdoor is to measure the time average flow of particles through the middle wall opening when a large density difference is maintained artificially. In contrast to the equilibration studies above, this study characterizes the steady state behavior of the trapdoor. The experiments are set up as follows. We reverse bias the system by constantly removing all particles that hit the rightmost wall of the right chamber and re-inserting them in the left side of the left chamber. This results in a density difference that tends to close the trapdoor. Conversely we forward bias the system by re-inserting molecules from the leftmost wall into the right chamber.

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

Table 1: 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 negative, and those crossing from right to left are counted positive.

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 negative and molecules passing right to left are counted positive. We list the results for two different systems, a system of 500 particles and a system of 100 particles. The time interval over which we averaged was about $10^{-5} sec$ for the 100 particle system and $10^{-6} sec$ for the 500 particle system, which are both large enough to guarantee that 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. Therefore 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. For some geometries the rectifying behavior may almost vanish. Experimentally we have found that our trapdoor system becomes a better rectifier the longer the trapdoor is, and the more molecules there are near the trapdoor. A possible explanation is the following: If many collisions take place exclusively on one side of the trapdoor in the time interval that the door needs to move from one door stop to the other, then the trapdoor will be kept exclusively near one door stop, and the probability of moving significantly away from that door stop will be very small. For example if many collisions take place exclusively on the left side of the trapdoor, then the trapdoor will be kept near the middle wall bouncing between the door stop there and the large number of particles on the left. We have also found that the trapdoor performance can be improved 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 left chamber into the 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.

4 Verification of the Second Law

The question we discuss now is whether our trapdoor mechanism can violate the second law of thermodynamics. The trapdoor can open to the left but not to the right, and this intends to hinder the passage of molecules from left to right, while providing an easy access from right to left. The goal of the trapdoor is to exploit the naturally occurring variations in density between the two chambers, and to make states of higher density in the left chamber last longer than the corresponding states of higher density in the right chamber. Section 3 showed that the trapdoor indeed acts as a rectifier when large density differences are imposed by external means. One might expect that the rectifying behavior will also work when the trapdoor is left to operate on its own inside an isolated system of molecules. In other words one might expect that a trapdoor that opens to the left will create a higher density in the left chamber than the right chamber on the average. Our simulations however have shown the opposite. 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 average number of molecules in the right chamber. Further it turns out the excess of particles in the right chamber is not a true density difference between the two chambers. We have checked this by opening an additional hole to the middle wall that separates the two chambers, in addition to the hole covered by the trapdoor. If the trapdoor acted as a pump of molecules from one chamber to the other, then a flow from one chamber to the other should be observed on the average. In our simulations we did not observe any flow.

The reason for having a lower number of particles in the left chamber on the average is that the presence of the trapdoor in the left chamber takes up volume. From the point of view of the molecules, the available area in the left chamber is slightly smaller than the available area in the right chamber. To measure the effect of the excluded area by the trapdoor, we performed an experiment of 20 particles where each chamber measured $13.5 \times 10^{-7} cm$ in length and $18 \times 10^{-7} cm$ in height. The particle radius was $R = 6 \times 10^{-8} cm$ giving a mean free path in the order of $20 \times 10^{-7} cm$. The length of the trapdoor (vertical direction) was $10 \times 10^{-7} cm$. Given these numbers one can calculate 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 average 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 we must consider the motion of the *center* of the particles. For the right chamber we have $[(13.5 \times 18) - (13.5 + 13.5 + 18) \times 0.06] \times 10^{-14} cm^2$. For the left chamber we must subtract from the above the area taken up by the trapdoor $[(10 \times 0.06) + \pi(0.06)^2] \times 10^{-14} cm^2$. Putting it all together we find $N_L = 0.484$. In our simulations we found the time average number of particles in the left chamber to be 0.486 in good agreement with the theoretical estimate. We note that there is an additional small correction to the available area in each chamber because the presence of one particle in some location excludes other particles from that location. However this correction is small in our system, less than $10\pi(0.06)^2 \times 10^{-14} cm^2$, and does not change the first three decimal places of the theoretical estimate.

We see that the operation of our 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. In addition we have found in our simulations that the time average of the temperature (kinetic energy averaged over particles and divided by the number of degrees of freedom, two for particles and one for the trapdoor) is identical in each chamber and equal to the temperature of the trapdoor. Finally the time average velocity distributions in each chamber are Gaussian distributions in v_x and v_y identical to each other and identical between the two chambers, consistent with the Maxwell-Boltzmann distribution and equipartition of energy. We conclude that our trapdoor system can not rectify the naturally occurring differences in density between the two chambers, and does not violate the second law.

An intuitive explanation of why our trapdoor fails to work when operating in an isolated system of gas molecules, is that the trapdoor gets thermalized — its temperature equals the temperature of the particles — and its thermal motion prevents the rectifying behavior [13, 15]. By contrast, a macroscopic trapdoor works successfully as a rectifier because it can get rid of excess energy through dissipation. Following this analogy further we expect that our trapdoor would work successfully if a reservoir of lower temperature than the particles in our system were used to cool the trapdoor. In that case our

trapdoor would act as a heat engine, pumping molecules from one chamber to the other. We have performed simulations to test this idea, and we report our results in the next section.

5 The Trapdoor as a Heat Engine

To convert our trapdoor system into a heat engine, we remove energy from the trapdoor in small increments, scaling the trapdoor's velocity by 0.5 every Δt time interval where Δt is chosen 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. The slowing down of the trapdoor is performed only when the trapdoor is near the closed position, which makes the trapdoor tend to remain closed. We note that the mass of the trapdoor in relation to the mass of each particle is crucial for efficient operation of this heat engine. 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 can open the trapdoor and let the particle through, even though some energy is lost by interacting with the trapdoor. On the other hand if the trapdoor mass is much larger than the mass of one particle, then many particles from the right chamber must collide with the trapdoor in a short amount of time, in order to open the trapdoor. Clearly the latter situation occurs much less frequently than the former, and makes the trapdoor less efficient. 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 $4.7 \times 10^{-24} gm$, or one tenth of the mass of one particle. The time interval Δt which controls the rate of energy dissipation is $2.5 \times 10^{-13} sec$, while the mean free path and mean collision time in the left chamber are of the order of $20 \times 10^{-7} cm$ and $5 \times 10^{-11} sec$. The length of the trapdoor is $6 \times 10^{-7} cm$ and each chamber measures $13.5 \times 10^{-7} cm$ by $18 \times 10^{-7} cm$. In this experiment we have also included a second hole in the middle wall, of size $1 \times 10^{-7} cm$, in addition to the hole covered by the trapdoor. The purpose of the additional hole is to verify that the trapdoor can act as a pump of molecules from right to left, by exhibiting the *return*

flux of molecules. The graph in figure 4(a) shows how the normalized density in the left chamber builds up as soon as the system is released starting from uniform density. The time average of the density in the left chamber over long periods of time ($10^{-5}sec$) is around 0.76. The graph in figure 4(b) shows the accumulated flux of particles through the trapdoor hole (negative slope) and the accumulated flux of particles through the second hole that allows free passage. The slope of the accumulated flux (measured over $10^{-5}sec$) is approximately 2×10^{9}particles/sec. The time average temperature of the trapdoor is 11 degrees Kelvin, compared to 270 degrees Kelvin averaged over all particles. These results show that the trapdoor can operate successfully as a rectifier when a reservoir of lower temperature is available, but as discussed previously it can not operate successfully when run at the same temperature as the gas particles, in accordance with the second law of thermodynamics.

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Figure 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.

Figure 2: The absolute value of the relative density difference between 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.

Figure 3: The flux of particles from one chamber to the other is plotted against the density difference. $N1$ is the number of particles in the left chamber, $N2$ the right chamber, and N the total number of particles. The y-axis is in units of 25×10^9particles/sec.

Figure 4: The trapdoor as a heat engine includes a mechanism for cooling the trapdoor. The graph on the top (a) shows how the normalized density in the left chamber builds up after the system is released from uniform density. The graph on the bottom (b) shows the accumulated flux of particles through the trapdoor opening (negative slope) and the accumulated flux through an additional opening that allows free passage (positive slope).

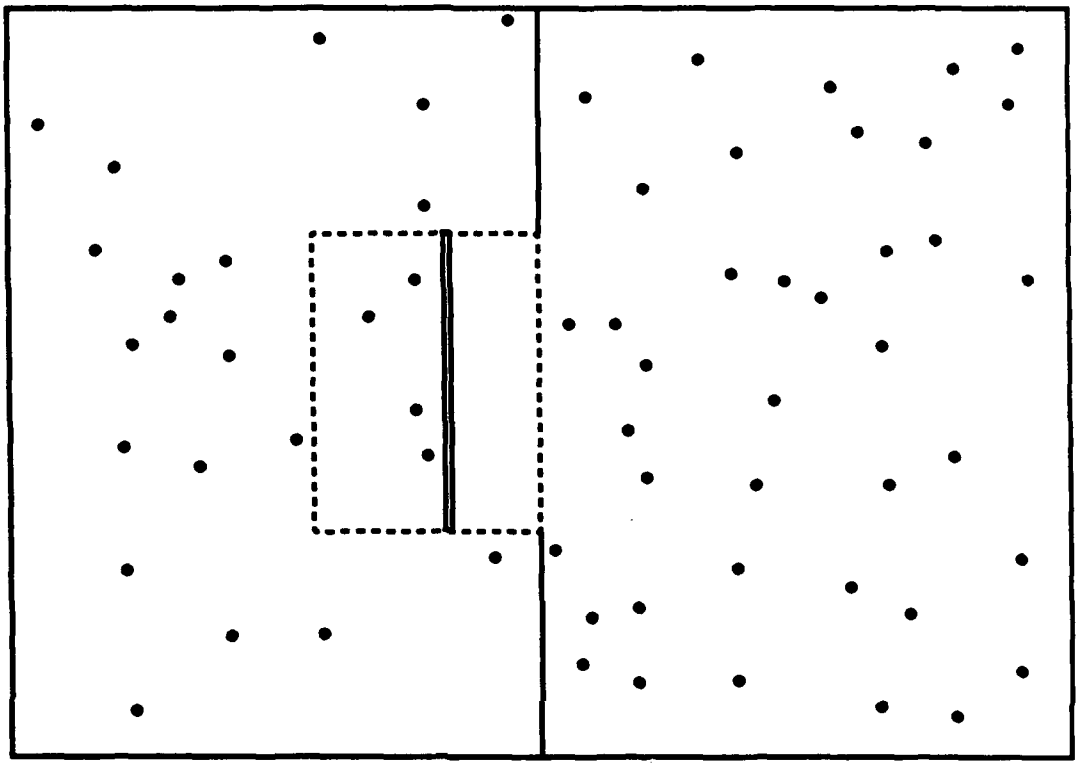

fig. 1

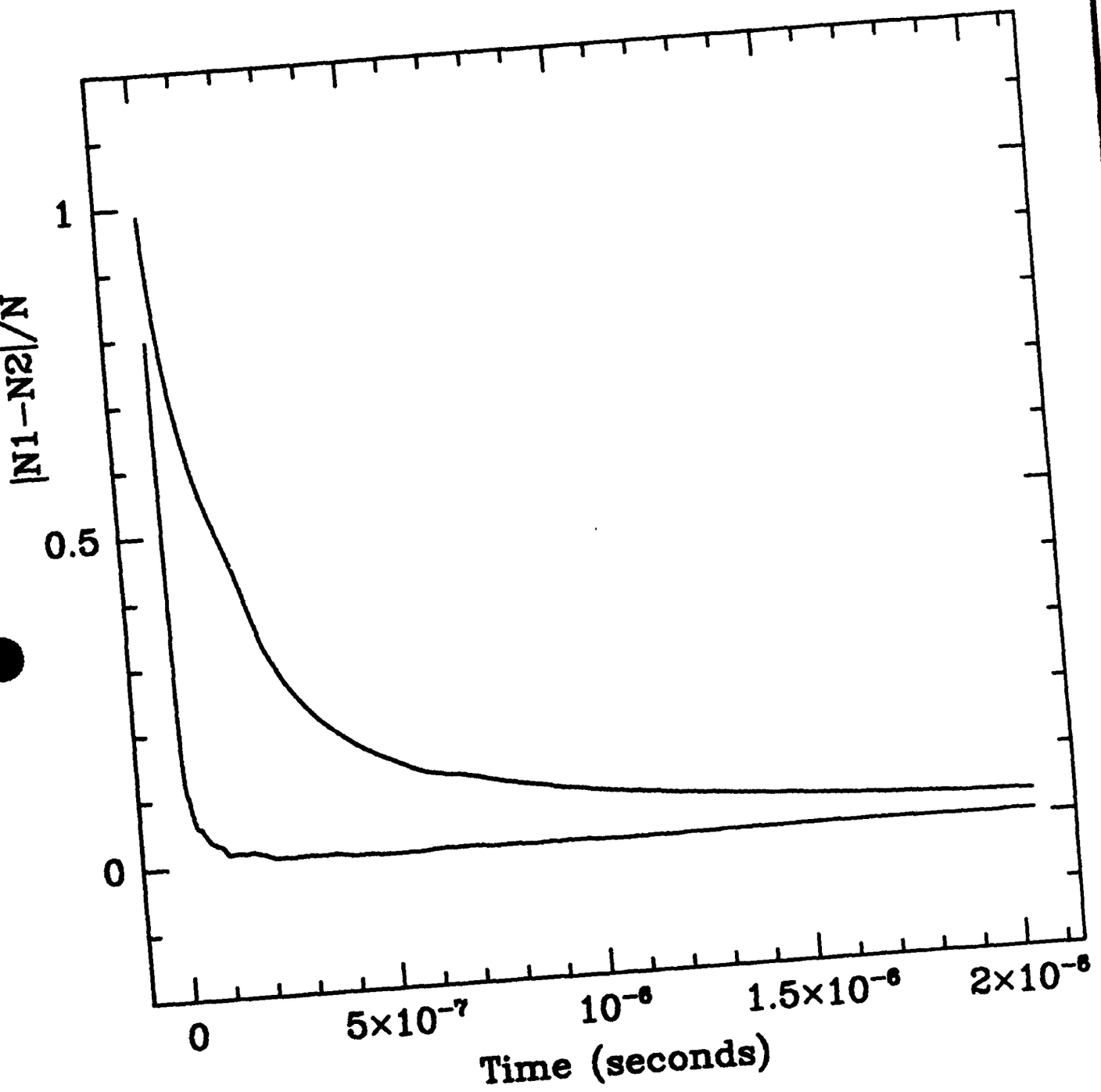

fig. 2

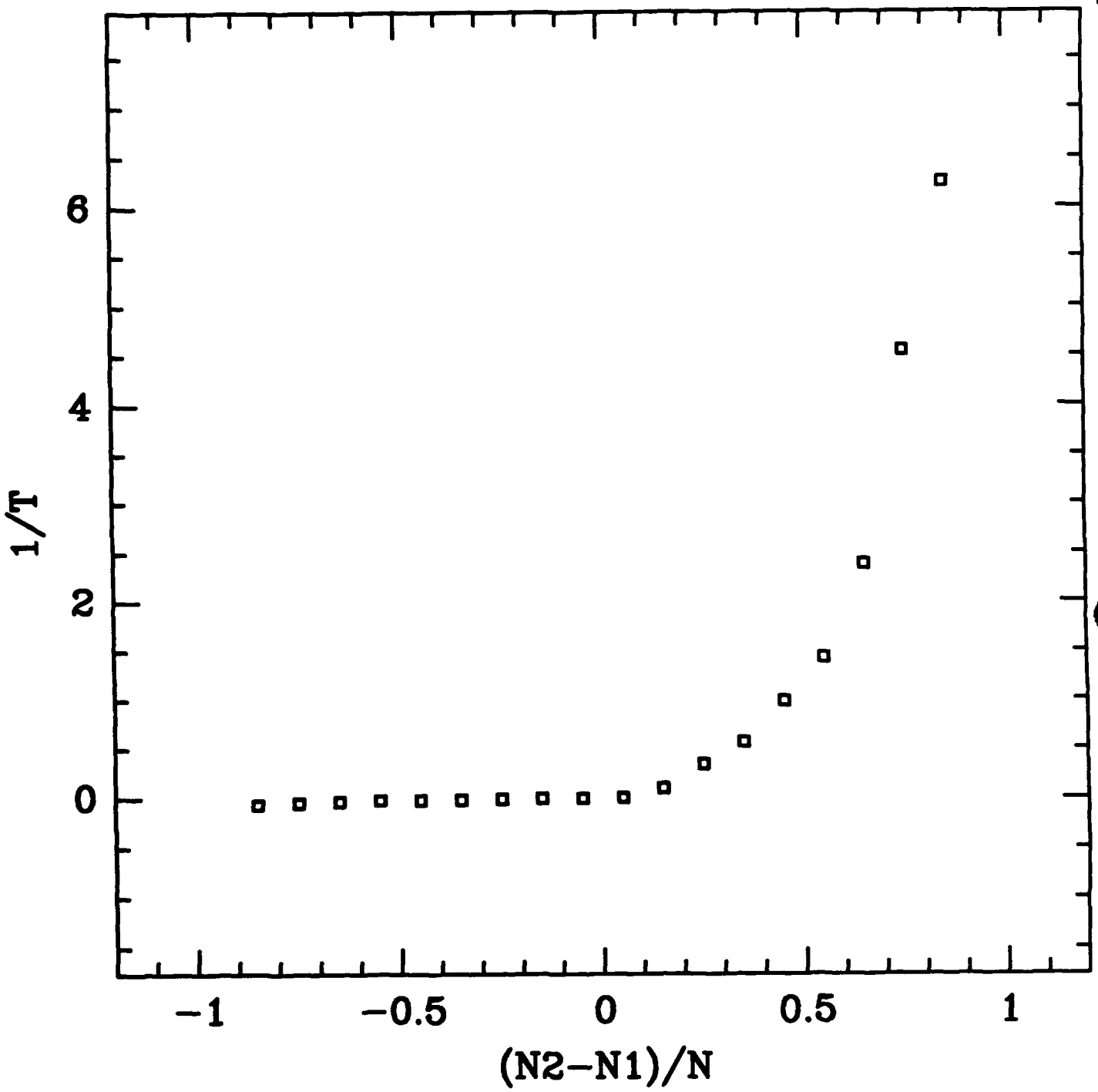

fig. 3

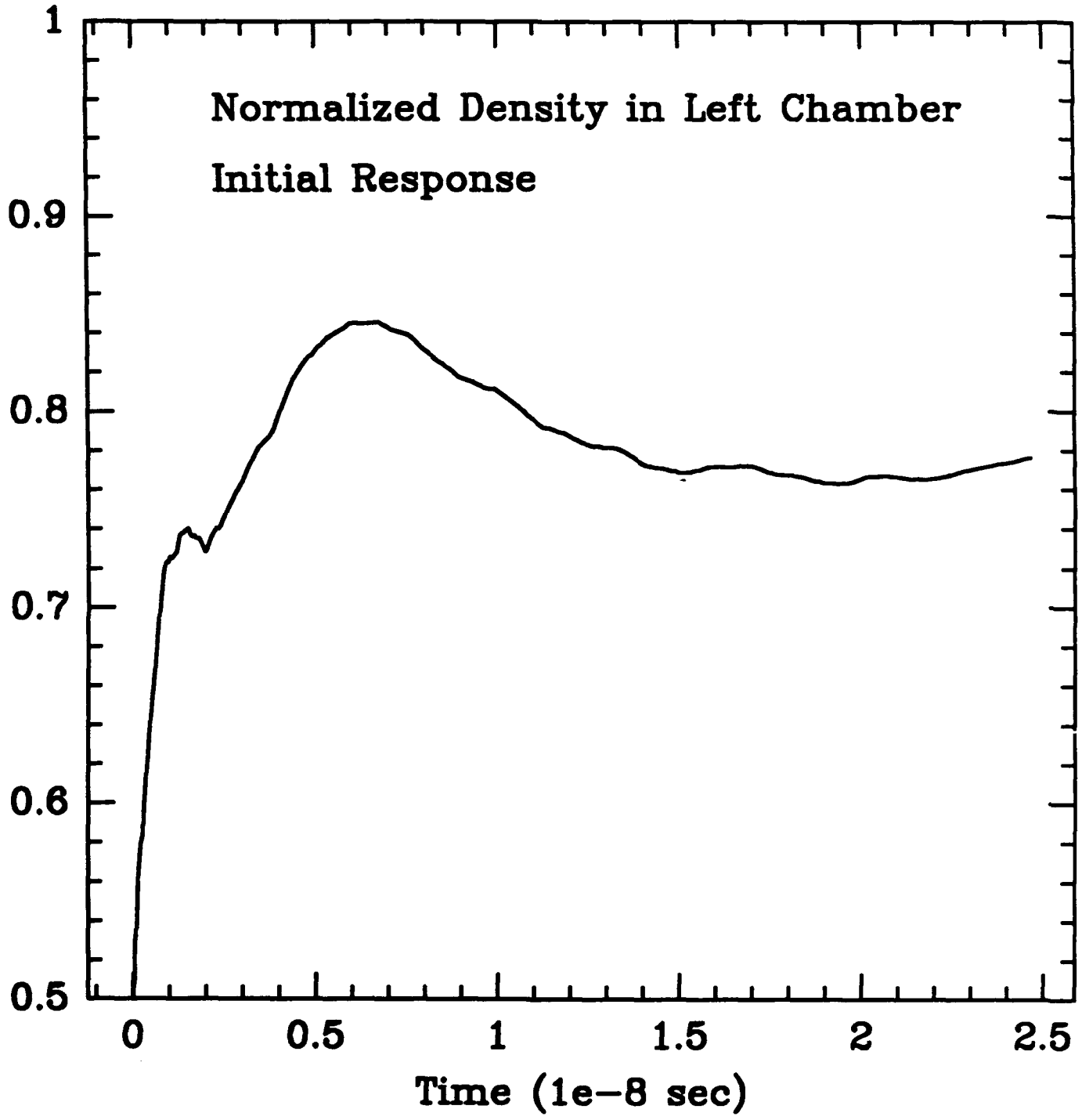
Normalized Density in Left Chamber
Initial Response
1
0.9
0.8
0.7
0.6
0.5
0
0.5
1
1.5
2
2.5
Time (1e−8 sec)

fig 4a

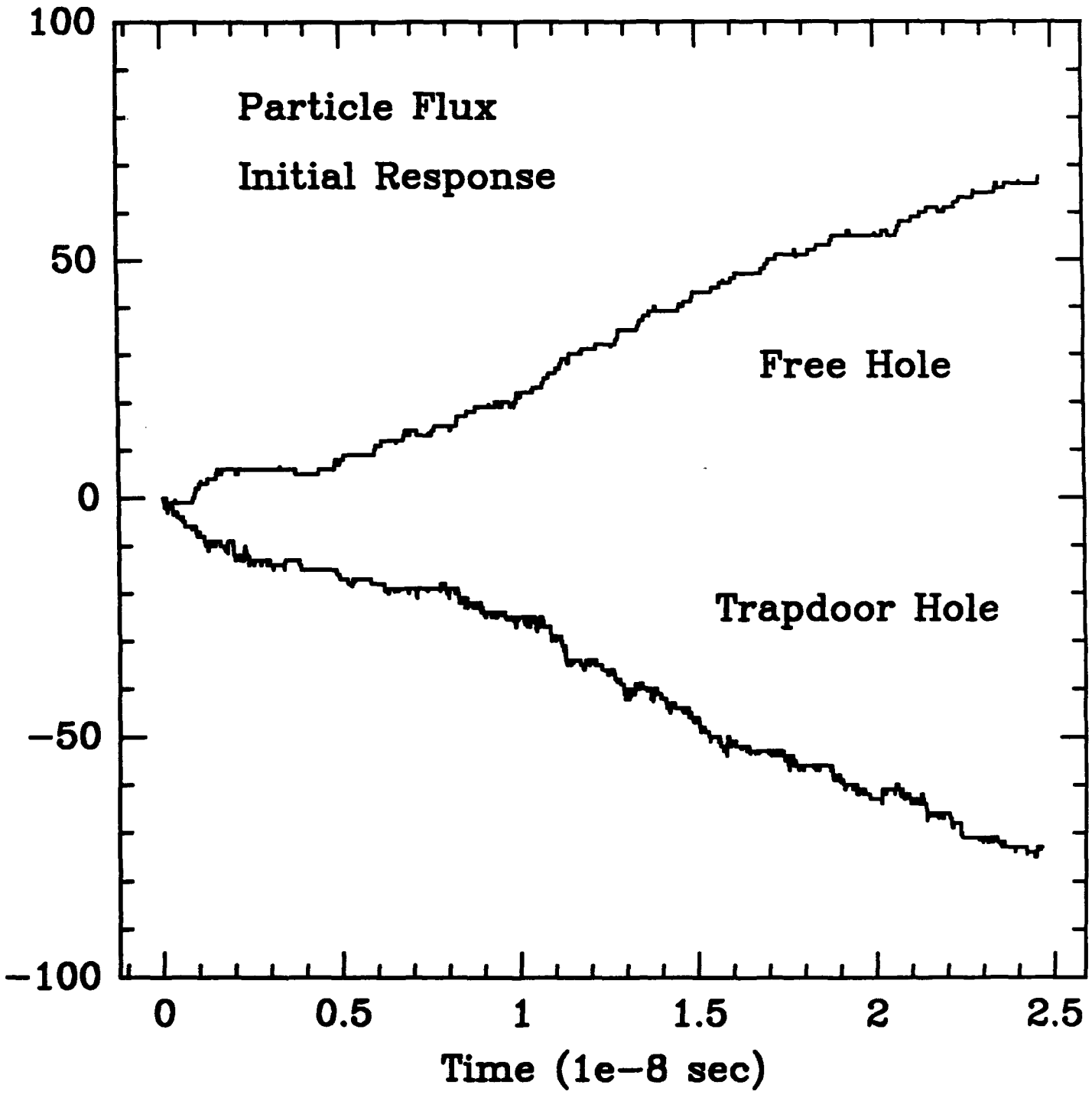
Particle Flux
Initial Response
Free Hole
Trapdoor Hole
100
50
0
−50
−100
0
0.5
1
1.5
2
2.5
Time (1e−8 sec)

fig. 4b