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Author
Wheeler, John C

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Resolution of a Classical Gravitational Second–Law Paradox

John C. Wheeler*

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Sheehan and coworkers have claimed [D. P. Sheehan e. al. Found Phys. **30**, 1227 (2000); **32**, 441 (2002); D. P. Sheehan in Quantum imits to the Second Law, AIP Conference Proceedings **643** (American Institue of Physics, Melville, NY, 2002, p. 391] that a dilute gas trapped between an external shell and a gravitator can support a steady state in which energy flux by particles in one direction is balanced by energy flux by radiation in the opposite direction, and in which work can be extracted from an isothermal heat reservoir, thereby violating the second law of thermodynamics. In this paper, we identify a fundamental error in their simulation and analysis of their model system that vitiates their conclusions. We analyze a simpler, exactly soluble, three-dimensional model of a very dilute gas in a gravitational field between two thermal reservoirs, and show that their conclusions are not supported for the simple model. We show that their method of simulation, when applied to either the simple model or their more complex model under simpler conditions where the answers are known, leads to unphysical results. We also show that, when appropriate sampling is done, their model gives results in accord with the second law and detailed balance.

KEY WORDS: thermodynamics; second law; gravitation; paradox; resolution; kinetic theory.

1 INTRODUCTION

Recently Sheehan and coworkers have claimed[(1–3)] that a dilute gas trapped between an external shell and a gravitator will support a steady state in which the shell and gravitator are at essentially the same temperature, but in which the gas transports

*Department of Chemistry and Biochemistry 0340; University of California, San Diego; La Jolla CA 92093-0340; e-mail: jwheeler@ucsd.edu

energy in one direction while the black–body radiation field transports energy in the opposite direction, maintaining essentially equal temperatures of the walls. They assert, in addition, that this steady state results in a net force on the gravitator that can be used to extract work isothermally from the heat in the outer reservoir. This assertion conflicts with one of the most trusted principles of physics, namely, the second law of thermodynamics. There is a widespread and understandable response among scientists to dismiss such results simply as "therefore clearly in error" and ignore them. However, as pointed out in Ref. 1, systems with gravitational fields require extra care in thermodynamics and can lead to surprising results. More generally, there is an obligation on the part of the scientific community to demonstrate where the error occurs in claims of violation of physical laws so that it will be apparent that the claims are rejected on the basis of scientific argument and not mere prejudice. It is therefore of interest to identify the errors, if any, in their analysis.

In this paper, we identify a fundamental error in both the simulation and analysis presented in Refs. 1–3 that renders their conclusions inapplicable to any system of physical interest. We analyze a simpler three–dimensional model of a very dilute gas in a uniform gravitational field, trapped between two plates at altitudes 0 and H that serve as thermal reservoirs at temperatures T_0 and T_H, respectively, under conditions where the mean free path of the particles is much greater than H. This model is simpler, and in some ways, perhaps, less realistic than that considered in Refs. 1–3, but it has the virtue of being exactly soluble, given the underlying assumptions, and therefore easily allows one to consider various limits not considered by those authors. Treated properly, this model exhibits none of the anomalous behavior seen in Refs. 1–3. However, if their method of simulation and analysis is applied to this simpler model, the same unphysical results observed in Refs. 1–3 are obtained. Moreover, their method of simulation leads to unphysical results when applied to either model in the *absence* of gravity, where the answers are known. If their model is treated appropriately, it gives results in accord with the second law and with detailed balance.

In the remainder of this section, we briefly describe their model and their method of simulation, and identify the fundamental error in their simulation and analysis that invalidates their conclusions. In Sec. 2, we describe the simpler model and give its solution under steady–state conditions. We show that if $T_0 \neq T_h$, then energy transport by the gas takes place from the higher to the lower temperature, *i.e.*, in the direction tending to remove the temperature difference, in accordance with second–law expectations. We also show that when $T_0 = T_h$, no flow of energy takes place in either direction between the reservoirs, and the gas density is described by an equilibrium Maxwell–Boltzmann distribution of velocities, with densities and pressures that vary with height according to the barometric law, again, in accordance with second–law expectations. In Sec. 3, we justify in detail our identification of the error made by Sheehan *et al.* and show how it is responsible for the unphysical results they obtain. We show that if their method is applied to the simpler model in Sec. 2, then that model, too, exhibits the same pathologies as they find for their model. We show that if either model is treated by their method in the absence of gravity, an unphysical distribution of velocities is obtained for the density of particles in the container. We also show there that if their model is treated correctly, it is consistent with second law expectations. A discussion of the results appears in Sec. 4.

The model described in Refs. 1–3 consists of a large spherical cavity of radius r_c, the outer wall of which is clamped at temperature T by an infinite heat reservoir. The cavity contains a planet–sized spherical gravitator of radius r_G and mass m_G and a very dilute gas. The gravitator is coated on two opposite hemispheres with materials of different trapping probability for the gas particles. Gas particles striking the outer wall of the cavity are absorbed and re-emitted thermally. Gas particles striking the gravitator are either reflected specularly or absorbed with a probability that depends upon the coating material and the particle velocity, in which case they are re-emitted with a velocity distribution characteristic of the temperature of the gravitator surface. The gas particles are taken to be structureless, with mass m_A and radius r_A, and with particle density, $n_{\rm cav}$, sufficiently low that their mean free path in the cavity is large compared with the cavity diameter, so that particle–particle collisions are rare compared with particle–wall and particle–gravitator encounters. In addition, the gas is taken to be sufficiently dilute that black–body radiation maintains the temperature of the gravitator essentially uniform and equal to that of the cavity wall, regardless of what the particles may do. Particles leaving the outer wall of the cavity are attracted to the gravitator by the universal gravitational force, and so arrive at the gravitator with greater kinetic energy than that with which they left the wall. The authors argue that the detailed dynamics of the particles, coupled with the thermalization at the outer wall and at the gravitator, leads to a steady state in which there is a net force on the gravitator and a flux of energy from the gravitator to the cavity wall carried by the particles that is balanced by a net flux from the wall to the gravitator carried by the black–body radiation. The authors make reference to a "standard gravitator" with the parameters $m_A = 4$ amu, $m_G = 2 \times 10^{23}$ kg, $r_A = 10^{-10}$ m, $r_G = 1.6 \times 10^6$ m, $r_c = 3.21 \times 10^6$ m, $T = 2000$ K, $n_{\rm cav} = 5 \times 10^{10}$ m^{-3}. [Additional parameters are also specified, having to do with details of the trapping probabilities, but they will not be needed here.]

Although the "standard gravitator" described by the authors contains about 6×10^{30} gas particles at an average density of about 5×10^{10}m^{-3}, the authors' simulation involves only a single particle, which the authors follow over many excursions through the cavity between the cavity wall and the gravitator. There is, in principle, nothing wrong with such a procedure, provided that the simulation of the dynamics is carried out correctly, that averages are taken correctly, and that the sampling of the velocities of particles emitted from the cavity wall and gravitator is appropriate to the property being simulated. As a practical matter, there are some troubling difficulties with this procedure. Because they find that some trajectories leaving the gravitator or cavity wall result in near–orbiting trajectories, in which the particle orbits nearly indefinitely at some intermediate altitude, the authors invoke rare collisions between the particles to eliminate these. Because there is no ensemble of such particles in the simulation, the authors simply thermally randomize the velocity of the particles on an infrequent basis. This fails to satisfy conservation of momentum, so that Newton's equations of motion are not strictly being followed. This fact was not mentioned in Refs. 1–3, and we became aware of it only through discussions with Sheehan [D. P. Sheehan, private commun.] Sheehan acknowledges that this is a weakness of the procedure but argues that the authors tested the model extensively and found that the results were insensitive to the details of this randomization in the range of conditions in which the unusual phenomena occurred. This may well be so, and in any case, that weakness in their method is not the error that we suggest is responsible for their unphysical results.

Even the presence of these orbiting trajectories is troublesome, because the trajectories of the particle in the cavity are Keplerian orbits,[(4)] following conic sections, each of which should result in collision with either the gravitator or the cavity wall within a relatively short time. Sheehan speculates [D. P. Sheehan, private commun.] that they may arise from roundoff errors in the simulation. In any case, this also is not the problem responsible for the unphysical results they obtain.

The fundamental error committed by the authors of Refs. 1–3 that is responsible for the unphysical results they obtain is that they did not sample the velocities of the particles emitted from the cavity wall and gravitator from a distribution appropriate to the property being simulated. This error resulted because they did not make a clear distinction — either for themselves or for the reader — between the distribution over velocities of the particle *density*, on the one hand, and of the particle *flux*, or rate of production of particles by a reservoir, on the other. As a result, they sample from a velocity distribution appropriate for a particle *density* when, in fact, the property for which they are sampling plays the role of a particle *flux*. We justify this assertion in detail in Sec. 3.

This has the consequence that, with the distribution of velocities from which Sheehan *et al.* have sampled, neither the cavity wall nor the gravitator is capable of attaining equilibrium with a gas that is itself in internal equilibrium at the same temperature, *even in the absence of any gravitational field.* It is not surprising, therefore, that this sampling also leads to an inability of the system to reach equilibrium when a gravitational field is present. This last observation is important because the inability of the particles to reach equilibrium by themselves — or even to attain a steady state with equal temperatures of the cavity wall and gravitator without the dominating influence of black–body radiation — was a feature of their results almost as puzzling and counterintuitive as the violation of the second law itself. Both are explained by the identification of the error in sampling, and both are corrected by correction of the sampling procedure. These points are developed in more detail in Secs. 3 and 4.

The authors of Ref. 1 stress the point that the behavior they report is "emergent," and "in no way 'programmed' into the following numerical simulations." While we do not question the honesty of their intentions, their selection of a distribution from which to sample the velocities of the particles emitted by the cavity wall and gravitator does constitute a choice by those investigators that was, quite literally, programmed into the simulations. That choice requires scientific judgment to ensure that the results are consistent with known physical behavior. In particular, a choice that prohibits equilibrium with detailed balance between an equilibrium gas and the cavity wall or gravitator in the absence of gravitational forces can be expected to lead to unphysical behavior of the model more generally.

That Sheehan *et al.* have sampled from a distribution inappropriate for the property being sampled does not prove that their device obeys the second law when appropriate sampling is done. It does, however, vitiate any conclusions from their results about their device under physically relevant conditions. In the next section, we examine a simpler model and show explicitly that it obeys the second law when treated properly. In Sec. 3, we show that it exhibits the same pathologies as the more complicated model when sampled in the manner corresponding to that employed by Refs. 1–3, that both models exhibit pathologies in the *absence* of any gravitational field when this sampling is used, and that their model is consistent with the second law when treated appropriately.

2 SIMPLE MODEL AND SOLUTION

We consider a sample of a fixed number of monatomic gas particles in a three–dimensional cubic box of edge length H, with floor and ceiling at height $z = 0$ and $z = H$ in a uniform gravitational field with acceleration g downward along the z axis. The vertical walls may be taken as either perfectly reflecting or following periodic boundary conditions. The upper wall is perfectly absorbing and serves as a thermal bath at temperature T_H. That is, any particle striking the upper wall is absorbed and re-emitted with a distribution of velocities characterized by the temperature T_H. The lower wall reflects specularly with probability α, and absorbs with probability $1 - \alpha$, re–emitting with a velocity distribution characterized by the temperature T_0. We take the reflection probability α to be independent of the particle velocity. This is not essential; the problem can be formulated with α as a function of the component of the velocity normal to the surface, as in Refs. 1–3. The only consequence is that certain integrals can no longer be computed in closed form. We assume that the gas is so dilute that collisions between gas particles can be neglected: a particle emitted from the upper wall inevitably strikes the lower wall; a particle emitted from the lower wall either strikes the upper wall, if it leaves the lower wall with z component of its velocity satisfying $v_z > +(2gH)^{1/2}$, or else rises until the gravitational acceleration brings it to a halt and then falls back to strike the bottom wall with the same kinetic energy with which it left. The model is fully three–dimensional although much of the analysis is essentially one–dimensional, and the model is easily reduced to a two– or one–dimensional version. The vector position and velocity of a particle are $\mathbf{r} = (x, y, z)$ and $\mathbf{v} = (v_x, v_y, v_z)$. We will indicate throughout the development the way in which results differ in one and three dimensions.

This is a much simpler model than the one studied in Refs. 1–3, but the one–dimensional version is essentially identical to that in the one–dimensional argument presented there to justify their results. It retains the essential feature that it is possible to compare the forces exerted on partially reflecting surfaces with different trapping probabilities. Sheehan confirms [D. P. Sheehan, private commun.] that, on the basis of his arguments, he expects nonzero energy flux by the particles in this model in a steady state with $T_0 = T_H$, and a force on the “gravitator” (*i.e.*, the lower wall) that depends upon α. We show here that, for a physically reasonable choice of particle flux from the upper and lower walls, this is not the case. Rather, under conditions of steady state with respect to particle flux, the energy flux when $T_H \neq T_0$ is in the direction tending to equalize the temperatures of the reservoirs, and when $T_H = T_0$ there is no energy flux, and the force on the lower wall is independent of α. In the following section, we show that, if an unphysical choice for the flux is made, corresponding to the sampling choice made in Refs. 1–3, then the same unphysical consequences observed there follow.

Let $n(\mathbf{r}, \mathbf{v})d\tau_v$ be the (spatial) number density of particles at location $\mathbf{r}$ in the velocity volume element $d\tau_v$ centered at velocity $\mathbf{v}$. In three dimensions, this is the number of particles per unit volume in the velocity volume element $d\tau_v = dv_x dv_y dv_z$. In one dimension, it is the number of particles per unit length in $d\tau_v = dv_z$. In a similar manner, let $j(\mathbf{r}, \mathbf{v})d\tau_v$ be the number flux of particles in the upward direction through the horizontal surface at height $h = z$ at location $\mathbf{r}$ in the velocity volume element $d\tau_v$. This flux is a number per unit time per unit area in three dimensions, and a number per unit time in one dimension.

It will turn out that the steady–state solutions for $n(\mathbf{r}, \mathbf{v})$ and $j(\mathbf{r}, \mathbf{v})$ are independent of x and y, and so it is convenient to have an alternative notation that reflects this. Accordingly, we will use $n_h(\mathbf{v})d\tau_v$ for the number density in the specified velocity range at height $z = h$ and $j_h(\mathbf{v})d\tau_v$ for the upward flux in the indicated velocity range through the horizontal plane at height $z = h$. We will adopt the convention that $n_0(\mathbf{v}) \equiv \lim_{h \searrow 0} n_h(\mathbf{v})$ is the density just above height 0 and $n_H(\mathbf{v}) \equiv \lim_{h \nearrow H} n_h(\mathbf{v})$ is the density just below height H. We adopt the corresponding conventions for the meaning of $j_0(\mathbf{v})$ and $j_H(\mathbf{v})$. The particle density and particle flux are related by the *continuity equation*,[5,6]

$$j(\mathbf{r}, \mathbf{v}) = v_z n(\mathbf{r}, \mathbf{v}) \,, \tag{1}$$

in both the three– and one–dimensional versions of the problem.

Following Refs. 1 and 3, we start with the particles just below height H with $v_z < 0$ and with velocities in the range $d\tau_v$. These necessarily come from the reservoir with $T = T_H$, and so are described by a distribution characterized by temperature T_H. The fundamental assumption of our treatment is that the particle flux from the reservoir with $T = T_H$ in the velocity volume element $d\tau_v$ about $\mathbf{v}$ is the same as that in the gas at $h = H$ and is given by

$$\begin{aligned} j_{H,\mathrm{res}}(\mathbf{v})d\tau_v &= j_H(\mathbf{v})d\tau_v = j(x, y, z = H, \mathbf{v})d\tau_v \\ &= B v_z \exp\left(-\frac{\frac{1}{2}mv^2}{kT_H}\right) d\tau_v \qquad (v_z < 0) \,, \end{aligned} \tag{2}$$

where m is the mass of the particles, T_H is the Kelvin temperature of the upper wall and k is Boltzmann's constant; where $v^2 = |\mathbf{v}|^2 = v_x^2 + v_y^2 + v_z^2$ in three dimensions and $v^2 = v_z^2$ in one dimension; and where B is a normalization constant having to do with the total particle density at H that remains to be determined. The corresponding density in the gas is then given, via Eq. (1), as

$$n_H(\mathbf{v})d\tau_v = B \exp\left(-\frac{\frac{1}{2}mv^2}{kT_H}\right) d\tau_v \qquad (v_z < 0) \,. \tag{3}$$

Note that the flux is independent of the horizontal coordinates, x and y, and independent of the azimuthal angle of the velocity around the z axis. As a consequence, the density is also independent of horizontal position and is isotropic in $\mathbf{v}$ apart from the requirement that, for the moment, we are considering only particles with $v_z < 0$.

Our choice for the flux in Eq. (2) plays the same role in this model that the choice for the distribution of velocities of particles leaving the cavity wall plays in Refs. 1–3. In each model, a choice must be made for the way in which statistics is used to avoid describing the detailed dynamics of the absorption and emission process from the wall. There are compelling arguments for accepting a form like (2) as reasonable for the flux emanating from a thermal reservoir that is in internal equilibrium. We will develop those further in Secs. 3 and 4. We note here, however, that if the reservoir is ever to be in equilibrium with a gas that is itself in internal equilibrium at the same temperature, then the flux from the reservoir under *those* conditions *must* be of the form in Eq. (2). This is because the density of the gas will be of the form in Eq. (3) for *all* v, and so its flux will be of the form (2) for all v. The choice we have made guarantees that the the upper reservoir is capable of establishing equilibrium, with detailed balance at every velocity, with a gas that is itself in internal equilibrium at the same temperature. This seems to us to be a reasonable requirement to place upon the choice of statistics of particles emanating from the upper wall. The choice made by Sheehan, *et.al.* does not satisfy this requirement, as we show in Sec. 3.

Each particle at height $z = H$ and with $v_z = v_{z,H} < 0$ will reach the bottom reservoir, at height $z = 0$, with a larger negative z component of its velocity, $v_{z,0}$, determined by conservation of energy,

$$\frac{1}{2}mv_{z,0}^2 = \frac{1}{2}mv_{z,H}^2 + mgH \,, \tag{4}$$

and with the x and y components of the kinetic energy unchanged, so that

$$\frac{1}{2}mv_0^2 = \frac{1}{2}mv_H^2 + mgH \,. \tag{5}$$

We observe that $n(\mathbf{r}, \mathbf{v})$ is essentially (within a factor of m^3) the *density in phase space* of the particles. [Because we employ Cartesian coordinates for position and velocity, the components of the momentum vector are just m times the corresponding components of the velocity.] We may therefore invoke *Liouville's theorem*[7]

$$n(\mathbf{r}, \mathbf{v}, t) = n(\mathbf{r}', \mathbf{v}', t') \,, \tag{6}$$

where $\mathbf{r}'$ and $\mathbf{v}'$ are obtained from $\mathbf{r}$ and $\mathbf{v}$ via the equations of motion over the time interval $t' - t$, during which the trajectory remains entirely between the upper and lower walls. Strictly, this relates the densities at two different times. For a steady state, however, the densities are independent of time, so the equation also applies to the two locations in phase space at the same time. We may then conclude that, in a steady state, particles starting at height $h = H$ with density $n_h(\mathbf{v})$ given by Eq. (3)

will arrive at height 0 at with with density given by

$$
\begin{aligned}
n_0(\mathbf{v}_0) &= n_H(\mathbf{v}_H) && (7)\\
&= B\exp\left(-\frac{\frac{1}{2}mv_H^2}{kT_H}\right) && (8)\\
&= B\exp\left(-\frac{\frac{1}{2}mv_0^2 - mgH}{kT_H}\right) \qquad \left(v_{0,z} < -(2gH)^{1/2}\right)\,. && (9)
\end{aligned}
$$

This implies that

$$
n_0(\mathbf{v}) = B\exp\left(\frac{mgH}{kT_H}\right)\exp\left(-\frac{\frac{1}{2}mv^2}{kT_H}\right) \qquad \left(v_z < -(2gH)^{1/2}\right)\,. \tag{10}
$$

The independence of $n_H(\mathbf{v})$ from x, y and azimuthal angle implies the same for $n_0(\mathbf{v})$ when $v_z < -(2gH)^{1/2}$. This point is actually slightly subtler than it might seem at first. At any point on the surface $z = 0$, and for any incoming velocity $\mathbf{v}$ with $v_z < -(2gH)^{1/2}$, one can trace back the trajectory to find a unique point on the surface $z = H$ from which it came. However, given the location, $\mathbf{r}$, of the arriving particle, the magnitude of its velocity, v, and the vertical component v_z, there are still many possible azimuthal angles at which it may arrive. Each of these will trace back to a different initial spot on the surface $z = H$ and to a different initial azimuthal angle there. However, all these initial conditions will have the same initial v_z and v. Because of the independence of the density at $z = H$ on location in the plane and azimuthal angle, the resulting density at $z = 0$ is also independent of position in the plane and azimuthal angle.

We may now use the continuity equation (Eq. (1)) to find the corresponding flux at $h = 0$:

$$
j_0(\mathbf{v}) = Bv_z\exp\left(\frac{mgH}{kT_H}\right)\exp\left(-\frac{\frac{1}{2}mv^2}{kT_H}\right) \qquad \left(v_z < -(2gH)^{1/2}\right)\,. \tag{11}
$$

We have thus begun to make the connection between the distributions in the immediate vicinity of the two reservoirs.

Of the particles arriving at height $z = 0$ with $v_z < -(2gH)^{1/2}$, a fraction α will reflect specularly, and thus contribute to the density $n_0(\mathbf{v})$ for $v_z > +(2Hg)^{1/2}$. The remaining fraction $1-\alpha$ is absorbed by the reservoir and re-emitted with a distribution characterized by the temperature T_0. For particles just above height $z = 0$ with $v_z^2 < 2gH$, we can say with certainty that they emanated, either directly or indirectly via specular reflections, from the reservoir at T_0. Of the particles in this velocity range with negative v_z, a fraction α will reflect specularly at the lower wall, and so a fraction α of the particles with positive v_z are actually reflected particles. Only fraction $(1-\alpha)$ of the flux consists of particles emitted directly from the reservoir. We therefore assume that the particle flux *emitted from the reservoir* is given by

$$
j_{0,res}(\mathbf{v})d\tau_v = A(1-\alpha)v_z\exp\left(-\frac{\frac{1}{2}mv^2}{kT_0}\right)d\tau_v \qquad (v_z > 0)\,, \tag{12}
$$

where A is another normalization constant, yet to be determined. This is a second fundamental assumption of our treatment, parallel to the sampling assumption by Sheehan, *et al.* concerning the velocities of particles leaving from their gravitator. Again, note the independence of the flux from x and y and from the azimuthal angle of $\mathbf{v}$. This choice allows the reservoir at $h = 0$ to achieve equilibrium with a dilute gas that is itself in internal equilibrium at the same temperature.

It then follows from Liouville's theorem, applied to particles with $v_z^2 < 2gH$, that the total flux just above $h = 0$, both specularly reflected and from the reservoir, in the range $-(2gH)^{1/2} < v_z < +(2gH)^{1/2}$, is given by

$$j_0(\mathbf{v})d\tau_v = Av_z \exp\left(-\frac{\frac{1}{2}mv^2}{kT_0}\right) d\tau_v \qquad (v_z^2 < 2gH)\,. \tag{13}$$

For velocities with $v_z > (2gH)^{1/2}$, there is no reflected component from the reservoir at T_0, but there is a reflected component from the reservoir at T_H. Therefore, the flux just above $h = 0$ in this range of v_z is given by

$$\begin{aligned} j_0(\mathbf{v})d\tau_v &= (1-\alpha)v_z A \exp\left(-\frac{\frac{1}{2}mv^2}{kT_0}\right) d\tau_v + \\ &\quad \alpha B v_z \exp\left(-\frac{\frac{1}{2}mv^2 - mgH}{kT_H}\right) d\tau_v \qquad (v_z > +(2gH)^{1/2})\,. \end{aligned} \tag{14}$$

The particle densities corresponding to Eqs. (13) and (14) are

$$n_0(\mathbf{v})d\tau_v = A \exp\left(-\frac{\frac{1}{2}mv^2}{kT_0}\right) d\tau_v \qquad (v_z^2 < 2gH) \tag{15}$$

and

$$\begin{aligned} n_0(\mathbf{v})d\tau_v &= (1-\alpha)A \exp\left(-\frac{\frac{1}{2}mv^2}{kT_0}\right) d\tau_v + \\ &\quad \alpha B \exp\left(-\frac{\frac{1}{2}mv^2 - mgH}{kT_H}\right) d\tau_v \qquad (v_z > +(2gH)^{1/2})\,. \end{aligned} \tag{16}$$

All of the particles with $v_z > +(2gH)^{1/2}$ will reach the ceiling at $h = H$, so we may now use Liouville's theorem once again to follow this last density upward to $h = H$. This gives

$$\begin{aligned} n_H(\mathbf{v}) &= (1-\alpha)A \exp\left(-\frac{\frac{1}{2}mv^2 + mgH}{kT_0}\right) + \\ &\quad \alpha B \exp\left(-\frac{\frac{1}{2}mv^2}{kT_H}\right) \qquad (v_z > 0)\,. \end{aligned} \tag{17}$$

The corresponding flux is then given by

$$
\begin{aligned}
j_H(\mathbf{v}) &= (1-\alpha) v_z A \exp\left(-\frac{\frac{1}{2}mv^2 + mgH}{kT_0}\right) + \\
&\quad \alpha B v_z \exp\left(-\frac{\frac{1}{2}mv^2}{kT_H}\right) \qquad (v_z > 0)\,. \qquad (18)
\end{aligned}
$$

We now have $n_0(\mathbf{v})$, $n_H(\mathbf{v})$, $j_0(\mathbf{v})$ and $j_H(\mathbf{v})$ over the entire range of velocities in terms of the two as–yet–unspecified constants A and B, and the presumed known parameters of the system, m, H, T_0 and T_H. Moreover, they are expressed in terms of the *local velocities*. We are therefore now in a position to calculate the net fluxes of particles, energy and momentum through the planes at heights 0 and H. Before doing this, however, we note that the same idea could be used to obtain the velocity distribution of the particle density, and thereby of the particle flux, at any altitude h between 0 and H using the energy conservation relation $v_{z,0}^2 = v_{z,h}^2 + 2gh$ between $\mathbf{v}_0$ and $\mathbf{v}_h$, along with the corresponding energy conservation relation $v_{z,h}^2 = v_{z,H}^2 + 2g(H-h)$ between $\mathbf{v}_h$ and $\mathbf{v}_H$. We quote the results here, both for completeness and to provide a compact presentation of the results for $h = 0$ and $h = H$.

$$
\begin{aligned}
n_h(\mathbf{v}) &= B \exp\left(-\frac{\frac{1}{2}mv^2 - mg(H-h)}{kT_H}\right) \qquad \left(v_z < -\left(2g(H-h)\right)^{1/2}\right) \qquad (19) \\
&= A \exp\left(-\frac{\frac{1}{2}mv^2 + mgh}{kT_0}\right) \qquad \left(v_z^2 \leq 2g(H-h)\right) \qquad (20) \\
&= \alpha B \exp\left(-\frac{\frac{1}{2}mv^2 - mg(H-h)}{kT_h}\right) + \\
&\quad (1-\alpha) A \exp\left(-\frac{\frac{1}{2}mv^2 + mgh}{kT_0}\right) \qquad \left(v_z > \left(2g(H-h)\right)^{1/2}\right)\,. \qquad (21)
\end{aligned}
$$

In all of these formulas, $v^2 = v_x^2 + v_y^2 + v_z^2$ for the three–dimensional model, with the range $-\infty < v_x, v_y < \infty$. For the one–dimensional model, $v^2 = v_z^2$. The corresponding flux distribution is obtained, in either one or three dimensions, by simply multiplying the density distribution by v_z.

We now turn to evaluating the total particle and energy flux at height h. The total particle flux at height h is obtained by integrating $j_h(\mathbf{v}) = v_z n_h(\mathbf{v})$ over all velocity components from $-\infty$ to ∞ using Eqs. (19)-(21). The integral of v_z over the range $v_z^2 < 2gH$ cancels to zero by symmetry, and the integral of v_z over the range $(-\infty, -(2gH)^{1/2})$ is equal to minus the integral of the same integrand over the range $(+(2gH)^{1/2}, +\infty)$. The result is

$$
\begin{aligned}
J_h &= \int j_h(\mathbf{v}) d\tau_v \qquad (22) \\
&= (1-\alpha)(2\pi)^{\frac{d-1}{2}} \left[A e^{-\frac{mgH}{kT_0}} \left(\frac{kT_0}{m}\right)^{\frac{d+1}{2}} - B \left(\frac{kT_H}{m}\right)^{\frac{d+1}{2}} \right], \qquad (23)
\end{aligned}
$$

where $d = 1, 2, 3$ is the spatial dimensionality of the model. Note that the result is independent of h, as required for a steady state.

Because particles are conserved, a steady state requires zero net particle flux at every height h. Requiring that the net particle flux be zero imposes one condition between A, B, T_H and T_0, fixing A in terms of B and the two T's:

$$A = \left(\frac{T_H}{T_0}\right)^{\frac{d+1}{2}} B \exp\left(\frac{mgH}{kT_0}\right) . \tag{24}$$

The energy flux at altitude h is obtained by putting an extra factor of $\frac{1}{2}mv^2$ inside the integral in Eq. (22). The computation is slightly more involved, owing to the necessity to integrate by parts from a finite limit and to the presence of three terms in the integrand, but one finds without too much difficulty that

$$J_{E,h} = \int \tfrac{1}{2}mv^2 j_h(\mathbf{v}) d\tau_v \tag{25}$$

$$\begin{aligned} &= (1-\alpha)(2\pi)^{\frac{d-1}{2}} m \times \\ &\left\{ \left[A \left(\frac{kT_0}{m}\right)^{\frac{d+3}{2}} e^{-\frac{mgH}{kT_H}} \left(\frac{mg(H-h)}{kT_0} + 1\right) - B \left(\frac{kT_H}{m}\right)^{\frac{d+3}{2}} \left(\frac{mg(H-h)}{kT_H} + 1\right) \right] + \right. \\ &\left. \frac{d-1}{2} \left[Ae^{-\frac{mgH}{kT_H}} \left(\frac{kT_0}{m}\right)^{\frac{d+3}{2}} - B \left(\frac{kT_H}{m}\right)^{\frac{d+3}{2}} \right] \right\} . \end{aligned} \tag{26}$$

The first term in square brackets arises from the "diagonal" term in which $\frac{1}{2}mv_z^2$ multiplies $j_h(\mathbf{v}) = v_z n_h(\mathbf{v})$. The second term in square brackets results from the "off–diagonal" terms in the kinetic energy with v_x^2 or v_y^2 multiplying $v_z n_h(\mathbf{v})$. Substituting the requirement Eq. (24) for zero net particle flux into Eq. (26), this becomes

$$J_{E,h} = \left[(1-\alpha)B\frac{kT_H}{m}\left(\frac{2\pi kT_H}{m}\right)^{\frac{d-1}{2}}\right]\left[\left(\frac{d+1}{2}\right)(kT_0 - kT_H)\right] . \tag{27}$$

Again, the result is independent of h.

Eq. (27) has an interesting physical interpretation. The first factor in square brackets is just the total upward flux of particles arriving at $h = H$ that were *emitted from the reservoir at* $h = 0$. This is equal to the total downward flux of particles at $h = H$ from the reservoir at H *that will be absorbed by the reservoir at* $h = 0$. The downward moving particles just below $h = H$ have an average kinetic energy (averaged using the particle density) of $(d/2)kT_H$, while those just below $h = H$ that arrived from the reservoir at T_0 have an average kinetic energy (again, averaged using the particle density) of $(d/2)kT_0$. [This may be seen by calculating the average energy using suitable parts of the density given in Eqs. (19)–(21).] The second factor in square brackets is $(d+1)/d$ times the difference in average kinetic energy per particle between these arriving and leaving particles. The reason for the factor of $(d + 1)/d$ is that the energy and the rate of transport are coupled: particles with large v_z both transport more energy per particle and transport that energy faster. This coupling arises from the fact that we integrate over v_z^3 times the density rather than taking the product of integrals over v_z times the density and v_z^2 times the density divided by the integral of the density. This amplification occurs only for the z component; the terms in the kinetic energy involving v_x^2 and v_y^2 are not amplified in this way. The factor $(d+1)/2$ can be written as $(d-1)/2+1$. The terms involving the x and y components of the velocity contribute just their average kinetic energy times the particle flux rate. The term involving the z component contributes twice this amount. This enhancement of the energy flux for the component parallel to the direction of flux is quite general. For example, a gas effusing through a pinhole from a container into a vacuum has higher average kinetic energy per particle than does the gas from which it effuses by exactly the same factor of $(d+1)/d$ in d dimensions. Similarly, the energy flux in either direction through a plane in an equilibrium gas is $[(d+1)/2]kT$ times the particle flux in the same direction through that plane, a result we shall use in Sec. 3.

Regardless of dimensionality, Eq. (27) shows that if $T_0 = T_H$, the energy flux is zero at every altitude, including $h = 0$ and $h = H$. There is, therefore, no tendency for the temperatures of the reservoirs to change if they have finite heat capacity. If $T_0 < T_H$, then the (upward) energy flux is negative, so energy flows from the higher temperature, at height H, to the lower temperature, at 0. If $T_0 > T_H$, then the energy flux is positive, so again, the energy flows from higher to lower temperature. That is, whenever $T_0 \neq T_H$, energy flows in the direction that would tend to equalize the temperatures of the two reservoirs if the thermal capacity of either were finite.

The total number density, n_h, and the total vertical momentum flux, $J_{p,h}$, at any altitude may be evaluated by integration over $n_h(\mathbf{v})$ in (19) – (21) to give

$$n_h = \int n_h(\mathbf{v}) d\tau_v \tag{28}$$

and

$$J_{p,h} = \int m v_z^2 n_h(\mathbf{v}) d\tau_v /, . \tag{29}$$

When $T_H \neq T_0$, these give fairly complicated and uninformative expressions that depend upon α as well as on both T_H and T_0. However, regardless of the dimensionality of the problem, the energy flux is zero if $T_H = T_0$ and the direction of energy flow is always such as to tend to equalize the temperatures. If either reservoir has finite heat capacity — the case envisioned by Refs. 1–3, with a gravitator of finite mass — then the temperatures of the reservoirs will approach each other with time, and the final steady state will be one with $T_H = T_0$. We shall therefore restrict ourselves to this final steady state condition in the following discussion. In this case, the expressions for the number density and momentum flux become particularly simple and elegant. Under these circumstances, Eq. (24) reduces to

$$A = B e^{\frac{mgH}{kT}} \qquad (T_H = T_0 = T) \,. \tag{30}$$

Substituting this into (19) – (21), we find that

$$n_h(\mathbf{v}) = Ae^{-\frac{mgh}{kT}} \exp\left(-\frac{mv^2}{2kT}\right) \qquad (-\infty < v < +\infty)\,. \tag{31}$$

That is, the distribution at each altitude is a simple Maxwellian distribution over the entire velocity range, and so may be taken as if at equilibrium. Moreover, the constant A may now be expressed in terms of the total particle density at height 0 as simply

$$A = \left(\frac{m}{2\pi kT}\right)^{d/2} n_0\,, \tag{32}$$

where d is the dimensionality of the model. Also, the total density at $z = h$ is related to that at $z = 0$ by

$$n_h = n_0 \exp\left(-\frac{mgh}{kT}\right)\,, \tag{33}$$

which is simply the barometric law for densities.

The momentum flux through a horizontal plane at height h in the case $T_0 = T_H = T$ is also very simple and elegant. It is simply given by

$$J_{p,h} = \int mv_z^2 n_h(\mathbf{v}) d\tau_v = n_h kT\,. \tag{34}$$

The momentum flux is a force in one dimension and a force per unit area, *i.e.*, a pressure, in three dimensions. The quoted result, together with Eq. (33), amounts to the barometric law for pressure. It is interesting to note that, because the result for the momentum transfer through a horizontal plane is just the usual result for a gas at density n and temperature T, this would also be the answer for the momentum flux through a vertical plane. That is, the horizontal pressures against the vertical walls will be the same at heights 0 and H as on the floor and ceiling, respectively, and the pressure is independent of direction at every altitude. Thus, the gas behaves exactly as would a gas in which the mean free path was very small compared with the distance between the walls.

Also notable is the fact that the momentum transfer to the floor (the "gravitator" in analogy to Refs. 1–3) is independent of α. That is, there is no differential force exerted on two floors of different reflectivity. Changing α affects the *rate* at which energy is transferred in the case where $T_H \neq T_0$ [*cf.* Eq. (27),] but does not affect the properties of the distribution or the pressure exerted by the gas once the limit $T_H = T_0$ is reached.

In summary, under steady state conditions and the flux assumptions from the reservoirs we have made, the exact solution to the simple model considered here, has the property that the energy flux by the particles is nonzero when $T_H \neq T_0$ and in the direction that tends to equalize the temperatures, and is zero when $T_H = T_0$. The force on the floor of the container is independent of the trapping probability of the floor for the particles when $T_0 = T_H$. We emphasize that these conclusions hold for the full three–dimensional version of the model as well as for the one–dimensional case. The steady state in the case of either the ceiling or the floor having finite heat capacity is one of a uniform temperature throughout, with an equilibrium Maxwell–Boltzmann distribution of velocities for the particles, with the density and pressure of the particles satisfying the barometric law. This is the case even though the gas is so dilute that collisions in the gas phase can be completely neglected. The particles approach thermal equilibrium by themselves and do not require a separate mechanism such as black–body radiation in order to arrive at even a steady state, much less a state of equilibrium. This is in stark contrast with the consequences of the method of simulation used in Refs. 1–3. Moreover, the system exhibits no tendency to violate the second law by allowing the extraction of work from an isothermal reservoir — again, unlike the results of that simulation method.

3 RESOLUTION OF THE PARADOX

None of the results obtained in Sec. 2 is particularly surprising. Each is precisely what would be expected from a second law point of view. They are, however, in serious disagreement with the findings of Sheehan, *et al.*[1–3]

As stated in the introduction, this is because Sheehan, *et al.* have made a serious conceptual error in both the simulation and analysis of their model. They sample for the distribution of velocities of particles leaving the cavity and gravitator walls from a distribution appropriate to a particle *density*, when, in fact, these particles play the role of a particle *flux* in the model. We now justify that assertion.

Sheehan, *et al.* select the velocities of the particles leaving the outer wall of the cavity and the gravitator surface from a three–dimensional half–Maxwell–Boltzmann distribution in the form of a product of three one-dimensional Gaussian distributions $f(v_k) \sim \exp(-m_A v_k^2/2kT) \quad (k = x, y, z)$, with exclusion of resulting velocities that do not enter the cavity. [This is not entirely obvious from the description supplied in Refs. 1,2, but it is clear from examination of their code, which is publicly available,[1,2] and has been independently confirmed [D. P. Sheehan, private commun.] by one of the authors.] This choice might seem plausible at first thought, but is, in fact, a serious error.

The distributions f_i that the authors sample for and measure are the velocity distributions of particles *leaving from* and *arriving at* the cavity wall and gravitator surface. The first of two crucial observations is that the particles leaving from and arriving at these surfaces play the role of particle *fluxes* in this model, not particle *densities*. This may be seen by asking how one would calculate from the simulation, on the one hand, the particle flux, $j(\mathbf{r}, \mathbf{v})d\tau_v$, through a surface just inside the cavity from the outer wall or gravitator surface in a specified velocity volume element, $d\tau_v$, and, on the other hand, the particle density, $n(\mathbf{r}, \mathbf{v})d\tau_v$, in the same velocity volume element just inside the cavity from these surfaces. For the flux, one could simply take the number of particles leaving an element of the surface in the small but finite velocity volume element $\delta\tau_v = \delta v_x \delta v_y \delta v_z$ over some time during which the system was in a steady state, and divide by the area of the surface element and the time interval to obtain an estimator for the particle flux in that velocity volume element. [We use

δv_x, *etc.* to emphasize that these are small but non-infinitesimal velocity ranges, as is required in a simulation.] This, normalized, is precisely what the authors quote as their f_i. Indeed, in Ref. 2, where they attempt to determine the velocity distribution in the interior of the cavity, they explicitly state that they do so by counting the number of particles in a specified velocity range passing through a surface element in the form of a spherical cap and normalizing by, among other things, the time the particle spends in the cavity and the area of the cap. In other words, they are determining the distribution over velocities of a particle *flux* through the cap.

To obtain the particle *density* in a given velocity volume element, one would, instead, choose a small spatial volume element in the cavity and define a dynamical variable $N(\mathbf{r}, \mathbf{v}, t)\delta\tau_v$ equal to the number of particles in the spatial volume element that are in the velocity volume element $\delta\tau_v = \delta v_x \delta v_y \delta v_z$ at time t. In their simulation, this variable would always be either zero or one because there is only one particle involved. A time average of this dynamical variable divided by the spatial volume of the element would give an estimator for the particle density, $n(\mathbf{r}, \mathbf{v})\delta\tau_v$. The authors of Refs. 1–3 make no mention of any attempt to sample for this observable.

The second crucial observation is that the half–Maxwell–Boltzmann distribution of velocities from which the authors of Refs. 1–3 sample for particles emanating from the cavity wall and gravitator is appropriate for the *density* of particles in a gas in equilibrium, but not for a *flux* of particles through a surface. The flux of particles, $j(\mathbf{r}, \mathbf{v})d\tau_v$, through a surface in a velocity volume element $d\tau_v$ centered about vector velocity $\mathbf{v}$, is related to the density, $n(\mathbf{r}, \mathbf{v})d\tau_v$, in the same velocity volume element centered at the same velocity by the *continuity equation*,[5,6] which in the present case takes the form

$$j(\mathbf{r}, \mathbf{v}) = v_\perp n(\mathbf{r}, \mathbf{v}) \,, \tag{35}$$

where $v_\perp$ is the component of the velocity normal to the surface in the direction of positive flux. Thus, the appropriate distribution for a flux requires a factor of $v_\perp$ multiplying the half–Maxwell–Boltzmann distribution. This factor of $v_\perp$ is essential if the reservoir is ever to be capable of existing in equilibrium with a dilute gas of particles that is itself in internal equilibrium. This is because such a gas will necessarily have a Maxwell–Boltzmann distribution of velocities for its particle density and, therefore, have a particle flux at the surface with the factor $v_\perp$ multiplying this density. For a perfectly absorbing surface to be in detailed balance with the gas, its flux must match that in the gas at its surface at every velocity.

In addition to this gross requirement of a factor of $v_\perp$, there is a subtler requirement in connection with the gravitator. Because the trapping probability at the gravitator surface is a function of the velocity of the particle, the flux of particles from an equilibrium gas that is actually absorbed at the gravitator surface will contain an additional factor of $P_{\text{trap}}(v_\perp)$. As a consequence, for detailed balance in the equilibrium between the gravitator and a dilute gas, the emission probability from the gravitator must contain a factor of $P_{\text{trap}}(v_\perp)$ as well as of $v_\perp$ itself. Curiously, Sheehan, *et al.* include the factor of $P_{\text{trap}}(v_\perp)$ in their emission distribution from the gravitator, but not the factor of $v_\perp$.

As a consequence, with the distribution of velocities from which Sheehan, *et al.*

have sampled, neither the cavity wall nor the gravitator is capable of attaining local equilibrium with a gas that is itself in internal equilibrium at the same temperature *even in the absence of any gravitational field.* It is not surprising, therefore, that this sampling also leads to an inability of the system to reach equilibrium when a gravitational field is present.

It is possible to work out the consequences for the model of Sec. 2 of assuming the faulty flux distribution used in Refs. 1–3. If we assume that

$$j_H(\mathbf{v}) = -B \exp\left(-\frac{\frac{1}{2}mv^2}{kT_H}\right) \qquad (v_z < 0) \tag{36}$$

and

$$j_{0,\mathrm{res}}(\mathbf{v}) = A(1-\alpha) \exp\left(-\frac{\frac{1}{2}mv^2}{kT_0}\right) \qquad (v_z > 0)\,, \tag{37}$$

then the same reasoning as employed in Sec. 2 leads to the following result for the flux density $j_h(\mathbf{v})$ at height $z = h$

$$\begin{aligned} j_h(\mathbf{v}) &= B\frac{v_z}{(v_z^2 - 2g[H-h])^{1/2}} \exp\left(-\frac{\frac{1}{2}mv^2 - mg(H-h)}{kT_H}\right) \qquad \left(v_z < -[2g(H-h)]^{1/2}\right) \\ &= A\frac{v_z}{[v_z^2 + 2gh]^{1/2}} \exp\left(-\frac{\frac{1}{2}mv^2 + mgh}{kT_0}\right) \qquad \left(v_z^2 < 2g[H-h]\right) \\ &= \alpha B\frac{v_z}{(v_z^2 - mg[H-h])^{1/2}} \exp\left(-\frac{\frac{1}{2}mv^2 - mg(H-h)}{kT_H}\right) + \\ &\quad (1-\alpha)A\frac{v_z}{[v_z^2 + 2gh]^{1/2}} \exp\left(-\frac{\frac{1}{2}mv^2 + mgh}{kT_0}\right) \qquad \left(v_z > (2g[H-h])^{1/2}\right)\,, \end{aligned} \tag{38}$$

where $v^2 = v_x^2 + v_y^2 + v_z^2$ in three dimensions and $v^2 = v_z^2$ in one dimension. The corresponding particle densities are obtained by dividing by v_z.

The particle flux, the energy flux and the momentum flux that follow from the faulty flux distributions in Eqs. (36), (37) and (38), corresponding to the sampling choice of Refs. 1–3, can be calculated. With T_0 set equal to T_h, one finds that the condition for a steady state with respect to particle flux gives a nonzero energy flux and a momentum flux that depends upon both h and α. The integrals can no longer be carried out in closed form, but rather must be expressed in terms of incomplete error functions and related integrals. Using power series, asymptotic expansions and numerical evaluation of the integrals, it can be shown that, over the entire physical range of the parameter $\frac{mgH}{kT}$, the particles carry an energy flux upward in the gravitational potential, and the surface at $h = 0$ experiences a momentum flux that increases with decreasing α (*i.e.*, with increasing absorption probability). These results are in accord with the findings of Refs. 1–3. [The details of these calculations are available from the author upon request.] That is, use of the unphysical flux distributions from the reservoirs used by the authors of Refs. 1–3 leads to exactly the same unphysical consequences that they observe. This strengthens the conclusion that their unphysical results are the consequence of their unphysical sampling for the fluxes.

Another way to see just just how unphysical are the distributions of velocities leaving the reservoirs used in Refs. 1–3 is to consider what would result from these if the simple model in Sec. 2 were simulated in the *absence* of a gravitational field and with $T_H = T_0 = T$ and $\alpha = 0$ so that both walls were perfectly absorbing. Taking the limit $g = 0$ and dividing by v_z, in Eq. (38), one obtains for $n_h(\mathbf{v})$,

$$
\begin{aligned}
n_h(\mathbf{v}) &= B\frac{1}{|v_z|}\exp\left(-\frac{\frac{1}{2}mv^2}{kT}\right) \qquad (v_z < 0) \\
&= A\frac{1}{|v_z|}\exp\left(-\frac{\frac{1}{2}mv^2}{kT}\right) \qquad (v_z > 0)\,. \qquad (39)
\end{aligned}
$$

A steady state with respect to particle flux immediately requires $A = B$. The resulting density is not even integrable over the velocity.

In a simulation using a single particle, one would choose the velocity of this particle, on each absorption and re-emission, from the half–Gaussian Maxwell–Boltzmann distribution. Velocities with small v_z would be selected more often than those with large, and the particle would spend a time H/v_z in transit between the horizontal walls for a particle with z component of velocity v_z. One could estimate the density of particles in the velocity volume element $\delta\tau_v$ in any little spatial volume δV — or in the entire volume V — by defining the dynamical variable $N(\mathbf{v}, t)\delta\tau_v$ in analogy with the description above of $N(\mathbf{r}, \mathbf{v}, t)$, averaging over time and dividing by V. One will find that slow particles are the most probable, and they will contribute to the average proportionally to $1/v_z$, so one will obtain the very unrealistic velocity distribution in Eq. (39) for the relative density of particles in the box with different velocities. In addition, one will also spend an inordinate amount of the computational time simply waiting for the very slow particles to cross the box. The mean time to pass between floor and ceiling is infinite with this choice of fluxes.

If, instead, one uses the flux distributions $j(\mathbf{r}, \mathbf{v})$ in Eqs. (2) and (12) to generate the velocities of the particles emanating from the walls, one will generate very few particles with very small v_z. They will take a very long time to cross, but the product of their probability and their residence time will give a result varying smoothly with v_z and leading to a density of particles in the velocity volume element $\delta\tau_v$ in agreement with the Maxwell–Boltzmann distribution.

Similar, but less calamitous, conclusions follow for the more complicated model of Refs. 1–3 in the *absence of the gravitator*. With the gravitator absent, and the particle density low enough that inter-particle collisions and self–gravitation of the gas are negligible, the particles travel in straight lines, and it is possible to deduce the density of particles in the cavity resulting from a particle flux from the cavity wall of the form

$$
j_c(\mathbf{v}) = -A\exp\left(-\frac{\frac{1}{2}mv^2}{kT_c}\right) \qquad (v_\perp < 0) \qquad (40)
$$

with the convention that flux and $v_\perp$ are positive if outwardly directed. This corresponds to the sampling choice in Refs. 1–3. Consider a point at a distance r from the center of the cavity and a particle passing through that point with velocity $\mathbf{v}$. This particle left the cavity surface with the same velocity, $\mathbf{v}$, from a point obtained by tracing back along the velocity vector to the cavity wall. The density at that point on the cavity wall (and every other point on the cavity wall) is given, *via* the continuity equation (35), by

$$\begin{aligned} n_c(\mathbf{v}) &= \frac{A}{|v_\perp|} \exp\left(-\frac{\frac{1}{2}mv^2}{kT_c}\right) \\ &= \frac{A}{v\cos(\theta_c)} \exp\left(-\frac{\frac{1}{2}mv^2}{kT_c}\right) \qquad (41) \\ &, \qquad (42) \end{aligned}$$

where θ_c is the angle the velocity vector $\mathbf{v}$ makes with the *inwardly directed* normal to the cavity wall. Let θ be the angle that the velocity vector $\mathbf{v}$ makes with the outwardly directed radius from the cavity center through the point of interest. The law of sines relates θ_c and θ by $r/\sin(\theta_c) = r_c/\sin(\theta)$, where r_c is the cavity radius. As a consequence, by Liouville's theorem(7) (Eq. (6) above) we may conclude that, for a steady state, the particle density in the velocity volume element $d\tau_v$ at any point in the container is given by

$$n(\mathbf{r}, \mathbf{v})d\tau_v = \frac{A}{v\left[1 - \left(\frac{r}{r_c}\right)^2 \sin^2\theta\right]^{1/2}} \exp\left(-\frac{\frac{1}{2}mv^2}{kT_c}\right) d\tau_v. \qquad (43)$$

This distribution is highly non-Maxwellian and very unphysical, although it is non-integrable over velocity only at $r = r_c$, and gives a finite residence time in the cavity. Nevertheless, it is completely inconsistent with a gas in internal equilibrium. It diverges proportionally to $1/v$ as $v \to 0$ at every r and for every angle θ between 0 and π.

Curiously, this gas is formally "in equilibrium" with the flux coming from the walls in the sense that, provided no collisions occur between molecules in the gas, the corresponding flux is in detailed balance with the walls at every velocity. It does not, however, correspond to a gas in *internal* equilibrium. If the density of the gas were increased to the point where particles experienced many more collisions with other particles than with the wall [a wide range of densities gives this condition with negligible self–gravitation of the gas], then the particles near the center of the cavity would establish a local equilibrium through inter-particle collisions, with a velocity distribution of particle density given by the Maxwell–Boltzmann distribution. This distribution is *not* in detailed balance with that from the walls. To attain a steady state, the total particle and energy flux in the interior of the gas must match that at the walls. By choosing the density and temperature of the gas in the interior, this can be achieved. However, the energy flux from the walls resulting from the distribution of velocities chosen by Sheehan, *et al.* can be evaluated as $(3/2)kT_c$ times the total particle flux from the wall, while the energy flux across any surface in the interior of an equilibrium Maxwell–Boltzmann gas is found to be $2kT$ times the particle flux across that surface, due to the coupling between v^2 and $v_\perp$ noted in Sec. 2. As a consequence, if the particle flux is to balance between the gas in the interior of the cavity and that coming from the walls, then for the energy flux to balance, the temperature of the interior gas must be *lower* than that of the walls. Alternatively, if black–body radiation were to maintain the temperature of the interior of the gas equal to that of the walls, as occurs with the gravitator present, then there would be a steady–state flux of energy from interior to walls carried by the particles, balanced by a steady–state flux of energy from the walls to the interior carried by the black–body radiation. This is precisely the behavior seen by Sheehan, *et al.* in the presence of the gravitator. Thus, this unphysical feature of the model with the gravitator present is also exhibited in the absence of the gravitator and any influence of its gravitational field. Therefore, it seems reasonable to conclude that the reason for this unphysical behavior is not the presence of any gravitational "Maxwell Demon," but rather the unphysical nature of the distribution from which Sheehan, *et al.* have sampled for the velocities of the particles leaving the cavity wall.

In contrast, if the flux at the cavity wall is taken to be of the form

$$j_c(\mathbf{v}) = A v_\perp \exp\left(-\frac{\frac{1}{2}mv^2}{kT_c}\right) \qquad (v_\perp < 0), \tag{44}$$

as we suggest it should, then the density everywhere in the container is simply given by

$$n(\mathbf{r}, \mathbf{v}) = A \exp\left(-\frac{\frac{1}{2}mv^2}{kT_c}\right) , \tag{45}$$

which is the Maxwell–Boltzmann distribution for a gas in internal equilibrium, independently of the assumption that the density is so low that inter-particle collisions are unimportant. If the density of the gas were increased in this case, no difficulty would arise, because the dilute gas already has the distribution required for equilibrium in the more dense case.

There are three reasons why the authors did not notice the inappropriateness of the half–Gaussian Maxwell–Boltzmann distribution for the purpose to which they put it. First, the presence of a gravitational field makes the resulting anomalies in the density distribution of velocities more subtle. In the presence of such a field, there is a maximum residence time in the cavity of $2(2H/g)^{1/2}$ for the simple model studied in Sec. 2 and an analogous limit for the model studied in Refs. 1–3. Thus, the extraordinarily long wait times for particles emitted with very low velocities in the model considered in Sec. 2 are not present. As a consequence, the velocity distribution of the particle density is singular at $v_z = 0$ only at heights $h = H$ and $h = 0$ in the simple model, and at $v = 0$ only at the cavity surface and the surface of the gravitator in the more complex model. Second, even in the absence of the gravitator, the singular nature of the density is more subtle in their three–dimensional cavity because of absorbing surfaces in all directions, and in any case, they apparently did no simulations in the absence of the gravitator. Third, because those authors simulate a single particle, they would have noticed the pile–up in density at zero velocity only by calculating, in the manner described above, the particle density distribution over velocity. They did no sampling for the density in their simulations.

The one-dimensional distributions shown as $f_1 - f_4$ in Fig. 2 of Refs. 1 and 3 and described in Eqs. (1) and (2) of Ref. 3 are revealing about the nature of the distributions calculated by Sheehan, *et. al.* The distributions f_1 and the dashed curve in f_3 are both given (for appropriate ranges of the velocity) by the form in Eq. (1) of Ref. 3,

$$f_1(v) \quad [= f_3(v)] \quad = \alpha^{1/2} \exp\left(-\alpha v^2\right) \,, \tag{46}$$

where, here, $\alpha = m_A/2kT$. The dashed curve in distribution f_4 is given by Eq. (2) of Ref. 3

$$f_4(v) = \left[\frac{\alpha}{v^2+\beta}\right]^{1/2} v \exp\left(-\alpha(v^2+\beta)\right) \,, \tag{47}$$

where $\beta = 2Gm_G\left[\frac{1}{r_G} - \frac{1}{r_c}\right]$. These formulas, if correct, immediately rule out the possibility that the distributions f_i are distributions of *density* over velocity because if they were, then Liouville's theorem[(7)] (see Eq. (6) above) would require that $f_4(v) = \alpha^{1/2}\exp\left(-\alpha(v^2+\beta)\right)$. Sheehan [D. P. Sheehan, private commun.] justifies his Eq. (2) with the argument that every particle that leaves the gravitator with sufficient velocity arrives at the cavity wall, so that the distribution of velocities is over the same set of particles. It then follows that the appropriate transformation is, for a steady state,

$$f_3(v)d\tau_v = f_4(v')d\tau'_v \,, \tag{48}$$

where v and v' are related by the conservation of energy relation

$$\tfrac{1}{2}m_A v^2 = \tfrac{1}{2}m_A(v')^2 + \frac{m_A m_G G(r_c - r_G)}{r_c r_G} \,. \tag{49}$$

Applied to dv and dv', in the one–dimensional version of his model in which particles only move radially and the gravitator is centered in the cavity, this gives Eq. (47). In fact, Eq. (48) is essentially a flux conservation equation for steady states:

$$j_G(\mathbf{v})d\tau_v dA = j_c(\mathbf{v}')d\tau'_v dA' \,, \tag{50}$$

where j_G and j_c are the flux just above the gravitator and just below the cavity wall at the velocities $\mathbf{v}$ and $\mathbf{v}'$, respectively, related by Eq. (49), and where dA is an element of area on the gravitator and dA' is the corresponding element of area on the cavity wall, transformed under the equations of motion. Eq. (50) may be derived from Liouville's theorem by combining the theorem for the transformation of the density in Eq. (6) with that for the conservation of volume in phase space:[(7)] $d\tau_r d\tau_v = d\tau'_r d\tau'_v$. The latter may be written in the form

$$v_\perp dA d\tau_v = v'_\perp dA' d\tau'_v \,. \tag{51}$$

Multiplying by dt, the volume in space swept out in time dt at the gravitator wall is $v_\perp dAdt$, and so the volume in phase space is $v_\perp dAd\tau_v dt$. The same reasoning holds at the cavity wall. Combining this with Eq. (6) gives Eq. (50). [As in Sec. 2, the time t' differs from t by the time needed to evolve from $\mathbf{r}, \mathbf{v}$ to $\mathbf{r}', \mathbf{v}'$. For a steady state, however, the properties in question are independent of time, and so the equation may be taken as correct for the properties at any single time.] Because the f_i in Refs. 1–3 are taken as normalized probability distributions, the ratio $dA'/dA = (r_c/r_G)^2$ cancels out.

Examining Eq. (38) for $v_z > 0$ and $h = H$ we see that it takes the form

$$\begin{aligned} j_H(\mathbf{v}) &= (1-\alpha)A\frac{v_z}{(v_z^2+2gH)^{1/2}}\exp\left(-\frac{\frac{1}{2}mv^2+mgH}{kT_0}\right)+ \\ &\quad \alpha B\exp\left(-\frac{\frac{1}{2}mv^2}{kT_H}\right) \qquad (v_z>0)\ . \end{aligned} \tag{52}$$

The first term is of the same form as Eq. (47), while the second term is the Gaussian arising from the particles emanating originally from the cavity wall that are reflected back from the gravitator. This reinforces in one more way the conclusion that the distributions f_i in Refs. 1–3 are, in fact, distributions of flux, not distributions of density, over velocities.

The relationship between the solid curves in f_1, f_2, and f_3 of Fig. 2 of Refs. 1,3 is in error. They give no formula for their distribution f_2, but the same logic they use to obtain f_4 from f_3 would lead to distributions f_2 and f_3 of the form

$$f_2 = \left[\frac{\alpha}{v^2-\beta}\right]^{1/2} v\exp\left[-\alpha(v^2+\beta)\right] \qquad (v < -(\beta)^{1/2}) \tag{53}$$

and

$$f_3 = \left[\frac{\alpha}{v^2-\beta}\right]^{1/2} v\exp\left[-\alpha(v^2+\beta)\right] \qquad (v > (\beta)^{1/2}) \tag{54}$$

for the solid curves in the graph of f_2 and f_3 in Fig. 2 of Refs. 1 and 3. This predicts a strongly up–curving distribution that actually diverges as $v^2 \searrow \beta$. This is quite unlike the appearance of their f_2 or the solid curve in their f_3. Apparently, the failure to produce an accurate (according to their arguments) f_2 and f_3 in their Fig. 2 was simply an oversight by the authors of Refs. 1 and 3. Sheehan has acknowledged this [D. P. Sheehan, private commun.]

At $h = 0$, and for $v_z < -(2gH)^{1/2}$, Eq. (38) gives precisely the form predicted for f_2 and f_3 in Eqs. (53) and (54), provided appropriate translation of parameters between the two models is made, that allowance is made for the fact that the f_i are normalized to unity rather than to give total particle fluxes, and that Eq. (38) includes contributions from both reservoirs.

If one interprets the distributions $f_1 - f_4$ of Refs. 1–3 as flux distributions, then these papers are both internally and mutually consistent in their analysis (with the exception of the error just noted). They are then, however, inapplicable to any physical system because of the unphysical choice of the flux distributions f_1 and f_3 from the thermal reservoirs. On the other hand, if f_1–f_4 are interpreted as distributions of the *density* of particles over velocity, then these papers contain both internal errors and mutual inconsistencies that render their conclusions invalid, even though the distributions f_1 and f_3 would then be physically appropriate. In particular, the transformation embodied in Eqs. 1 and 2 of Ref. 3 is then in conflict with Liouville's

Theorem, as noted above.

We now show that, with a physically sensible choice for the flux distribution from the cavity walls and gravitator, Liouville's theorem[(7)] (see Eq. (6) above), together with the continuity equation and reasoning concerning flux balance at the walls, implies that the model of Refs. 1–3 is consistent with the second law of thermodynamics and with an equilibrium state in which the gas obeys Maxwell–Boltzmann statistics throughout the container with total particle density and pressure given by the barometric law and with detailed balance in the equilibrium between the gas and the surfaces. We restrict ourselves to the case where the gravitator and cavity wall have the same temperature: $T_G = T_c = T$.

Consider a particle density in the velocity volume element $d\tau_v$ of the form

$$n(\mathbf{r},\mathbf{v})d\tau_v = A\exp\left(-\frac{m_A m_G G(r-r_G)}{r r_G kT}\right)\exp\left(-\frac{\frac{1}{2}m_A v^2}{kT}\right)d\tau_v\,, \tag{55}$$

where $\mathbf{r}$ is the vector position *relative to the center of the gravitator*, where $r = |\mathbf{r}|$ is the distance of the point of interest from the gravitator center, and, following the notation of Refs. 1–3, where r_G is the radius of the gravitator, m_A is the mass of the gas atoms, m_G the mass of the gravitator, and G is the universal gravitational constant. We emphasize that the constant A in Eq. (55) is chosen small enough that collisions between particles in the container can be neglected; we are concerned with the equation of motion of the particles under the gravitational influence of the gravitator alone. For this density profile, the particle flux in the gas just above and normal to the gravitator surface is given by

$$j_G(\mathbf{r},\mathbf{v})d\tau_v = Av_\perp\exp\left(-\frac{\frac{1}{2}m_A v^2}{kT}\right)d\tau_v\,. \tag{56}$$

Of the particles with velocity directed inward, a fraction $P_{\rm trap}(k,v_\perp)$ given by Eq. (1) of Ref. 1 are absorbed by the surface k, where $k = 1,2$ indexes the two hemispheres. [We use k here to index the hemispheres, rather than the index j used by Sheehan, *et al.* to avoid confusion with the symbol for flux.] We take the flux in the velocity volume element $d\tau_v$ emanating from the two hemispheres of the gravitator to be of the form

$$j_{G,k,{\rm res.}}(\mathbf{v}) = Av_\perp P_{\rm trap}(k,v_\perp)\exp\left(-\frac{\frac{1}{2}m_A v^2}{kT_c}\right)\qquad(v_\perp > 0)\,, \tag{57}$$

This flux produces a local equilibrium, with detailed balance at every velocity, between the rate of particles being absorbed and emitted at the gravitator surface. Because the inward flux is independent of position and azimuthal angle on the gravitator surface, and fraction $P_{\rm trap}(k,v_\perp)$ is absorbed, fraction $(1-P_{\rm trap}(k,v_\perp)$ is reflected, and the remaining fraction $P_{\rm trap}(k,v_\perp)$ is re-emitted. For exiting velocities that will re-collide with the gravitator, they will reach the gravitator with their kinetic energy unchanged. Whichever hemisphere they collide with, the inward flux multiplied by the absorption probability is exactly matched by the emissive flux. It remains, then, to establish the appropriate flux out of the cavity wall that will just balance that coming from the gravitator and from other points on the cavity wall.

For particles leaving the gravitator with a velocity such that they collide with the cavity wall, the velocities at the gravitator and cavity wall are related through the general conservation of energy equation, applying for any trajectory within the cavity between cavity wall and gravitator,

$$\tfrac{1}{2} m_A v_f^2 = \tfrac{1}{2} m_A v_i^2 - \frac{m_A m_G G (r_f - r_i)}{r_f r_i} \, . \tag{58}$$

Here, the initial velocity, $\mathbf{v}_i$, is that at the gravitator surface, $\mathbf{v}_G = \mathbf{v}_i$, the final velocity, $\mathbf{v}_f$ is the velocity at the cavity wall, $\mathbf{v}_c = \mathbf{v}_f$, with $v^2 = v_x^2 + v_y^2 + v_z^2$. Also, here, r_i is the initial distance from the center of the gravitator, here, r_G, the radius of the gravitator, and r_f is the final distance from the center of the gravitator, here, the distance, r, of the point on the cavity wall from the center of the gravitator. If the gravitator is at the center of the cavity, then $r = r_c$, the cavity radius, for all $\mathbf{r}$ on the cavity surface. If the gravitator is off–center, then r varies with the vector position $\mathbf{r}$ on the cavity wall. In either case, however, Liouville's theorem(7) (see Eq. (6) above) guarantees that the density there is given exactly by Eq. (43). Note that this density is, apart from a prefactor setting the magnitude of the total density at the point $\mathbf{r}$, simply a Maxwell–Boltzmann distribution appropriate to a gas in internal equilibrium. The flux into the cavity wall in the velocity volume element $d\tau_v$ is then given by

$$j_c(\mathbf{r}, \mathbf{v}) d\tau_v = A v_\perp \exp\left(- \frac{m_A m_G G (r - r_G)}{r r_G k T} \right) \exp\left(- \frac{\tfrac{1}{2} m_A v^2}{kT} \right) d\tau_v \qquad (v_\perp > 0) \, , \tag{59}$$

where $\mathbf{v}$ is the velocity of the particle arriving at the cavity wall and where $v_\perp$ is the component of $\mathbf{v}$ perpendicular to the cavity wall, taken as positive in the outward direction. Note that this flux is independent of azimuthal angle of the velocity vector around the normal to the surface.

According to the assumptions of Refs. 1–3, every particle arriving at the cavity wall is absorbed. We now take the flux *from* the cavity wall to be

$$j_{c,\mathrm{res}}(\mathbf{r}, \mathbf{v}) d\tau_v = A v_\perp \exp\left(- \frac{m_A m_G G (r - r_G)}{r r_G k T} \right) \exp\left(- \frac{\tfrac{1}{2} m_A v^2}{kT} \right) d\tau_v \qquad (v_\perp < 0) \, . \tag{60}$$

By the independence of azimuthal angle, this guarantees detailed balance at every vector velocity between absorbed and emitted particles that pass between the gravitator surface and the cavity wall.

The flux in Eq. (60) also guarantees detailed balance for particles passing from one point to another on the cavity surface. This follows from the observation that Eq. (60) is consistent with the density in Eq. (55), and that this density is consistent with Liouville's theorem. Given any two points on the cavity surface and a designation of one as the initial point and the other as final, then for any initial velocity that leads from the initial point to the final point, the final velocity will be given by the energy conservation equation (58) where r_i and r_f are the distances of the initial and final points on the cavity wall from the center of the gravitator and where v_i and v_f are the initial and final velocities. Liouville's theorem then guarantees that the densities at the two points are related as in Eq. (55).

As a consequence, we conclude that the proposed density in Eq. (55) is an equilibrium steady–state solution to the equations of motion in the cavity and the postulated absorption probabilities and emission fluxes. On the other hand, the proposed emission fluxes are precisely those which are required in order that the gravitator and cavity wall be in *local* equilibrium with a gas that is itself in internal equilibrium at temperature T and the *local density* given by Eq. (55) *in the absence of any gravitational field*. They are, thus, completely in the spirit of those proposed in Section 2.

The proposed density is an equilibrium Maxwell–Boltzmann distribution for a gas in a spherical gravitational field, satisfying the barometric law for dependence of density on altitude. We thus conclude that the equilibrium distribution expected on the basis of the second law is a steady state distribution for the dynamics of this problem, satisfying detailed balance of particle flux at every velocity. It therefore also satisfies detailed balance of *energy flux* at every velocity. As a consequence, there is no tendency for energy to flow in either direction between gravitator and cavity wall.

There will also be no net force on the gravitator *from particle collisions with the gravitator*. There is, however, one consideration that was irrelevant in the model considered in Sec. 2, but that must be considered here. In calculating the force on the floor of the cavity in Sec 2 and on the gravitator here, we have calculated only the force arising from momentum transfer from collisions with the particles. There is also a gravitational force exerted on the gravitator by the particles at a distance. In the model of Sec. 2, this was the same, independent of α because the density profiles were the same. It gives zero net force on the gravitator in the more complicated model considered here when the gravitator is at the center of the cavity because of the spherical symmetry. When the gravitator is off center in the cavity, however, there will be a force on the gravitator due to the imbalance of gravitational attraction of atoms in the cavity. This will, however, be directed along the radius of the cavity, attracting the gravitator to the center of the cavity. If van der Waals interactions between the gas particles and the material making up the cavity walls were included, there would also be a force due to these interactions, also directed along the cavity radius, but (typically) pushing the gravitator toward the cavity wall. Neither of these forces, however, can be harnessed to provide an ongoing source of work at the expense of heat from the cavity wall, so they lead to no contradiction of the second law of thermodynamics.

In the argument above, we consider each of the possible kinds of trajectory: gravitator to gravitator (both to the same kind of surface and to the opposite kind), gravitator to cavity wall, cavity wall to gravitator, and cavity wall cavity wall. We find that the proposed density is in a steady state with respect to each of the possible kinds of exchange: gravitator surface to the same kind of gravitator surface and return, gravitator surface to the opposite kind of gravitator surface and return, gravitator surface (of either kind) to cavity wall and return, and cavity wall to cavity wall and return. Together, these give detailed balance at each surface element and at every velocity between the particle flux arriving at any vector velocity and the flux leaving at minus that vector velocity. As a consequence, we have *deduced* that the proposed density is an equilibrium solution of the equations of motion and the proposed absorption and emission probabilities.

Our analysis of the more complicated model of Refs. 1–3 is necessarily less complete than that of the model in Sec. 2. We do not (and are not able to) solve the case where $T_G \neq T_c$, and so do not show that the equilibrium steady state obtained is a stable steady state (although this seems very plausible). We are also unable to consider in detail the consequences of making their faulty choice for the particle flux at the cavity wall and gravitator. These limitations make the solution of the simpler model considered in Sec. 2 a worthwhile investment. We have shown, however, that with the physically sensible choice for particle fluxes from the cavity wall and gravitator, there is no tendency for the more complicated model of Refs. 1–3 to deviate from the proposed density, and that this density satisfies detailed balance between the walls and the gas at every velocity, and so is an equilibrium state. This is not the case if the fluxes used by those authors are employed.

We conclude that the reason the authors of Refs. 1–3 obtain unphysical results in the analysis of the gravitator is that they use an unphysical distribution over velocities for the flux of particles leaving the reservoirs. When this flux is used in the simple model, the same unphysical results are obtained. When the physically correct flux is used, both the simpler model and the model considered by those authors are consistent with the second law of thermodynamics and with detailed balance at equilibrium.

4 DISCUSSION

We have argued, we believe compellingly, that the authors of Refs. 1–3 obtain their highly controversial results as a consequence of making a fundamental error in their choice for the distribution over velocity of what turns out on careful examination to be the flux of particles through a surface. We did so by examining a simpler model, obtaining an exact solution for its steady states, and reasoning about what the authors' method would yield if applied to this simpler model. We do not claim that our method of analysis gives the complete solution to the model in Refs. 1–3. It does, however, allow us to show that the physically sensible choice for the flux from the walls proposed here gives a steady state solution for that model that satisfies detailed balance between the gas and the cavity wall and gravitator at every velocity, and has a density that is the expected equilibrium density for particles in a gravitational field.

Our simpler model provides a legitimate testing ground for the methods employed by those authors. The analytic solution to our model in three dimensions with the reservoir fluxes we propose is in complete accord with the principle of detailed balance and with the second law of thermodynamics. Their method, when applied to our model, gives exactly the same unphysical results as they find in their more complicated model. Moreover, their method leads to unphysical answers for the properties of both their model and our model when applied in the *absence* of gravity, where the answers are well known.

We note that throughout our treatment, both of the simpler model introduced in Sec. 2 and of the model of Sheehan *et al.*, we restrict the application of Liouville's theorem to trajectories that lie entirely between the absorbing surfaces. That is, given the density just inside the cavity from an absorbing surface, whether the upper or lower wall of the simpler model of Sec. 2 or the cavity wall or gravitator surface of the model of Sheehan, *et al.*, particles with velocities that will necessarily carry them away from that surface are followed using Liouville's theorem to obtain the corresponding density just inside the cavity from the destination surface. For particles adjacent to an absorbing surface and with velocities that will carry them into that surface, the *continuity equation* is used to obtain the corresponding flux, and then the absorption and emission probabilities are used to determine the flux balance at the wall. We do *not* use Liouville's theorem to describe the collisions of the particles with any absorbing surface. [We *do* apply Liouville's theorem to trajectories in which particles strike the vertical, specularly reflecting side walls of the simpler model. Such collisions are purely mechanical and conservative, preserving phase space density and volume, so that Liouville's theorem applies to these trajectories.] In treating the model of Sheehan *et al.*, Liouville's theorem is not applied to particle–surface collisions of *any* sort. Zhang and Zhang[8] have pointed out that interactions between particles and membranes or surfaces can be devised that are purely mechanical but that do not preserve phase–space volume. They conclude that such interactions do not occur in nature. Sheehan *et al.* do not describe their particle–surface interactions in terms of equations of motion, so that no such analysis of their particle–surface collisions is possible. Rather, one must reason by balancing the fluxes based on the assumed relative probabilities of absorption and emission. Their choice of relative emission probabilities has an effect analogous to choosing a particle–surface interaction that does not preserve phase space volume. It makes their model unphysical even in the absence of gravity.

Quite apart from the argument based on consistency with the Maxwell–Boltzmann distribution for particle density, there is another sound theoretical reason to choose a velocity distribution of particle production rates proportional to $v_\perp \exp(-\frac{1}{2}mv^2/kT)$. The particles are escaping from a potential well provided by the "trap." According to *activated complex theory*,[9] the rate of escape from such a potential well is equal to the number of trapped particles (or the number per unit area for the flux from a two–dimensional surface in three dimensions) times the probability that the particle has the required energy, times the *rate of passage* through the transition state for such particles. The probability that the particle has the required energy, for a particle escaping with velocity v, will be proportional to $\exp(-[V_{\text{well}} + \frac{1}{2}mv^2]/kT)$, where V_{well} is the minimum energy needed to escape the well, while the rate of passage through the transition state may be taken as $v_\perp/d$, where d is a length characteristic of the transition state. This naturally leads to a rate equal to $N(v_\perp/d)\exp(-[V_{\text{barrier}} + \frac{1}{2}mv^2]/kT)$, which is precisely of the form $j(v) = Av_\perp \exp(-\frac{1}{2}mv^2/kT)$.

The foregoing discussion is appropriate if there is no potential barrier to particle absorption or if that barrier is either zero or infinite with probabilities $1-\alpha$ and α, respectively. If there is a finite barrier to absorption, then the particle may "ride downhill" in energy from the transition state, and there may be a threshold energy (and corresponding velocity) below which there is no flux from the surface. In addition, if there are transition–state recrossings, then activated complex theory is only an approximation, and additional dependence on particle velocity may appear in the rate of escape. The factor of $v_\perp$, however, is always present.

The model of Sec. 2 is of some interest beyond the issue of resolving the paradox presented by Refs. 1–3. The treatment applies equally well to a potential energy well $\phi(h)$ that varies nonlinearly with height h. The essential ingredient is the change in potential energy, there mgH. We might therefore, model the traps at the surfaces by imagining that they consist of a potential well in which the potential drops very rapidly just below 0 and just above H by an amount large enough that the density increases to a value large enough that the mean free path of the molecules between collisions with each other drops to a small value typical of a gas at 1 atm. In that case, the gas can easily thermalize, both internally and with whatever reservoir we choose to employ. Because the velocity distribution and particle density vary in a manner independent of whether the mean free path is large or small, the formulas for the density, $n(\mathbf{r}, \mathbf{v})$, and flux, $j(\mathbf{r}, \mathbf{v})$, can be expected to remain valid through the potential change. This gives yet another argument for the form chosen for $j_0(\mathbf{v})$ and $j_H(\mathbf{v})$. Moreover, it provides an aid in understanding why the vapor evaporating from an adsorbed solid layer or a liquid in an equilibrium state is described by a Maxwell–Boltzmann velocity distribution with the same temperature as the solid or liquid.

The authors of Ref. 1 make the point that the scientific community has an obligation to keep an open mind on the validity of the second law, and to test it rigorously. They lament that this has not been the case. While the scientific community does have an obligation to address purported violations of the second law, scientists who make such claims have an obligation to test their own algorithms thoroughly to ensure that their assumptions are sound and consistent with known physics. If the authors of Refs. 1–3 had tested their simulation on simpler models, such as the one presented in Sec. 2, and under simpler conditions, such as in the absence of gravity, they probably would have come to realize that there was an inconsistency between their assumptions and physical reality. It would seem likely that others of the "growing number" of unresolved second law paradoxes quoted by the authors of 1 and 3 are worthy of closer inspection.

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REFERENCES

1. D. P. Sheehan, J. Glick, and J. D. Means, *Found. Phys.* **30**, 1227 (2000)

2. D. P. Sheehan, J. Glick, T. Duncan, J. A. Langton, M. J. Gagliardi, and R. Tobe, *Found. Phys.* **32**, 441 (2002)

3. D. P. Sheehan, in *Quantum Limits to the Second Law* D. P. Sheehan, ed. *AIP Conference Proceedings* **643** (American Institute of Physics, Melville, NY, 2002), p. 391.

4. H. Goldstein, *Classical Mechanics 2nd Ed.* (Addison–Wesley, Reading, 1980), pp 94–102.

5. J. Jeans, *An Introduction to the Kinetic Theory of Gases*, (Cambridge at the University Press, Cambridge, 1962) p. 225.

6. S. Chapman, T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases* (Cambridge at the University Press, Cambridge, 1970), p 30.

7. *ibid.* pp 426–428.

8. K. Zhang, and K. Zhang, *Phys. Rev. A* **46**, 4598 (1992).

9. K. J. Laidler, *Chemical Kinetics, 3d ed.* (Harper Collins, New York, 1987).