Thermal equilibrium of an ideal gas in a free-floating box

SCOTT TREMAINE,1,2 BENCE KOCSIS,3 AND ABRAHAM LOEB4

1Institute for Advanced Study, Princeton, NJ 08540, USA
2Canadian Institute for Theoretical Astrophysics, University of Toronto, 60 St. George Street, Toronto, ON M5S 3H8, Canada
3Rudolf Peierls Centre for Theoretical Physics, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, UK
4Astronomy Department, Harvard University, 60 Garden St., Cambridge, MA 02138, USA

ABSTRACT

The equilibrium and fluctuations of an ideal gas in a rigid container are studied by every student of statistical mechanics. Here we study the less well-known case when the box is floating freely; in particular we determine the fluctuations of the box in velocity and position due to interactions with the gas it contains. This system is a toy model for the fluctuations in velocity and position of a black hole surrounded by stars at the center of a galaxy. These fluctuations may be observable in nearby galaxies.

1. INTRODUCTION

The determination of the equilibrium state of a dilute gas in a box is perhaps the most famous problem in statistical mechanics, and usually the first one to which students are exposed (Landau & Lifshitz 1980). The problem is usually solved with the assumption that the box is fixed, or at least very massive compared to the gas it contains. The purpose of this short paper is to describe the equilibrium state when the box is free to move and the mass of the box is comparable to the mass of the gas.

This system offers both a simple analytic problem in statistical mechanics and a toy model for a more complicated, and still poorly understood, problem from astrophysics: the Brownian motion of the supermassive black holes found at the centers of galaxies due to the gravitational forces from the surrounding stars (see §4 for more detail).

We consider an isolated rigid box of mass $M$ containing $N$ particles of mass $m$, so the total gas mass is $M_\text{g} = Nm$. The particles collide via short-range forces and we neglect the self-gravity of the gas. The box is freely floating and there is a heater attached to the box that maintains its temperature at a fixed value $T$ (thus we are working with a canonical ensemble in which the “heat bath” exchanges energy but not momentum with the system; we could instead have used an insulating box and worked with the microcanonical ensemble, with very similar results). The center of mass of the system (box plus gas) is at rest. We can assume that the box is cubical, with its symmetry axes parallel to the coordinate axes $(x, y, z)$. Then the dynamics along each axis is independent. What is the root-mean-square velocity of the box along each axis?

There are two simple arguments leading to different answers, and both turn out to be correct only in limiting cases.

First, we can argue that the box is in thermal equilibrium with the gas. The mean-square velocity of the gas particles in one dimension—say along the $x$-axis—is $\langle v_x^2 \rangle = k_B T/m$ where $k_B$ is Boltzmann’s constant. Then equipartition implies that the mean-square velocity of the box along the $x$-axis should be

$$\langle V_x^2 \rangle = \frac{k_B T}{M}. \quad (1)$$

The second argument starts with the observation that the center of mass of the system is at rest so momentum conservation implies that $MV_x = -m \sum_{i=1}^{N} v_{xi}$ where $v_{xi}$ is the $x$-velocity of particle $i$ and the sum is over all the particles. From the central limit theorem, the mean-square value of the right-hand side should be $m^2 N \langle v_x^2 \rangle = mN k_B T = M_\text{g} k_B T$ so

$$\langle V_x^2 \rangle = \frac{M_\text{g}^2}{M^2} k_B T, \quad (2)$$

obviously not the same as (1).

2. THE MEAN-SQUARE VELOCITY OF THE FREE-FLOATING BOX

Each microstate of the system we are examining is specified by the $N$ particle velocities $v_{xi}$ and the box velocity $V_x$, both measured along the $x$-axis. Momentum conservation restricts the phase space to the hyperplane $mv_{x1} + \cdots + mv_{xN} + MV_x = 0$. 


The canonical ensemble assigns to each microstate a probability proportional to \( \exp[-E/(k_B T)] \), where the kinetic energy \( E = \frac{1}{2} m (v_{x1}^2 + \cdots + v_{xN}^2) + \frac{1}{2} MV_x^2 \). Therefore the probability distribution of the velocities is given by

\[
p(V_x, v_{x1}, \ldots, v_{xN}) dv_{x1} \cdots dv_{xN} dv_x \propto \exp \left( - \frac{mv_{x1}^2 + \cdots + mv_{xN}^2 + MV_x^2}{2k_B T} \right),
\]

\[\times \delta(mv_{x1} + \cdots + mv_{xN} + MV_x)dv_{x1} \cdots dv_{xN}dv_x \]

where \( \delta(\cdot) \) is the Dirac delta function. The probability distribution of \( V_x \) is then obtained by integrating over the \( N \) particle velocities,

\[
p(V_x) \propto \int_{-\infty}^{\infty} dv_{x1} \cdots \int_{-\infty}^{\infty} dv_{xN} \exp \left( - \frac{mv_{x1}^2 + \cdots + mv_{xN}^2 + MV_x^2}{2k_B T} \right) \delta(mv_{x1} + \cdots + mv_{xN} + MV_x).
\]

To evaluate this integral we use the relation

\[
\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \exp(i \kappa x).
\]

Then

\[
p(V_x) \propto \exp \left( - \frac{MV_x^2}{2k_B T} \right) \int_{-\infty}^{\infty} dk \exp(i \kappa MV_x) \left[ \int_{-\infty}^{\infty} dv \exp \left( - \frac{mv^2}{2k_B T} + i \kappa mv \right) \right]^N.
\]

We use the result

\[
\int_{-\infty}^{\infty} du \exp(i \alpha u - \beta u^2) = 2 \int_{0}^{\infty} \cos(\alpha u) \exp(-\beta u^2) = \left( \frac{\pi}{\beta} \right)^{1/2} \exp \left( - \frac{\alpha^2}{4\beta} \right), \quad \beta > 0.
\]

The integral inside the square brackets is then

\[
\int_{-\infty}^{\infty} dv \exp \left( - \frac{mv^2}{2k_B T} + i \kappa mv \right) = \left( 2\pi k_B T/m \right)^{1/2} \exp \left( - \frac{1}{2} mk_B T \kappa^2 \right).
\]

Thus

\[
p(V_x) \propto \exp \left( - \frac{MV_x^2}{2k_B T} \right) \int_{-\infty}^{\infty} dk \exp \left( i \kappa MV_x - \frac{1}{2} Nmk_B T \kappa^2 \right).
\]

The integral can be evaluated using equation (7), and yields

\[
p(V_x) \propto \exp \left[ - \frac{MV_x^2}{2k_B T} \left( 1 + \frac{M}{M_g} \right) \right].
\]

The mean-square velocity of the box along the \( x \)-axis is thus

\[
\langle V_x^2 \rangle = \frac{k_B T}{M} \frac{M_g}{M + M_g}.
\]

This result agrees with equation (1) when the gas mass is much larger than the box mass \((M_g \gg M)\) and agrees with (2) when the gas mass is much less than the box mass. When \( M_g \ll M \), the argument leading to equation (1) is wrong because it neglects the constraint imposed by momentum conservation. When \( M_g \gg M \) the argument leading to equation (2) is wrong because it neglects energy equipartition between the gas and the box.

Although equation (11) was derived for a cubical box it should hold for a box of arbitrary shape.

There is a simple heuristic derivation of this result (Lin & Tremaine 1980). Approximate the system as consisting of two bodies, the box with mass \( M \) and the gas with mass \( M_g \). The reduced mass of the two-body system is \( \mu = M M_g/(M + M_g) \). In thermal equilibrium the kinetic energy per degree of freedom is \( \frac{1}{2} k_B T \) so the relative velocity \( V_{x,\text{rel}} \) between the two bodies satisfies

\[
\langle V_{x,\text{rel}}^2 \rangle = \frac{k_B T}{\mu}.
\]

Since the center of mass is fixed, the one-dimensional velocity of the box is \( V_x = M_g V_{x,\text{rel}}/(M + M_g) \) so

\[
\langle V_x^2 \rangle = \frac{M_g^2}{(M + M_g)^2} \langle V_{x,\text{rel}}^2 \rangle = \frac{k_B T}{M} \frac{M_g}{M + M_g},
\]

the same as equation (11).
3. THE MEAN-SQUARE DISPLACEMENT OF THE FREE-FLOATING BOX

We can use similar methods to calculate the mean-square displacement of the box. Assume that the center of mass of the system is at the origin so \( MX = -m \sum_{i=1}^{N} x_i \) where \( x_i \) is the position of particle \( i \) and \( X \) is the position of the center of mass of the box. We assume that the box is cubical, with thin walls of length \( L \) in each dimension.

Since we are only concerned with the position of the box, we can integrate the probability distribution in phase space over the velocities, so

\[
p(X, x_1, \ldots, x_N) \propto \delta(m x_1 + \cdots + x_N + MX) \prod_{i=1}^{N} \Theta(\frac{1}{2}L + X - x_i) \Theta(\frac{1}{2}L - X + x_i),
\]

where \( \Theta(x) \) is the step function, equal to 1 if \( x > 0 \) and 0 if \( x < 0 \). The delta function constrains the mass of the system to remain at the origin and the step functions constrain the particles to remain inside the box. Using the identity (5),

\[
p(X, x_1, \ldots, x_N) \propto \int_{-\infty}^{\infty} d\kappa \exp(i\kappa MX) \prod_{i=1}^{N} \int_{-\infty}^{L/2+X} dx_i \exp(i\kappa x_i)
\]
\[
\propto \int_{-\infty}^{\infty} d\kappa \exp[i\kappa X(M + M_g)] \left( \sin \frac{\pi mL\kappa}{\kappa} \right)^N.
\]

To evaluate the integral we assume that the gas mass \( M_g = N m \) is fixed and let \( N \to \infty \) or \( m \to 0 \). We replace the dummy variable \( \kappa \) by \( u \equiv \kappa / \sqrt{N} \). Then

\[
p(X, x_1, \ldots, x_N) \propto \int_{-\infty}^{\infty} du \exp[iuN^{1/2}(M + M_g)] \left( \sin \frac{\pi M_g LN^{-1/2}u}{u} \right)^N.
\]

Since \( |\sin x/x| \) is less than unity except near \( x = 0 \), \( (\sin x/x)^N \) is negligible as \( N \to \infty \) except near \( x = 0 \). Here it can be approximated by the first two terms in its Taylor series, \( \sin x/x = 1 - \frac{1}{6}x^2 \), and we have

\[
\left( \sin \frac{\pi M_g LN^{-1/2}u}{u} \right)^N \propto \left( 1 - \frac{M_g^2 L^2 u^2}{24N} \right)^N \to \exp \left( -\frac{M_g^2 L^2 u^2}{24} \right),
\]

in which we have used the identity \( (1 - z/N)^N \to \exp(-z) \) as \( N \to \infty \). The integral in equation (16) can now be evaluated using equation (7), and we find

\[
p(X) \propto \exp \left[ -\frac{6NX^2(M + M_g)^2}{L^2 M_g^2} \right].
\]

Note that as \( N \to \infty \) this derivation converges to the correct answer at a fixed value of \( XN^{1/2} \) but not necessarily at a fixed value of \( X \) (obviously, \( |X| \) cannot exceed \( \frac{1}{2} LM_g/(M + M_g) \), the value it would have if all of the gas were on one wall of the box). The mean-square displacement of the box from the original center of mass is

\[
\langle X^2 \rangle = \frac{L^2}{12N} \left( \frac{M_g}{M + M_g} \right)^2.
\]

The factor \( L^2/12 \) is simply the variance of a uniform distribution between \( -\frac{1}{2}L \) and \( \frac{1}{2}L \), given by \( \int_{-L/2}^{L/2} x^2 dx/L \). For a box of general shape the factor \( L^2/12 \) should be replaced by \( \frac{1}{3} \) of the mean-square distance of the box wall from its center of mass.

4. NUCLEAR STAR CLUSTERS

“Supermassive” black holes with masses between \( M_\bullet = 10^6 \) and \( M_\bullet = 10^{10} \) solar masses are found in the centers of most galaxies (Kormendy & Ho 2013). The black holes are typically surrounded by nuclear star clusters (Neumayer et al. 2020), systems of stars orbiting the black hole. These are the densest stellar systems in the universe, exceeding \( 10^7 \) times the stellar number density in the solar neighborhood. The mass of stars in the nuclear cluster can be comparable to or even exceed the mass of the black hole. Because the star cluster is usually much denser than the surrounding galaxy, it is reasonable to approximate the cluster plus black hole as an isolated system.
The dynamics and statistical mechanics of stars in a nuclear star cluster differ from those of a gas in a box in several important respects: (i) the stars are bound to the black hole because of their own gravity and the gravity from the black hole, rather than being confined in a box; (ii) relaxation occurs through gravitational encounters, rather than collisions, similar to relaxation through Coulomb encounters in a plasma; (iii) the mean free path is much longer than the size of the system; (iv) even the oldest, densest clusters have only lived for a few tens of relaxation times; (v) the cluster cannot approach thermodynamic equilibrium, since it has negative heat capacity (Binney & Tremaine 2008; Bahcall & Wolf 1976).

The velocity and displacement of the black hole from the center of the nuclear star cluster are accessible to observations, at least in the nearest galaxies. The supermassive black hole at the center of the Milky Way is nearly stationary: its velocity components perpendicular to the line of sight are only $0.5 \pm 2.2 \, \text{km s}^{-1}$ in the Galactic plane and $0.9 \pm 0.8 \, \text{km s}^{-1}$ normal to the plane (Reid & Brunthaler 2020), and the component along the line of sight (Gravity Collaboration et al. 2019) is $3 \pm 2 \, \text{km s}^{-1}$. The supermassive black hole in the nearest giant galaxy, M31, is displaced from the center of the large-scale galaxy (Kormendy & Bender 1999) by $0.07 \pm 0.01$ arcseconds or $0.23 \pm 0.03$ parsecs, although this offset is probably due to the gravitational influence of the eccentric stellar disk that orbits the black hole. The black hole in the giant elliptical galaxy M87, which has been imaged by the Event Horizon Telescope, appears to be offset from the photo-center of the galaxy by $7 \pm 1 \, \text{pc}$ (Batcheldor et al. 2010; Broderick et al. 2011).

The free-floating box provides a toy model that captures some but not all of the dynamics that determines the Brownian motion of the black hole due to its interactions with the surrounding stars, both within the cluster and outside it. The nuclear star cluster is not in thermal equilibrium, so the “temperature” or mean-square velocity of the stars varies with radius, given roughly by the Kepler relation $\langle v^2 \rangle \approx GM/r$. If the number of stars in a small radius range $dr$ is $dN$, and the mass of the star cluster is small compared to the mass of the black hole, then equation (11) suggests that these contribute $\langle V^2 \rangle = \langle v^2 \rangle m^2 dN/M^2_\bullet$ where $m$ is now the typical stellar mass. The mean-square velocity of the black hole due to interactions with the cluster stars is then

$$\langle V^2 \rangle \approx \frac{Gm^2}{M_\bullet} \int \frac{dN}{r},$$  \hspace{1cm} (20)

Similarly the mean-square displacement should be roughly

$$\langle R^2 \rangle \sim \frac{m^2}{M^2_\bullet} \int r^2 dN, \quad N m \lesssim M_\bullet. \hspace{1cm} (21)$$

For the usual Bahcall–Wolf model of an equilibrium cluster (Bahcall & Wolf 1976), $dN \sim r^{1/4} dr$, both the velocity and the displacement are dominated by the effects of stars in the outer parts of the cluster, and the mean-square velocity and radius of the black hole are smaller than those of the stars in this region by a factor of order $m^2 N/M^2_\bullet$. A more quantitatively reliable approach, of course, is to use N-body simulations (Lin & Tremaine 1980; Chatterjee et al. 2002; Reid & Brunthaler 2020).

5. SUMMARY

We have described aspects of the Brownian motion of a free-floating box containing an isothermal gas. The mean-square velocity and displacement of the box are given by equations (11) and (19); the mean-square velocity is independent of the size and shape of the box, and the mean-square displacement is independent of the temperature. This system provides a toy model that describes some aspects of the Brownian motion of a supermassive black hole in a nuclear star cluster.

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