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A Universal Asymptotic Velocity Distribution for Independent Particles in a Time-Dependent Irregular Container

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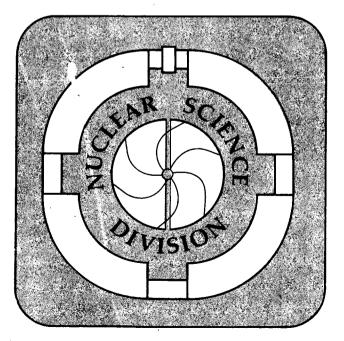
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A Universal Asymptotic Velocity Distribution for Independent Particles in a Time-Dependent Irregular Container

C. Jarzynski and W.J. Swiatecki

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## A Universal Asymptotic Velocity Distribution for Independent Particles in a Time-Dependent Irregular Container

C. Jarzynski and W.J. Swiatecki

Nuclear Science Division Lawrence Berkeley Laboratory 1 Cyclotron Road Berkeley, California 94720

January 9, 1992

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## A Universal Asymptotic Velocity Distribution for Independent Particles in a Time-Dependent Irregular Container

C. Jarzynski and W.J. Swiatecki Nuclear Science Division Lawrence Berkeley Laboratory 1 Cyclotron Road Berkeley, California 94720

#### Abstract

We show that the velocity distribution f(v) for a gas of non-interacting particles bouncing around in a deforming irregular container of fixed volume tends to a universal function independent of its original form and of the container's shape or time evolution. This function turns out to be the *exponential* velocity distribution  $f(v) \propto e^{-v/c}$ . This may be contrasted with the *gaussian* Maxwell-Boltzmann distribution appropriate in the case of a gas of *interacting* particles.

#### 1. Introduction

The study of the dynamics of classical or quantized independent point particles bouncing about inside variously shaped static containers (so-called two- or three-dimensional billiards) has received much attention in recent years in connection with attempts to understand the characteristics of ordered and chaotic motions in dynamical systems in general (Refs. 1-5). In the context of nuclear physics, the study of independent particles in variously shaped 'meanfield' or 'single-particle' potential wells has served for a long time as the starting point for models of nuclear structure. The generalization of this problem to the case of *time-dependent* containers is of importance for understanding the order-to-chaos transition in the case of timedependent Hamiltonians. In nuclear physics the problem arises in the case of idealized models of fissioning or fusing nuclei. The understanding of the order-to-chaos transition is particularly relevant in this case, since there is evidence that the transition from ordered to chaotic nucleonic

motions is accompanied by a transition in the collective properties of nuclei from those of an elastic solid to those of a very viscous fluid (Refs. 6-24).

The present paper is a contribution to studies of idealized time-dependent dynamical systems of the above type, in particular to the long-term behaviour of a gas of independent classical particles in a time-dependent irregular container. (This could be regarded as a modification of the 'Fermi acceleration problem,' in which independent particles bounce between two oscillating parallel walls (Ref. 25). In our case the dynamics is three- rather than one-dimensional and, apart from the time dependence, chaotic rather than integrable.)

#### 2. The Wall Formula for dissipation

It was shown in Ref. (6) that, under certain assumptions, the rate of change of the energy E of such a gas is given by the so-called wall formula for nuclear dissipation, viz.

$$\frac{dE}{dt} = \rho \overline{v} \oint \dot{n}^2 d\sigma, \qquad (1)$$

where  $\rho$  is the mass density of the gas,  $\overline{v}$  the mean speed of the gas particles and n specifies the normal speeds of the surface elements d $\sigma$  of the container, assumed small compared to  $\overline{v}$ . Since the energy E is equal to half the total mass M of the gas times the mean square particle speed  $\overline{v^2}$ , Eq. (1) may be re-written as

$$\frac{d\overline{v^2}}{dt} = \frac{2\overline{v}}{V} \oint \dot{n}^2 \, d\sigma \,, \tag{2}$$

where V is the volume of the container, equal to M/p. This equation has been used in the past to calculate the short term increase of the energy (or of  $\overline{v^2}$ ) by using for  $\overline{v}$  its initial value  $\overline{v_0}$ . But for longer times,  $\overline{v}$  will also increase and Eq. (2) by itself is not able to predict the long term evolution of the energy. In a recent paper (Ref. 26) this problem was solved by the derivation of an equation for the rate of change of the first moment  $\overline{v}$  (in effect a second wall formula), viz

$$\frac{d\overline{v}}{dt} = \frac{3}{4V} \oint \dot{n}^2 d\sigma , \qquad (3)$$

so that

$$\overline{\mathbf{v}} = \overline{\mathbf{v}}_0 \left( 1 + \frac{3}{4} \mathbf{I}(\mathbf{t}) \right), \tag{4}$$

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where I(t) stands for the following dimensionless monotonically increasing function of time

$$I(t) = \frac{1}{\overline{v}_0 V} \int_0^t dt \oint \dot{n}^2 d\sigma \,.$$
 (5)

Multiplying Eq. (3) by  $2\overline{v}$  we also find

$$2\overline{v}\frac{d\overline{v}}{dt} \equiv \frac{d\overline{v}^2}{dt} = \frac{3\overline{v}}{2V} \oint \dot{n}^2 d\sigma,$$

$$\frac{\overline{dv^2}}{dt} = \frac{4}{3} \frac{\overline{dv}^2}{dt},$$
(6)

i.e.

$$\overline{\mathbf{v}^2} - \overline{\mathbf{v}_0^2} = \frac{4}{3} \left( \overline{\mathbf{v}}^2 - \overline{\mathbf{v}}_0^2 \right). \tag{7}$$

It follows that the time evolution of the relative energy is given, for arbitrarily long times, by the following closed formula (consistent with Ref. 27):

$$\frac{E}{E_0} = \frac{\overline{v^2}}{\overline{v_0^2}} = 1 + \frac{4}{3} \left[ \overline{v}_0^2 \left( 1 + \frac{3}{4} I \right)^2 - \overline{v}_0^2 \right] / \overline{v_0^2}$$

$$= 1 + \frac{2\overline{v}_0^2}{\overline{v_0^2}} \left( I + \frac{3}{8} I^2 \right).$$
(8)

From Eq. (7) we also deduce that after a sufficiently long time, when  $\overline{v_0^2}$  and  $\overline{v}_0^2$  have become negligible compared to the monotonically increasing  $\overline{v^2}$  and  $\overline{v}^2$ , the following relation between the first and second moments holds asymptotically:

$$\overline{\mathbf{v}^2} \to \frac{4}{3} \,\overline{\mathbf{v}}^2 \,. \tag{9}$$

As is readily verified, this happens to be the relation between the first and second moments of an exponential velocity distribution  $f(v) \propto e^{-v/c}$ . Following up this hint we proceeded to generalize the wall formula, obtaining an expression for the rate of change of an arbitrary moment  $\overline{v^n}$ . We then deduced that, asymptotically, all the resulting moments agree with the moments of an exponential function!

### The Wall Formula for an Arbitrary Moment $\overline{v^n}$

The derivation of the generalized wall formula for  $\overline{v^n}$  proceeds along the lines of the derivation of  $\overline{v^2}$  in Ref. (6). Consider a gas of non-interacting particles characterized by an initial isotropic velocity distribution f(v), normalized so that

$$\int_0^\infty 4\pi \, \mathrm{d} v \, v^2 f(v) = 1 \,. \tag{10}$$

The gas is in a very long cylinder of cross-sectional area  $\Delta\sigma$ , closed off at one end by a piston which begins to move slowly with speed u towards the gas. (The cylinder may be thought of as an imaginary prism erected on an element of area  $\Delta\sigma$  of an infinite plane wall moving towards a semi-infinite volume of the gas.) After a while the gas in the vicinity of the piston will consist of two components; the undisturbed gas which is at rest in the laboratory frame of reference and a reflected component consisting of particles that have collided with the moving piston and are streaming away from it. In a reference frame moving with the piston the first component is streaming towards the piston with speed u and the second is identical with the first except that it is streaming away from the piston with speed u. Figure 1 illustrates the velocity distribution of both components as seen either from the piston or from the laboratory frame of reference. When the piston is at rest, u vanishes and the velocity distribution reduces to the spherically symmetric function f(v). The motion of the piston introduces an asymmetry in the figure (as seen in the laboratory frame) and this modifies the moments  $\overline{v^n}$  of the resulting velocity distribution in a readily calculable way.

Consider a time interval  $\Delta t$  during which a number of particles will have collided with the piston. These are particles whose distance l from the piston and speed towards the piston (given by u + z) satisfy the inequality  $l < (u+z)\Delta t$ . The number of particles in a slab of thickness l and cross-section  $\Delta \sigma$  is  $l \nu \Delta \sigma$ , where  $\nu$  is the number density of the undisturbed gas. Hence the number of particles colliding with the piston in time  $\Delta t$ , whose velocity components are restricted to lie between  $\rho$  and  $\rho + d\rho$ , and between z and z + dz (i.e., whose velocity vectors lie in a ring of volume  $2\pi\rho d\rho dz$  in velocity space) is given by

$$v\Delta\sigma\Delta t (u+z) f(v) 2\pi\rho d\rho dz$$
. (11)

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After colliding with the piston the above particles will have their z-components of velocity changed from z to -z-2u. The effect of this change on a particle's speed in the lab frame of reference is

$$\Delta v = v_{new} - v_{old} = \sqrt{\rho^2 + (z+2u)^2} - \sqrt{\rho^2 + z^2} ,$$

and the effect on the n-th power of the speed is

$$\Delta \mathbf{v}^{n} = \mathbf{v}_{new}^{n} - \mathbf{v}_{old}^{n} = \left[\rho^{2} + (z+2u)^{2}\right]^{n/2} - \left[\rho^{2} + z^{2}\right]^{n/2}$$

$$= 2n\mathbf{v}^{n-2}zu + 2\left[n\mathbf{v}^{n-2} + n(n-2)\mathbf{v}^{n-4}z^{2}\right]u^{2} + \cdots,$$
(12)

where  $v^2 = \rho^2 + z^2$ , and where we have kept only the first two terms in the expansion in u, considered small. Multiplying  $\Delta v^n$  by Eq. (11), integrating over  $\rho$  from 0 to  $\infty$ , over z from –u to  $\infty$ , and dividing by  $\Delta t$  gives the rate of increase of the summed n-th powers of v for the particles in the cylinder:

$$\frac{d}{dt} \Sigma v^{n} = v \Delta \sigma \int_{z=-u}^{\infty} dz \int_{\rho=0}^{\infty} d\rho \ \rho 4\pi f(v) \left[ nv^{n-2} z^{2}u + \left( 2nv^{n-2} z + n(n-2)v^{n-4} z^{3} \right) u^{2} + \cdots \right].$$
(13)

Changing the variable of integration from  $\rho$  to v, noting that  $\rho d\rho = v dv$  and that the lower limit  $\rho = 0$  corresponds to z = |z|, we find

$$\frac{d}{dt} \Sigma v^{n} = v \Delta \sigma \int_{z=-u}^{\infty} dz \int_{v=|z|}^{\infty} dv \ v 4\pi f(v) \left[ nv^{n-2} z^{2} u + \left( 2nv^{n-2} z + n(n-2)v^{n-4} z^{3} \right) u^{2} \right] .$$
(14)

We split the z integration into  $\int_{z=-u}^{0} dz$  and  $\int_{z=0}^{\infty} dz$  and note that the former, representing a small interval of size u, will lead to a contribution of higher order in u than u<sup>2</sup>. This leaves an expression for  $\frac{d}{dt} \sum v^n$  identical with Eq. (14), except that the lower limit in the z-integration is 0 and in the v-integration is now simply v = z rather than v = |z|. We evaluate the integrals by taking the factors  $z^2$ , z and  $z^3$  in the square bracket outside the v-integration and carrying out the z-integrations in each case by parts. (The first part is  $z^2$ , z or  $z^3$  and the second part is an integral over v whose dependence on z enters only through the lower limit v = z). The result is

$$\frac{d}{dt} \Sigma v^{n} = v \Delta \sigma \int_{z=0}^{\infty} dz \ z 4\pi f(z) \left[ n z^{n-2} \frac{z^{3}}{3} u + \left( 2n z^{n-2} \frac{z^{2}}{2} + n(n-2) z^{n-4} \frac{z^{4}}{4} \right) u^{2} \right].$$

Since z is now merely a dummy variable of integration, the result may be written in terms of the moments  $\overline{v^n}$  as follows

$$\frac{\mathrm{d}}{\mathrm{d}t} \Sigma \mathbf{v}^{\mathrm{n}} = \mathbf{v} \Delta \sigma \left[ \frac{1}{3} \operatorname{nu} \overline{\mathbf{v}^{\mathrm{n}}} + \left( n \overline{\mathbf{v}^{\mathrm{n-1}}} + \frac{1}{4} n(\mathrm{n-2}) \overline{\mathbf{v}^{\mathrm{n-1}}} \right) \mathbf{u}^{2} \right].$$
$$= \mathbf{v} \Delta \sigma \left[ \frac{1}{3} n \overline{\mathbf{v}^{\mathrm{n}}} \mathbf{u} + \frac{1}{4} n(\mathrm{n+2}) \overline{\mathbf{v}^{\mathrm{n-1}}} \mathbf{u}^{2} \right], \qquad (15)$$

 $\overline{\mathbf{v}^{\mathbf{n}}} = \int_0^\infty 4\pi d\mathbf{v} \, \mathbf{v}^2 \, \mathbf{v}^{\mathbf{n}} \, \mathbf{f}(\mathbf{v}) \; .$ 

where

We now apply this 'piston formula' to the case of a container whose surface elements do move with *outward* normal speeds specified by  $\dot{n}$ . Thus u is to be identified with  $-\dot{n}$ . Integrating over the surface of the container will give the rate of change of the summed n-th powers of all the particles' speeds in the container. If the number of particles in the container is N then the rate of change of the average of v<sup>n</sup>, i.e.  $dv^n/dt$ , is obtained by dividing eq. (15) by N. Since N/v = V, the container's volume, we find

$$\frac{d\overline{\mathbf{v}^{\mathbf{n}}}}{dt} = \frac{1}{\mathbf{V}} \oint d\sigma \left[ -\frac{1}{3} \, \mathbf{n} \, \overline{\mathbf{v}^{\mathbf{n}}} \, \dot{\mathbf{n}} + \frac{1}{4} \, \mathbf{n} \, (\mathbf{n+2}) \, \overline{\mathbf{v}^{\mathbf{n-1}}} \, \dot{\mathbf{n}}^2 \right]. \tag{16}$$

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For volume preserving deformations of the container the first term vanishes and we find the following generalized wall formula:

$$\frac{d\overline{\mathbf{v}^{n}}}{dt} = \frac{1}{4} n (n+2) \overline{\mathbf{v}^{n-1}} \frac{1}{V} \oint \dot{\mathbf{n}}^{2} d\sigma.$$
(17)

For n = 2 we obtain the standard wall formula in the form of Eq. (2). For n = 1 we recover the 'second wall formula' of Ref. (26) (our Eq. (3)), derived here in a different way. We shall now proceed to use Eq. (17) to derive the asymptotic form of the velocity distribution f(v).

#### 4. The Asymptotic Form of f(v) is an Exponential

Combining Eqs. (3) and (17) we have

$$\frac{\overline{dv^n}}{dt} = \frac{1}{3} n (n+2) \overline{v^{n-1}} \frac{\overline{dv}}{dt}.$$
(18)

For n = 2 we find

$$\frac{\overline{dv^2}}{dt} = \frac{4.2}{3} \overline{v} \frac{d\overline{v}}{dt} = \frac{4.2}{3} \frac{1}{2} \frac{d\overline{v}^2}{dt}$$

which is the same as Eq. (7) and leads asymptotically to

$$\overline{v^2} \rightarrow \frac{4.2}{3} \frac{1}{2} \overline{v}^2$$

For n = 3 we have

$$\frac{\mathrm{d}\mathbf{v}^{3}}{\mathrm{d}t} = \frac{5.3}{3} \overline{\mathbf{v}^{2}} \frac{\mathrm{d}\overline{\mathbf{v}}}{\mathrm{d}t} \to \frac{5.3}{3} \frac{4.2}{3} \frac{1}{2} \overline{\mathbf{v}}^{2} \frac{\mathrm{d}\overline{\mathbf{v}}}{\mathrm{d}t} = \frac{5.3}{3} \cdot \frac{4.2}{3} \cdot \frac{1}{2} \cdot \frac{1}{3} \frac{\mathrm{d}\overline{\mathbf{v}}^{3}}{\mathrm{d}t}$$
$$\therefore \overline{\mathbf{v}^{3}} \to \frac{5.3}{3} \cdot \frac{4.2}{3} \cdot \frac{1}{2} \cdot \frac{1}{3} \overline{\mathbf{v}}^{3} .$$

For general n we have, by induction

$$\overline{\mathbf{v}^{\mathbf{n}}} \rightarrow \frac{(\mathbf{n+2})\mathbf{n}}{3} \cdot \frac{(\mathbf{n+1})(\mathbf{n-1})}{3} \cdot \frac{\mathbf{n}(\mathbf{n-2})}{3} \cdots \frac{4.2}{3} \cdot \frac{1}{2} \cdot \frac{1}{3} \cdot \frac{1}{4} \cdots \frac{1}{\mathbf{n}} \overline{\mathbf{v}^{\mathbf{n}}} \,.$$

It follows that

$$\frac{\overline{\mathbf{v}^{\mathbf{n}}}}{\overline{\mathbf{v}}^{\mathbf{n}}} \to \frac{(\mathbf{n+2})!}{2.3^{\mathbf{n}}}.$$
(19)

Now for an exponential function  $f(v) \propto e^{-v/c}$ , the ratio of  $\overline{v^n}$  to  $\overline{v}^n$  is given by

$$\frac{\overline{v^{n}}}{\overline{v}^{n}} = \frac{\int_{0}^{\infty} dv v^{n+2} e^{-v/c} / \int_{0}^{\infty} dv v^{2} e^{-v/c}}{\left(\int_{0}^{\infty} dv v^{3} e^{-v/c} / \int_{0}^{\infty} dv v^{2} e^{-v/c}\right)^{n}} = \frac{(n+2)!}{2.3^{n}}.$$

This proves that, under the explicit and implicit assumptions made in arriving at Eq. (19), the asymptotic velocity distribution f(v) for particles bouncing about in an irregular, volume-conserving, time dependent container is an exponential.

#### 5. Discussion

The explicit approximation made in Section 3 concerned the slowness of the wall velocities n compared to the particle speeds. At first this seems like a serious limitation, suggesting that the theorem about the asymptotic velocity distribution being exponential holds only if the container is restricted to very slow deformations. On reflection one realizes that this is almost certainly not the case. Thus insofar as the particle velocities increase monotonically with time, they will

eventually become larger than the wall velocities and the approximation  $|\dot{n}| \ll \bar{v}$  will automatically continue to improve with time, becoming virtually perfect asymptotically. But could it be that if initially |n| is very large compared to  $\overline{v}$ , the particle speeds will not increase with time? Again this is most unlikely, since the simplest qualitative way of understanding why it is that the standard wall formula predicts an increase in the particle energies is based precisely on considering the limit of very large piston speeds. The argument is most transparent if one considers the gas in the cylinder to have initially a sufficiently sharply cut off velocity distribution, one that is essentially zero for  $v > v_c$ . In that case for piston speeds exceeding  $v_c$ there is a gross asymmetry between the cases of the inward or outward moving piston. In the former case the gas particles are speeded up dramatically by the large piston speed, but in the latter no particles ever collide with the piston and their speeds remain unaltered: there is no compensating slowing down at all. This is the qualitative way of understanding why the sign of the second term in Eq. (14) is positive and shows that the argument for the average speeding up of the gas particles is actually strongest when the wall velocities are *large*. (Of course, one needs to exclude pathological situations where the gas particles—or some finite fraction—are actually at rest and *never* hit the wall of the container. But for any finite particle speed, a particle will eventually begin hitting the wall elements and its average speed will begin to be boosted by the collisions. One must also exclude contrived situations where the container's deformations are continuously speeded up so that the approximation  $\overline{v} >> |n|$  is never satisfied.)

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The more serious, implicit, assumption underlying the present analysis concerns the application of the piston formula, Eq. (15), derived for a semi-infinite volume of a gas with standard density, initially at rest and isotropic in velocity space, to the surface elements of a finite container. What one is effectively assuming here is that also in the case of the finite container each surface element d $\sigma$  continues to be bombarded by particles as if they originated in a gas of standard density, at rest in the laboratory frame, and with an isotropic velocity distribution. For this assumption to be valid one clearly needs some kind of randomization hypothesis relying on the irregularity of the container and of its time dependence. As discussed already in Ref. 6, it is

very easy to construct counter-examples where the randomization hypothesis is *not* satisfied. One class of examples concerns containers whose shapes are such that the particle motions are integrable (e.g. boxes or spheroids). Another concerns containers whose motions are globally regular, i.e. overall translations or notations. (See Ref. 6.) Apart from such obvious exceptions, the randomization hypothesis relies on the observation that the particles about to collide with an element d $\sigma$  of the container arrive at the location of d $\sigma$  after collisions at many different instants with many irregularly oriented other surface elements, whose orientations and states of motion do not, by hypothesis, define any preferred directions in coordinate or velocity space. We expect that the randomization hypothesis will encompass a large class of irregular, time-dependent billiards, but the precise, mathematically rigorous specification of situations where the hypothesis might fail could turn out to be a difficult problem in theoretical dynamics.

1.1.1

A word about the limited relevance to the nuclear problem of the theorem concerning the long term behaviour of a gas. Even apart from the need in that case to study the effects of quantization, if a nuclear system were to deform for a time long enough to wash out its step-like velocity distribution (appropriate to a degenerate Fermi gas) into an exponential distribution, the justification for treating the nucleus as a gas of approximately independent particles would have disappeared. Thus the present finding should be viewed as a contribution to the abstract study of the dynamics of time-dependent systems of non-interacting particles, which only in some of its aspects does have relevance to the nuclear problem. The striking simplicity of the universal exponential velocity distribution for irregular billiards brings to mind the even more universal gaussian Maxwell-Boltzmann distribution. This raises the interesting question of how general the exponential distribution might, in fact, turn out to be. How does it generalize to the case of independent particles in a *smooth* time-dependent potential well?

#### Acknowledgement

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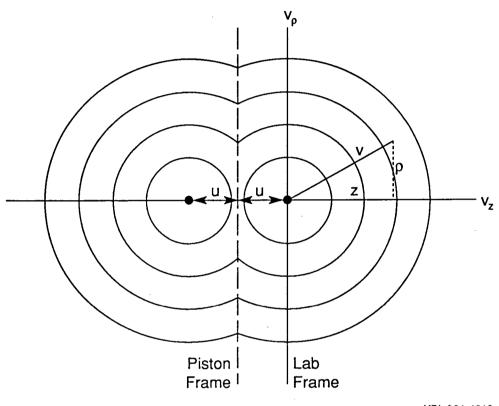
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#### **Figure Caption**

Fig. 1. The appearance of contour lines of the velocity distribution function for a gas in the vicinity of a piston moving with speed u towards the gas. Here z and  $\rho$  stand for  $v_z$  and  $v_{\rho}$ , the components of a particle's velocity  $\vec{v}$  along the z and  $\rho$  directions,  $\rho$  being the radial distance from the axis of the axially symmetric velocity-space distribution.



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Figure 1

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