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Energy Diffusion in a Chaotic Adiabatic Billiard Gas*

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Abstract

A diffusion equation is derived for the energy distribution of a gas of non-interacting point particles following chaotic trajectories inside a slowly-time-dependent container. We discuss the relevance of this problem to results concerning ergodic adiabatic Hamiltonian systems, as well as to one-body dissipation in nuclear dynamics.

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INTRODUCTION

This paper considers the problem of a *chaotic adiabatic billiard gas*, a gas of noninteracting point particles bouncing around chaotically inside a container whose shape changes slowly with time. (See Fig. 1.) Unlike an ordinary gas, where particle-particle collisions dominate, producing a Maxwell-Boltzmann distribution of energies, here the evolution of a particle's energy is determined solely by its collisions with the slowly moving walls of the container. Let $\eta(E,t)\,dE$ denote the number of particles with energy in a small interval dE around E, at time t. The main result of this paper is a diffusion equation governing the time evolution of η, the distribution of particle energies. We obtain such an equation for both the two- and three-dimensional versions of this problem.

Sec. I of this paper specifies the problem precisely, and introduces notation. In Sec. II we argue that the distribution of particle energies of a chaotic adiabatic billiard gas evolves diffusively; this suggests a Fokker-Planck equation for the evolution of $\eta(E,t)$. In Sec. III we derive explicit expressions for the drift and diffusion coefficients which determine this equation. These are given in terms of the dynamics of particles bouncing around inside time-*independent* containers, obtained by "freezing" the slowly-changing shape of the container at different instants in time. We show in Sec. IV that, under a certain approximation, our results may be further simplified so that the evolution of η is given entirely in terms of the changing shape of the container, without any reference to particle dynamics.

Our interest in this problem is twofold. First, as discussed in Sec. V, our gas can be treated as an example of an *ergodic adiabatic ensemble*, an ensemble of noninteracting systems evolving chaotically under a common, slowly time-varying Hamiltonian. Ott, Brown, and Grebogi [1–3] have used multiple time-scale analysis to study such systems. Their focus has been the goodness of the *ergodic adiabatic invariant*, i.e. the extent to which a certain quantity, shown by Ott [1] to be conserved in the limit of an infinitely slowly evolving Hamiltonian, remains conserved when the Hamiltonian evolves at a slow but finite rate. Recently [4], we have used an alternative approach to this problem to derive an evolution equation for the distribution of energies of an ergodic adiabatic ensemble. Such an equation was previously derived by Wilkinson [5], using Ott's results; regrettably, we were unaware of Wilkinson's work, and failed to give him due credit. In Ref. [4], we compared the predictions that follow from this equation with Ott's predictions concerning the goodness of the ergodic adiabatic invariant, and found disagreement. The results of the present paper will allow us to study this discrepancy numerically.

Our other motivation for studying this problem comes from the independent particle model of nuclear dynamics, in which a nucleus undergoing some dynamical process (e.g. fission, or collision with another nucleus) is imagined as a container, filled with a gas of independent point particles, whose shape is allowed to change with time. This simple model provides a mechanism, one-body dissipation, for friction in dynamical nuclear processes. A principal result of this approach to nuclear dynamics has been the wall formula [6,7], an expression for the rate at which one-body dissipation transfers energy from the collective degrees of freedom of one idealized nucleus to the individual nucleons. The results of the present paper, as discussed in Sec. VI, extend our understanding of one-body dissipation.

I. PRELIMINARIES

We take the time-dependent shape of the container to be an externally imposed, rather than a dynamical, quantity: the shape evolves in a pre-determined way, independently of the gas of particles. Each bounce of a particle off the moving walls of the container is taken to be specular (the angle of reflection is equal to the angle of incidence) in the instantaneous rest frame of the local piece of wall at which the collision occurs. Effectively, these bounces constitute elastic collisions in which the inertia of the wall is infinitely greater than that of the particle.

We are interested in observing our gas of noninteracting particles as the shape of the container changes slowly. To express "slow" shape evolution mathematically, we make the shape a function of ϵt, where t is time and ϵ is a slowness parameter, formally taken to be small. Thus, let $\mathrm{Sh}(\epsilon t)$ denote the shape of the container at time t. We will be interested in observing our gas for times of order ϵ^{-1}, over which the container changes by order unity. As the extreme limit of slow evolution, we will take the *adiabatic limit* to mean that in which we let ϵ go to zero, holding ϵt_i and ϵt_f fixed, t_i and t_f being the initial and final times over which we observe the system. In this limit, the container evolves infinitely slowly from the initial shape $\mathrm{Sh}(\epsilon t_i)$ to the final shape $\mathrm{Sh}(\epsilon t_f)$.

We will frequently refer to the motion of particles inside a *frozen* container, by which we mean the time-independent container obtained by arresting ("freezing") the slowly evolving shape $\mathrm{Sh}(\epsilon t)$ at some instant in time. Whenever discussing the dynamics of particles inside a frozen container, as opposed to the slowly changing one, we will emphasize the distinction by using Sh_α, with $\alpha = \epsilon t$, to denote the shape of the container frozen at ϵt. When discussing motion inside the time-dependent container, we will retain the notation $\mathrm{Sh}(\epsilon t)$. The slow evolution of the container from $\mathrm{Sh}(\epsilon t_i)$ to $\mathrm{Sh}(\epsilon t_f)$ defines a continuous sequence of frozen shapes Sh_α, with α ranging from ϵt_i to ϵt_f.

The motion of a particle bouncing around inside a frozen container is represented in phase space by a trajectory $(\mathbf{q}(t), \mathbf{p}(t))$ whose evolution is restricted to an *energy shell*, a surface of constant energy. We make the crucial assumption that, for any of the frozen shapes Sh_α, an arbitrary non-periodic trajectory will chaotically and ergodically explore the entire energy shell on which it is found. A consequence of this assumption is that the motion of particles in any of the frozen containers exhibits *chaotic mixing* over the energy shell: any distribution of initial particle positions and velocities will evolve into a uniform distribution of particles throughout the container, with an isotropic distribution of velocities. The time scale over which this mixing occurs is given by the Lyapunov time $t_L = 1/\lambda$, where λ is the Lyapunov exponent associated with the chaotic evolution of the trajectories.

We now discuss the relevance of chaotic mixing to a gas of particles in a slowly time-dependent container. First, consider the motion of two particles sharing identical initial conditions at time t_0, one subsequently evolving inside the time-dependent container $\mathrm{Sh}(\epsilon t)$, the other inside the frozen container Sh_α, with $\alpha = \epsilon t_0$. Let T be the length of time over which the paths followed by these two particles remain very close; after this time, they will diverge rapidly. T can be made arbitrarily large by choosing ϵ arbitrarily small, although, due to the assumed chaoticity, a value of T much larger than the Lyapunov time t_L would require an extremely small ϵ. (By treating motion inside the evolving container as a perturbed version of motion inside the frozen one, with the perturbations, proportional to

ϵ, introduced at collisions with the wall, T can be shown to scale like $t_L \ln(1/\epsilon)$, for small ϵ.) We will henceforth assume ϵ to be small enough that

$$T \gtrsim t_L. \tag{1.1}$$

Thus, motion inside the time-dependent container closely mimics that inside the frozen one over times on the order of the Lyapunov time. In this case, chaotic mixing occurs before the particles "realize" that the shape is changing; as the container slowly evolves, the continual process of chaotic mixing tends to maintain a uniform distribution of particles throughout the container, and an isotropic distribution of velocities.

We will use the term *chaotic adiabatic billiard gas* to describe a gas of noninteracting particles inside of a container whose slowly evolving shape satisfies the assumptions discussed above. Our goal is an evolution equation for the distribution of particle energies, $\eta(E,t)$.

II. DIFFUSION OF ENERGIES

The energy of a given particle changes in small, discrete amounts as the particle collides with the slowly moving walls of the container. We can think of this process in terms of the particle performing a "walk" along the energy axis, with steps determined by the underlying motion of the particle bouncing off the container's walls. Since this underlying motion is chaotic, correlations between these steps along the energy axis will exist only over a finite time, on the order of the Lyapunov time t_L. This consideration suggests [4,8] that the distribution of energies of a gas of such particles will, on a time scale much longer than t_L, evolve by a process of diffusion. We therefore postulate the following Fokker-Planck equation for the time-dependent distribution of energies, $\eta(E,t)$:

$$\frac{\partial \eta}{\partial t} = -\frac{\partial}{\partial E}(g_1\eta) + \frac{1}{2}\frac{\partial^2}{\partial E^2}(g_2\eta). \tag{2.1}$$

This is a generalized diffusion equation, in which the drift and diffusion coefficients g_1 and g_2 are functions of both energy and time. Specifically, we write $g_1(E,\epsilon t)$ and $g_2(E,\epsilon t)$; we use explicit functions of ϵt rather than simply t because we expect the evolution of η at a given time t to be determined by the instantaneous shape of the container and the way in which it is changing, which depend explicitly on ϵt.

Since we are interested in slow evolution of the shape of the container, we can expand g_1 and g_2 in powers of ϵ (making the assumption that integral powers suffice). As discussed below, retaining only $O(\epsilon^1)$ terms gives an evolution equation for η that corresponds to the adiabatic limit (infinitely slow shape evolution). We are interested in slow but finite evolution of the shape of the container, and therefore want expressions for g_1 and g_2 valid to $O(\epsilon^2)$.

In treating the evolution of η as a process of diffusion, we must keep in mind that this picture is valid only over times much longer than the Lyapunov time t_L. Thus, for Eq. 2.1 to be applicable to our problem, there must exist a time scale which is long compared to t_L, but short compared to that over which significant changes in the distribution of energies (as well as the shape of the container) occur. We will use the notation Δt to indicate a time on this scale, and will refer to this time as "short" or "long" depending on the context, i.e. whether we are discussing the evolution of $\eta(E,t)$, or the motion of particles in the container.

III. DERIVATION OF DRIFT AND DIFFUSION COEFFICIENTS

To derive expression for g_1 and g_2, note that a distribution of energies described initially by a δ-function along the energy axis,

$$\eta(E, t_0) = \delta(E - E_0), \tag{3.1}$$

will evolve under Eq. 2.1 so that, a short time Δt later, the average energy will have drifted away from E_0 by an amount $g_1 \Delta t$, and the distribution will have acquired a variance $g_2 \Delta t$, with g_1 and g_2 evaluated at E_0, ϵt_0. The second moment of this new distribution of energies with respect to E_0 is then

$$\begin{aligned} \mathcal{M}_2(\Delta t) &\equiv \int dE\ \eta(E, t_0 + \Delta t)\ (E - E_0)^2 \\ &= (g_1 \Delta t)^2 + g_2 \Delta t. \end{aligned} \tag{3.2}$$

By considering a gas of particles sharing a common energy E_0 at time t_0 (such a gas, with number of particles normalized to unity, is described by Eq. 3.1), then by solving, in terms of quantities characterizing the subsequent motion of these particles, for $\mathcal{M}_2(\Delta t)$, and finally by comparing the result with Eq. 3.2, we will obtain expressions for g_1 and g_2. We will solve only for the leading term of $\mathcal{M}_2(\Delta t)$, which is $O(\epsilon^2)$. From this will immediately follow the leading terms of g_1 and g_2, which are $O(\epsilon^1)$ and $O(\epsilon^2)$, respectively. To obtain the $O(\epsilon^2)$ term of g_1, we will invoke a trick using Liouville's theorem.

We therefore begin by considering, at time t_0, a gas of particles of energy E_0 distributed uniformly with the container, with an isotropic distribution of velocities. Let us introduce the *wall velocity field*, $\dot{n}$, a scalar field defined over the surface of the container: the value of $\dot{n}$ at a particular point on the surface gives the normal outward velocity of the moving wall at that point (see Fig. 1; a negative $\dot{n}$ indicates a portion of the wall which is moving into the gas). This field contains all information about how the shape of the container is changing at a given instant in time. Since this field changes with time along with the shape of the container, we will write it as $\dot{n}(\epsilon t)$ (suppressing the dependence on the position on the surface of the wall). We also introduce a *frozen* field $\dot{n}_\alpha$ — defined over the surface of the frozen shape Sh_α — which is simply the normal outward wall velocity at the moment of freezing; $\dot{n}_\alpha$ "remembers" how the shape $\mathrm{Sh}(\epsilon t)$ was changing at the instant in which it was frozen into Sh_α.

To lowest order in the wall velocity (proportional to ϵ), the change in the energy of a particle as it bounces off the wall is $-2mv\dot{n}\sin\theta$, where m is the particle mass, v is its speed prior to collision, $\dot{n}$ is the value of the wall velocity field at the point of collision, and θ is the angle between the incoming trajectory of the particle and a surface tangent to the wall. (See Figs. 2 and 3.) Between times t_0 and $t_0 + \Delta t$ the particle bounces many times off the walls of the container, whose shape changes negligibly during that time. The number of collisions, B, is approximated as

$$B \cong \Delta t / \tau, \tag{3.3}$$

where τ is the average time between bounces for a particle inside the container frozen at $\alpha = \epsilon t_0$. The total change in the energy of the particle over this time is

$$E - E_0 = -2mv \sum_{b=1}^{B} \dot{n}_b \sin\theta_b + O(\epsilon^2), \tag{3.4}$$

where the $\dot{n}_b$'s are the normal outward wall velocities sampled by the sequence of bounces $b = 1, 2, \cdots, B$, and the θ_b's are the corresponding angles of collision. We are justified in pulling $v = (2E_0/m)^{1/2}$ outside this sum by the fact that, to lowest order in ϵ, the speed of the particle remains constant over time Δt. To obtain $\mathcal{M}_2(\Delta t)$, we square the above sum, then average over all particles, i.e. over an ensemble of trajectories evolving from a uniform distribution of initial conditions on the energy shell E_0 at time t_0. Angular brackets will denote this average:

$$\mathcal{M}_2(\Delta t) = 4m^2v^2 \sum_{b=1}^{B} \sum_{b'=1}^{B} \left\langle \dot{n}_b \sin\theta_b \, \dot{n}_{b'} \sin\theta_{b'} \right\rangle + O(\epsilon^3). \tag{3.5}$$

Now, suppose temporarily that, for any initial condition corresponding to energy E_0 at time t_0, two trajectories evolving from that initial condition, one inside the slowly changing container, the other inside the container frozen at $\alpha = \epsilon t_0$, remain very close to one another for the entire length of time from t_0 to $t_0 + \Delta t$. (Since $\Delta t \gg t_L$, this puts a drastic limit, which we later relax, on the magnitude of ϵ.) If this condition holds, then, for puposes of evaluating the right hand side of Eq. 3.5, we may replace the gas of particles evolving for time Δt inside the time-dependent container, with a gas evolving inside the frozen one. With this replacement, Eq. 3.5 becomes

$$\mathcal{M}_2(\Delta t) = 4m^2v^2 \sum_{b=1}^{B} \sum_{b'=1}^{B} \left\langle \dot{n}_{\alpha b} \sin\theta_b \, \dot{n}_{\alpha b'} \sin\theta_{b'} \right\rangle_\alpha + O(\epsilon^3), \tag{3.6}$$

where the angular brackets $\langle \cdots \rangle_\alpha$ indicate an average over an ensemble of trajectories evolving inside the *frozen* Sh_α, with $\alpha = \epsilon t_0$ (as before, the ensemble is defined by a uniform distribution of initial conditions over the energy shell E_0), and $\dot{n}_{\alpha b}$ gives the value of the frozen field $\dot{n}_\alpha$ at the b'th bounce of one such trajectory.

We rewrite the quantity being summed in Eq. 3.6 as

$$\left\langle (\dot{n}_{\alpha b} \sin\theta_b - \xi_b)(\dot{n}_{\alpha b'} \sin\theta_{b'} - \xi_{b'}) \right\rangle_\alpha + \xi_b \xi_{b'} \equiv c_{b,b'} + \xi_b \xi_{b'}, \tag{3.7}$$

where $\xi_b \equiv \langle \dot{n}_{\alpha b} \sin\theta_b \rangle_\alpha$. As discussed in Appendix A, it is good approximation to treat ξ_b as independent of b, and so we write it simply as ξ. Furthermore the correlation function $c_{b,b'}$ depends, within the same approximation, only on the difference $b' - b$, and so may be written as $c_{\Delta b}$, with $\Delta b \equiv b' - b$. The double sum in Eq. 3.6 then becomes

$$\sum_{b=1}^{B} \sum_{b'=1}^{B} (c_{\Delta b} + \xi^2) = B^2\xi^2 + B \sum_{\Delta b=-B}^{B} \left(1 - \frac{|\Delta b|}{B}\right) c_{\Delta b}. \tag{3.8}$$

Now, $c_{\Delta b} \cong 0$ for $|\Delta b| > \nu_L$, where $\nu_L \cong t_L/\tau$ (again, see Appendix A). Having assumed $\Delta t \gg t_L$, we have $B \gg \nu_L$, and may therefore approximate the sum appearing on the right hand side of the above expression as $\sum_{-\infty}^{+\infty} c_{\Delta b}$; this is the discrete version of a standard result from the theory of stationary stochastic processes (see Ref. [9], and also Eqs. 4.11 and 4.12 of Ref. [4]). We assume that this sum converges. We now have, to $O(\epsilon^2)$,

$$\mathcal{M}_2(\Delta t) = 4m^2v^2\left(B^2\xi^2 + B\sum_{\Delta b=-\infty}^{+\infty} c_{\Delta b}\right)$$
$$= \left(\frac{2mv}{\tau}\xi\Delta t\right)^2 + \frac{4m^2v^2}{\tau}\Delta t\sum_{\Delta b=-\infty}^{+\infty} c_{\Delta b}. \tag{3.9}$$

Comparison with Eq. 3.2 yields

$$g_1 = \pm\frac{2mv}{\tau}\xi + O(\epsilon^2) \tag{3.10}$$
$$g_2 = \frac{4m^2v^2}{\tau}D + O(\epsilon^3), \tag{3.11}$$

where

$$D \equiv \sum_{\Delta b=-\infty}^{+\infty} c_{\Delta b}. \tag{3.12}$$

We now relax the assumption made immediately after Eq. 3.5, and assert that as long as motion inside the frozen container closely mimics that inside the time-dependent one over times on the order of t_L, rather than the much longer Δt, the steps leading to Eqs. 3.10 and 3.11 will remain valid. (We have already assumed, in Sec. I, that this more relaxed condition holds.) The justification for this assertion is similar to that presented in Ref. [4] (see the paragraph following Eq. 4.14 therein); its essence is as follows. Due to chaotic mixing, appreciable correlations exist only between bounces separated by times on the order of, or shorter than, the Lyapunov time t_L. However, since motion inside the frozen container closely resembles that inside the time-dependent one over times up to t_L, the correlations that do exist are nearly identical for the two cases. Since it is these correlations that determine the diffusion of particle energies, we are justified in evaluating the right hand side of Eq. 3.5 using particles inside the frozen rather than the time-dependent container.

We henceforth drop the subscript 0 from E_0 and t_0.

In Appendices A and B, we evaluate ξ and τ for both two- and three-dimensional containers. The results reduce Eq. 3.10 to

$$g_1(E, \epsilon t) = -\beta(\epsilon t)\,E + O(\epsilon^2), \tag{3.13}$$

where the factor $\beta(\epsilon t)$ depends on the dimensionality:

$$\beta = \dot{A}/A \qquad (2d \text{ container}) \tag{3.14a}$$
$$2\dot{V}/3V \qquad (3d \text{ container}), \tag{3.14b}$$

where A and V denote the area or volume enclosed by the container, and the dot signifies differentiation with respect to time. (A, $\dot{A}$, V, and $\dot{V}$ are evaluated at ϵt.) The ambiguity in sign appearing in Eq. 3.10 has been removed by physical considerations: since there is a net positive amount of work done by a gas inside a container whose area (in the $2d$ case) or volume ($3d$) is increasing, the energy drift g_1 associated with $\dot{A} > 0$ or $\dot{V} > 0$ must be negative.

In Eq. 3.11, the quantity D is determined by the frozen shape Sh_α and the associated frozen wall velocity field $\dot{n}_\alpha$, and hence may be written as a function of the value of α, in this case ϵt; thus, $D = D(\epsilon t)$. All dependence of g_2 on E is in the factor $4m^2v^2/\tau$. Using the results for τ from Appendix B, we get, to $O(\epsilon^2)$,

$$g_2(E, \epsilon t) = \gamma(\epsilon t)\, E^{3/2}, \tag{3.15}$$

with

$$\gamma = (8l/\pi A)\,(2m)^{1/2}\, D \qquad (2d) \tag{3.16a}$$

$$(2S/V)\,(2m)^{1/2}\, D \qquad (3d), \tag{3.16b}$$

where $l(\epsilon t)$ is the perimeter of the $2d$ container, and $S(\epsilon t)$ is the surface area of the $3d$ one.

It remains to obtain the $O(\epsilon^2)$ term of g_1. The strategy for doing so invokes Liouville's theorem, and is detailed in Sec. IV of Ref. [4]. There we find

$$g_1 = g_{11} + \frac{1}{2\Sigma}\frac{\partial}{\partial E}(g_2\Sigma), \tag{3.17}$$

where g_{11} is the leading term of g_1 (given above by Eq. 3.13), and

$$\Sigma(E, \epsilon t) \equiv \frac{\partial}{\partial E}\Omega(E, \epsilon t), \tag{3.18}$$

where $\Omega(E, \epsilon t)$ represents the volume of phase space enclosed by the energy shell E at time t. For a two-dimensional billiard system, this volume is the product of the area of ordinary space enclosed by the container, with the area in momentum space of a circle of radius $p = (2mE)^{1/2}$. Thus,

$$\Omega = 2\pi mAE \quad , \quad \Sigma = 2\pi mA. \tag{3.19}$$

In three dimensions, we get

$$\Omega = \frac{4}{3}\pi(2m)^{3/2}VE^{3/2} \quad , \quad \Sigma = 2\pi(2m)^{3/2}VE^{1/2}. \tag{3.20}$$

Using Eq. 3.17 we rewrite Eq. 2.1 as

$$\frac{\partial\eta}{\partial t} = -\frac{\partial}{\partial E}(g_{11}\eta) + \frac{1}{2}\frac{\partial}{\partial E}\Big[g_2\Sigma\frac{\partial}{\partial E}\Big(\frac{\eta}{\Sigma}\Big)\Big]. \tag{3.21}$$

Combining our results for g_{11}, g_2, and Σ with Eq. 3.21, we finally write the evolution equation for η, to $O(\epsilon^2)$, as

$$\frac{\partial\eta}{\partial t} = \beta\frac{\partial}{\partial E}(E\eta) + \frac{\gamma}{2}\frac{\partial}{\partial E}\Big(E^{3/2}\frac{\partial\eta}{\partial E}\Big) \qquad (2d) \tag{3.22a}$$

or

$$\frac{\partial\eta}{\partial t} = \beta\frac{\partial}{\partial E}(E\eta) + \frac{\gamma}{2}\frac{\partial}{\partial E}\Big[E^2\frac{\partial}{\partial E}\Big(E^{-1/2}\eta\Big)\Big] \qquad (3d). \tag{3.22b}$$

Eq. 3.22 represents the central result of this paper. The coefficients β and γ are given (Eqs. 3.14 and 3.16) in terms of: the particle mass m, quantities associated with the changing shape of the container (A, $\dot{A}$, and l; or V, $\dot{V}$, and S), and the function $D = \sum_{-\infty}^{+\infty} c_{\Delta b}$. Only the last of these directly involves the dynamics of particles bouncing around inside a container, and is given in terms of motion inside the *frozen* container Sh_α, $\alpha = \epsilon t$. Thus, the time-dependent problem (a gas of particles inside the slowly changing container $\mathrm{Sh}(\epsilon t)$) is solved in terms of the solutions of a continuous sequence of time-independent problems (motion inside the frozen shapes Sh_α). In the following section we show how, under a certain assumption (not always valid), the quantity D may be divested of any reference whatsoever to the dynamics of bouncing particles. In this case the evolution of η is given directly in terms of the changing shape of the container. First, however, we discuss the adiabatic limit.

The adiabatic limit, as defined in Sec. I, involves a time $t_f - t_i$ which approaches infinity like ϵ^{-1}. Over such a time, the term involving β ($\sim \epsilon$) in Eq. 3.22 will make an $O(\epsilon^0)$, i.e. finite, contribution to the change in η, while the term involving γ ($\sim \epsilon^2$) will make an $O(\epsilon^1)$, i.e. vanishing, contribution. Thus, in the adiabatic limit,

$$\frac{\partial \eta}{\partial t} = \beta \frac{\partial}{\partial E}\big(E\eta\big), \tag{3.23}$$

for both the $2d$ and the $3d$ case. This equation describes a distribution of particles moving along the energy axis under a "velocity" field $-\beta E$. The energy $\mathcal{E}(t)$ of any one of these particles satisfies

$$\frac{d}{dt}\mathcal{E}(t) = -\beta(\epsilon t)\,\mathcal{E}(t) = \quad -(\dot{A}/A)\,\mathcal{E}(t) \qquad (2d) \tag{3.24a}$$

$$-(2\dot{V}/3V)\,\mathcal{E}(t) \qquad (3d). \tag{3.24b}$$

From this, we get $(d/dt)\,\Omega(\mathcal{E}(t), \epsilon t) = 0$ (see Eqs. 3.19 and 3.20). Eq. 3.22 is therefore consistent with the adiabatic invariance of Ω, which was demonstrated by Ott [1] to hold generally for ergodic adiabatic Hamiltonian systems.

IV. A SIMPLIFICATION OF THE CENTRAL RESULT

It may sometimes be the case that the sum $D = \sum_{-\infty}^{+\infty} c_{\Delta b}$ which appears in γ is dominated by the term c_0:

$$D \cong c_0. \tag{4.1}$$

The validity of this approximation (which implies that correlations between the different bounces of a trajectory play a negligible role in the evolution of η) will depend on the details of the shape Sh_α and the frozen wall velocity field $\dot{n}_\alpha$, and may be difficult to assess *a priori*. Roughly speaking, it demands that the container's shape and its motion be sufficiently irregular. We do not pursue here the question of how to define "sufficiently irregular". Rather, for those systems for which Eq. 4.1 happens to be valid, we derive an evolution equation for η wholly in terms of the evolution of the shape $\mathrm{Sh}(\epsilon t)$, without explicit mention of particle dynamics. (See also Sec. VII for a situation in which the results of the present section may apply, without Eq. 4.1 being valid.)

Take Eq. 4.1 to be valid. Using Eqs. A6 to A8 from Appendix A, we get, in two dimensions,

$$c_0 = \frac{2}{3l} \oint ds \left[\dot{n}^2 - \frac{3\pi^2}{32} \bar{\dot{n}}^2\right] \equiv \frac{2}{3l} I_2(\epsilon t). \tag{4.2}$$

Here, $\bar{\dot{n}} = (1/l) \oint ds\, \dot{n} = \dot{A}/l$ is the average value of $\dot{n}$ over the surface of the container. In three dimensions, using Eqs. A11 to A13, we obtain

$$c_0 = \frac{1}{2S} \oint d\sigma \left[\dot{n}^2 - \frac{8}{9} \bar{\dot{n}}^2\right] \equiv \frac{1}{2S} I_3(\epsilon t), \tag{4.3}$$

with $\bar{\dot{n}} = (1/S) \oint d\sigma\, \dot{n} = \dot{V}/S$ again being the average value of $\dot{n}$ over the surface of the container. (Since these expressions no longer explicitly involve the dynamics of particles inside a frozen container, we have dropped the subscript α; $\dot{n}$ now refers to $\dot{n}(\epsilon t)$, the wall velocity field of the slowly-changing container.) Combining these results with Eqs. 3.14, 3.16, and 3.22, we have the simplified results

$$\frac{\partial \eta}{\partial t} = \frac{\dot{A}}{A} \frac{\partial}{\partial E}(E\eta) + \frac{8\sqrt{2m}}{3\pi A} I_2 \frac{\partial}{\partial E}\left(E^{3/2} \frac{\partial \eta}{\partial E}\right) \qquad (2d) \tag{4.4a}$$

and

$$\frac{\partial \eta}{\partial t} = \frac{2\dot{V}}{3V} \frac{\partial}{\partial E}(E\eta) + \frac{\sqrt{2m}}{2V} I_3 \frac{\partial}{\partial E}\left[E^2 \frac{\partial}{\partial E}\left(E^{-1/2}\eta\right)\right] \qquad (3d). \tag{4.4b}$$

V. RELATION TO PREVIOUS RESULTS

In Ref. [4] we considered the general problem of systems evolving in phase space under an *ergodic adiabatic Hamiltonian*, a slowly time-varying Hamiltonian which, if frozen at any instant, gives rise to trajectories that ergodically and chaotically explore their energy shells. This problem has been studied by Ott and coworkers [1–3], using multiple-time-scale analysis; by Koonin and Randrup [10], using linear response theory; and by Wilkinson [5], expanding on Ott's results. Let $\mathbf{z} = (\mathbf{q}, \mathbf{p})$ represent a point in phase space, let $H(\mathbf{z}, \epsilon t)$ denote the slowly-changing Hamiltonian, and let $H_\alpha(\mathbf{z})$, with $\alpha = \epsilon t$, denote the time-independent Hamiltonian obtained by freezing $H(\mathbf{z}, \epsilon t)$ at time t. A central result of Ref. [4] is an evolution equation (previously derived by Wilkinson) for $\eta(E, t)$, the distribution of energies of an ensemble of such systems, all governed by the same ergodic adiabatic Hamiltonian, differing from one another only by their initial conditions in phase space; we call such an ensemble an *ergodic adiabatic ensemble*. This equation is identical to Eq. 2.1 of the present paper, with

$$g_1(E, \epsilon t) = \bar{u} + \frac{1}{2\Sigma} \frac{\partial}{\partial E}\left(\Sigma g_2\right) \tag{5.1}$$

$$g_2(E, \epsilon t) = \int_{-\infty}^{+\infty} ds\, C(s), \tag{5.2}$$

where $\Sigma(E, \epsilon t)$ is defined as per Eq. 3.18, and the quantities $\bar{u}$ and $C(s)$, both functions of E and ϵt, are discussed below. (To avoid notational conflict with Sec. VI of the present paper, we use $\bar{u}$ to denote the quantity which in Ref. [4] is denoted by $\bar{v}$.)

In this section we show that one can consistently treat a chaotic adiabatic billiard gas as an example of an ergodic adiabatic ensemble, by treating the container as the limiting case of a smooth potential well. Thus, Eqs. 5.1 and 5.2 will be shown to reduce, in this limit, to the corresponding expressions derived in Sec. III for the billiard gas.

The quantities $\bar{u}$ and $C(s)$ are defined as follows. Let $\dot{H}(\mathbf{z}, \epsilon t)$ be the slowly time-dependent function obtained by differentiating $H(\mathbf{z}, \epsilon t)$ with respect to t; define $\dot{H}_\alpha(\mathbf{z})$, with $\alpha = \epsilon t$, as the time-independent function obtained by "freezing" $\dot{H}(\mathbf{z}, \epsilon t)$ at time t. Then

$$\bar{u} \equiv \left\{\dot{H}_\alpha(\mathbf{z})\right\} \tag{5.3}$$

$$C(s) \equiv \left\{\left[\dot{H}_\alpha(\mathbf{z}) - \bar{u}\right] O_\alpha(s) \left[\dot{H}_\alpha(\mathbf{z}) - \bar{u}\right]\right\}, \tag{5.4}$$

where the curly brackets indicate an average over all points $\mathbf{z}$ on the energy shell E of H_α, and $O_\alpha(s)$ is a time evolution operator which acts to the right, evolving a point $\mathbf{z}$ for a time s under the frozen Hamiltonian H_α.

For a particle moving inside a hard-walled container, it is intuitive to think of the container as a potential well $V(\mathbf{q})$ whose value is zero for $\mathbf{q}$ inside the container and infinite outside. This formulation, however, does not immediately lend itself to the calculation of $\bar{u}$ and $C(s)$ as defined above. We therefore soften the walls of the container by letting the potential rise smoothly from 0 inside to infinity outside, over a wall skin of thickness δ; we let δ be arbitrarily small.

The contours of $V(\mathbf{q})$ in the vicinity of some point on the surface of the wall will have the appearance shown in Fig. 4. If the wall at this point is moving with normal outward velocity $\dot{n}$, then, at a point $\mathbf{q}$ within the wall skin, we have

$$\dot{H} = -\dot{n}\, \hat{\mathbf{n}} \cdot \nabla V(\mathbf{q}) = -\dot{n}\, |\nabla V(\mathbf{q})|, \tag{5.5}$$

where $\hat{\mathbf{n}}$ is the unit vector pointing normally outward from the wall. The frozen value of $\dot{H}$ is then

$$\dot{H}_\alpha = -\dot{n}_\alpha\, \hat{\mathbf{n}} \cdot \nabla V(\mathbf{q}). \tag{5.6}$$

By the assumed ergodicity of motion inside the hard-walled container (and by extension in the soft-walled container, for arbitrarily small δ), the phase space average of $\dot{H}_\alpha$ over a particular energy shell is equal to the time average of $\dot{H}_\alpha(\mathbf{z}(t))$, where $\mathbf{z}(t)$ is any non-periodic trajectory of energy E:

$$\bar{u} = \left\{\dot{H}_\alpha\right\} = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, \dot{H}_\alpha(\mathbf{z}(t)). \tag{5.7}$$

Contributions to this integral occur only along the short segments of $\mathbf{z}(t)$ that constitute collisions with the wall. The contribution from one such bounce, occurring between times t_1 and t_2 as shown in Fig. 4, is, by Eq. 5.6,

$$\int_{t_1}^{t_2} dt\, \dot{H}_\alpha(\mathbf{z}(t)) = -\dot{n}_\alpha\, \hat{\mathbf{n}} \cdot \int_{t_1}^{t_2} dt\, \nabla V(\mathbf{q}(t)). \tag{5.8}$$

Since $-\nabla V$ is the force acting on the particle, its integral gives the total change in momentum:

$$\int_{t_1}^{t_2} dt\, \dot{H}_\alpha(\mathbf{z}(t)) \;=\; \dot{n}_\alpha\, \hat{\mathbf{n}} \cdot \big[\mathbf{p}(t_2) - \mathbf{p}(t_1)\big] \;=\; -2mv\dot{n}_\alpha \sin\theta. \tag{5.9}$$

Thus, Eq. 5.7 becomes

$$\bar{u} \;=\; -\frac{2mv}{\tau} \lim_{N\to\infty} \frac{1}{N} \sum_{b=1}^{N} \dot{n}_{\alpha b} \sin\theta_b, \tag{5.10}$$

the sum being over the bounces occurring between $t = 0$ and $t = T$. The quantity $\lim_{N\to\infty} (1/N) \sum_{b=1}^{N} \dot{n}_{\alpha b} \sin\theta_b$ is the average value of $n_\alpha \sin\theta$ sampled by a particle bouncing forever off the walls of the frozen container, which, as pointed out in Appendix A, is equal to the previously defined ξ. Thus,

$$\bar{u} \;=\; -\frac{2mv}{\tau}\, \xi \;=\; -\beta E. \tag{5.11}$$

To solve for $\int_{-\infty}^{+\infty} ds\, C(s)$, note that $C(s)$ may be written as

$$\Big\langle \big[\dot{H}_\alpha(\mathbf{z}(t)) - \bar{u}\big]\, \big[\dot{H}_\alpha(\mathbf{z}(t+s)) - \bar{u}\big] \Big\rangle_\alpha, \tag{5.12}$$

where $\mathbf{z}(t)$ is a trajectory of energy E evolving under H_α, and the angular brackets denote an average over all such trajectories, i.e. over a uniform distribution of initial conditions $\mathbf{z}(0)$ over the energy shell E in phase space. (Since such a distribution is unchanged by evolution in time, the above expression for $C(s)$ is independent of t.) With some manipulation, this allows us to write

$$\int_{-\infty}^{+\infty} ds\, C(s) \;=\; \lim_{T\to\infty} \frac{1}{T} \Big\langle \Big(\int_0^T dt\, \big[\dot{H}_\alpha(\mathbf{z}(t)) - \bar{u}\big] \Big)^2 \Big\rangle. \tag{5.13}$$

Using Eqs. 5.9 and 5.11, we have

$$\int_0^T dt\, \big[\dot{H}_\alpha(\mathbf{z}(t)) - \bar{u}\big] \;=\; -2mv \sum_{b=1}^{N} (\dot{n}_{\alpha b} \sin\theta_b - \xi), \tag{5.14}$$

where as before the sum is over the bounces of $\mathbf{z}(t)$ occurring between $t = 0$ and $t = T$. Thus,

$$\int_{-\infty}^{+\infty} ds\, C(s) \;=\; \lim_{T\to\infty} \frac{1}{T} \Big\langle \Big[-2mv \sum_{b=1}^{N} (\dot{n}_{\alpha b} \sin\theta_b - \xi)\Big]^2 \Big\rangle \tag{5.15}$$

$$\;=\; \frac{4m^2v^2}{\tau} \lim_{N\to\infty} \frac{1}{N} \sum_{b=1}^{N} \sum_{b'=1}^{N} c_{b'-b} \tag{5.16}$$

$$\;=\; \frac{4m^2v^2}{\tau}\, D \;=\; \gamma E^{3/2}, \tag{5.17}$$

where the steps taken are similar to those of Sec. III.

By treating the hard-walled container as a limiting case of a potential well [11], we have shown that, in this limit,

$$\bar{u} \rightarrow -\beta E \tag{5.18}$$

$$\int_{-\infty}^{+\infty} ds\, C(s) \rightarrow \gamma E^{3/2}. \tag{5.19}$$

When these expressions are plugged into Eqs. 5.1 and 5.2, they give an evolution equation for $\eta(E,t)$ identical to that obtained in Sec. III. This shows that a chaotic adiabatic billiard gas can be consistently treated as an example of an ergodic adiabatic ensemble, and so a numerical test of the results presented in the present paper would also stand as a test of the results of Ref. [4].

VI. ONE-BODY DISSIPATION IN NUCLEAR DYNAMICS

As discussed in Refs. [6,7], it may be instructive to treat a nucleus undergoing some dynamical process (such as fission or heavy-ion collision) as a container, whose shape (but not volume) is allowed to change with time, filled with a gas of noninteracting point particles. The container is an idealization of the mean field created by the nucleons; the particles represent the individual nucleons moving within this mean field. (Residual nucleon-nucleon interactions are suppressed by Pauli blocking, and are disregarded in this simple approximation.) The solution of this dynamical problem at the classical level is closely related to the problem considered in the present paper.

In applications of this model, one is typically interested in following the shape of the nucleus through some dynamical process. This involves choosing a few reasonable variables to describe the changing shape, then deriving Euler-Lagrange-Rayleigh equations for the evolution of these variables [6,12]. As pointed out in Ref. [6], the particles behave as a source of friction: as they interact with the changing shape of the container (bouncing elastically off its moving walls), there occurs a net flow of energy from the degrees of freedom of the shape, to the degrees of freedom of the gas of particles. This mechanism is known as *one-body dissipation*, and is an example (to our knowledge, the first) of deterministic friction, in which the energy of a few "slow" degrees of freedom is dissipated by their coupling to "fast" deterministic chaotic motion. To incorporate this friction into the equations of motion for the shape of the container, one needs an expression for the rate of this flow of energy, as a function of the way in which the shape is instantaneously changing. In Ref. [6], the wall formula is derived for this rate:

$$\frac{dE_T}{dt} = \rho\overline{v} \oint d\sigma\, \dot{n}^2. \tag{6.1}$$

Here, E_T is the total energy of the gas (the sum of the kinetic energies of the individual particles), ρ is the total mass density of particles inside the container, $\overline{v}$ is the average speed of the particles, and $\oint d\sigma\, \dot{n}^2$ is the surface integral of the square of the normal wall velocity.

The wall formula is derived by treating each infinitesimal area element on the surface of the container as a tiny piston, moving either into or away from the gas of particles. By calculating the work done on the gas by one such piston, then summing over the entire

surface (and taking the volume of the container to stay constant), one obtains Eq. 6.1. We will refer to this derivation as the "piston approach" to one-body dissipation. [13]

Two key assumptions that enter the derivation of the wall formula are, first, that the motion of the walls is slow compared to that of the particles, and second, that the gas is always distributed uniformly within the container, with an isotropic distribution of velocities. These assumptions are satisfied by a chaotic adiabatic billiard gas, and so the wall formula should be consistent with the results derived in the present paper. To show that this is the case, we first comment that the piston approach disregards any correlations that may exist between the bounces of a particle moving inside the container. Thus, in comparing the wall formula with our results, it is appropriate to use the simplified version of our central result given by Eq. 4.4b. The total energy of the gas may be expressed as $E_T(t) = \int dE\, \eta(E,t)\, E$, where η is the time-dependent distribution of energies. Differentiating with respect to time, then applying Eq. 4.4b (with $\dot{V} = 0$), we have

$$\frac{dE_T}{dt} = \frac{\sqrt{2m}}{2V} I_3 \int dE\, \frac{\partial}{\partial E}\Big[E^2 \frac{\partial}{\partial E}\big(E^{-1/2}\eta\big)\Big]\, E, \tag{6.2}$$

where $I_3 = \oint \dot{n}^2\, d\sigma$. After twice integrating by parts, this becomes

$$\frac{dE_T}{dt} = \frac{\sqrt{2m}}{V} I_3 \int dE\, \eta\, E^{1/2}. \tag{6.3}$$

The average speed of the particles is given by

$$\overline{v} = \frac{1}{\mathcal{N}} \int dE\, \eta\, (2E/m)^{1/2}, \tag{6.4}$$

where $\mathcal{N} = \int dE\, \eta$ is the total number of particles. This enables us to rewrite Eq. 6.3 as

$$\frac{dE_T}{dt} = \frac{m\mathcal{N}}{V} \overline{v} \oint \dot{n}^2\, d\sigma, \tag{6.5}$$

which is the wall formula.

Having demonstrated that the results of the present paper (in the simplified form of Sec. IV) agree with the wall formula, we now consider the factor $\overline{v}$ which appears in the latter. Differentiating both sides of Eq. 6.4 with respect to time, then applying Eq. 4.4b, then integrating by parts twice, we obtain

$$\frac{d\overline{v}}{dt} = \frac{3}{4V} \oint \dot{n}^2\, d\sigma. \tag{6.6}$$

Eqs. 6.5 and 6.6 constitute a closed set of equations, in the sense that, if we know how the shape of the container evolves with time, then Eq. 6.6 may be integrated to yield $\overline{v}(t)$, which may then be inserted into the wall formula, which in turn is integrated to give $E_T(t)$. Without Eq. 6.6, some assumption must be made about the evolution of $\overline{v}$ in order for the wall formula to be integrated over any finite length of time. The added understanding of one-body dissipation which one gains from the second wall formula is discussed in greater detail in Ref. [14].

We now consider a generalization of Eqs. 6.5 and 6.6. First, note that Eq. 6.5 may be rewritten as

$$\frac{d}{dt}\overline{v^2} = \frac{2}{V}\overline{v}\oint d\sigma\,\dot{n}^2, \tag{6.7}$$

where $\overline{v^2}$ is the average value of particle speed squared. Let $\overline{v^n}$ denote the average value of the nth power of particle speed:

$$\overline{v^n}(t) = \int dE\;\eta(E,t)\;(2E/m)^{n/2}. \tag{6.8}$$

Differentiating both sides with respect to time, applying Eq. 4.4b, and integrating twice by parts yields

$$\frac{d}{dt}\overline{v^n} = \frac{n(n+2)}{4V}\overline{v^{n-1}}\oint d\sigma\,\dot{n}^2; \tag{6.9}$$

Eqs. 6.6 and 6.7 are specific examples of this general formula.

In Ref. [14], Eq. 6.9 is obtained using a generalization of the piston approach described above. A consequence of Eq. 6.9, as shown in Ref. [14], and supported by numerical simulations [15], is that, asymptotically with time, a chaotic adiabatic billiard gas will achieve a distribution of particle velocities which has a universal form:

$$f(\mathbf{v}) \propto \exp(-v/c), \tag{6.10}$$

where $f(\mathbf{v})\,d^3v$ gives the number of particles with velocity in a small region d^3v around $\mathbf{v}$, and the quantity c is a velocity scale that grows with time. This exponential distribution of velocities stands in contrast to the Maxwell-Boltzmann distribution that occurs when the particles interact with one another.

VII. BRIEF DISCUSSION

We conclude with a brief discussion concerning one of the assumptions underlying our analysis. We assumed in Sec. I that the container's shape changed slowly enough that the evolution of a trajectory inside the slowly-evolving container resembled that inside the frozen one over times on the order of the Lyapunov time t_L; see Eq. 1.1. This allowed us in Sec. III to replace the correlations that exist between bounces in the time-dependent container, with correlations calculated in the frozen container. Now, for somewhat greater values of ϵ, Eq. 1.1 will no longer hold, and the two sets of correlations will differ significantly, although it may still be the case that the evolution of η will be well described as a process of diffusion. In such a case, we expect Eq. 3.22, our central result, to stand, only the factor D entering the coefficient γ will differ from that presented above; the new D will be a sum over correlations which must be calculated inside the time-dependent container. We have numerical evidence suggesting that, when ϵ is increased beyond the validity of Eq. 1.1, correlations between the different bounces of a trajectory in the time-dependent container tend to become "wiped out"; only c_0 remains significantly different from zero. In this case, the simplified results given by Eq. 4.4 work well, not because Eq. 4.1 (with D evaluated for motion inside the frozen container) is valid, but because we are within a range of values of ϵ in which we must evaluate correlations using trajectories inside the time-dependent container, and *these* correlations are dominated by c_0.

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APPENDIX A

In Sec. III, we considered the quantities

$$\xi_b(E,\epsilon t) \equiv \left\langle \dot{n}_{\alpha b} \sin\theta_b \right\rangle_\alpha \tag{A1}$$

$$c_{b,b'}(E,\epsilon t) \equiv \left\langle (\dot{n}_{\alpha b} \sin\theta_b - \xi_b)(\dot{n}_{\alpha b'} \sin\theta_{b'} - \xi_{b'}) \right\rangle_\alpha, \tag{A2}$$

where $\dot{n}_{\alpha b} \sin\theta_b$ is the value of $\dot{n}_\alpha \sin\theta$ at the bth bounce of a trajectory of energy E moving inside the container frozen at $\alpha = \epsilon t$. One specifies such a trajectory by its initial conditions on the energy shell E; the angular brackets denote an average over a uniform distribution of initial conditions over this energy shell.

The function $c_{b,b'}(E,\epsilon t)$ measures correlations (in the value of $\dot{n}_\alpha \sin\theta$) between the bth and the b'th bounce, for trajectories of energy E inside Sh_α. Due to chaotic mixing, we expect such correlations to exist only on the order of the Lyapunov time t_L. Let ν_L denote the number of bounces over which significant correlations exist (ν_L will be on the order of t_L/τ, where τ is the average time between bounces.) Then for $|b'-b| > \nu_L$ we get

$$c_{b,b'}(E,\epsilon t) \cong \left\langle \dot{n}_{\alpha b} \sin\theta_b - \xi_b \right\rangle \left\langle \dot{n}_{\alpha b'} \sin\theta_{b'} - \xi_{b'} \right\rangle = 0. \tag{A3}$$

Plotted on the b-b' grid, then, $c_{b,b'}$ is non-zero only in the diagonal band $|b'-b| \leq \nu_L$.

In this Appendix we show that, outside the small region $b, b' < \nu_L$, the function ξ_b is independent of b, and the correlation function $c_{b,b'}$ depends on b and b' only through their difference $\Delta b \equiv b' - b$ (see Fig. 5). This justifies approximating the sum $\sum_{b=1}^{B}\sum_{b'=1}^{B}(c_{b,b'} + \xi_b\xi_{b'})$ where $B \gg \nu_L$, by $\sum_{b=1}^{B}\sum_{b'=1}^{B}(c_{\Delta b} + \xi^2)$, as per Eq. 3.8. We obtain explicit expressions for $c_{\Delta b}$ and ξ, in both two and three dimensions.

Begin by considering the motion of a particle inside a two-dimensional frozen container. [17] This motion consists of straight line segments joining one bounce off the walls of the container to the next. Each bounce is completely specified by the point s at which it occurs (where s measures the distance along the perimeter from an arbitrarily chosen origin O), and by the angle θ of the collision. The value of s ranges from 0 to l, the perimeter of the container; θ ranges from 0 to π. Let K denote this finite region of the s-θ plane. The

dynamics of the motion of the particle can be reduced to a mapping $M : K \to K$; a given trajectory reduces to a sequence of points in K:

$$(s_1, \theta_1) \to (s_2, \theta_2) \to \cdots, \tag{A4}$$

with $(s_{b+1}, \theta_{b+1}) = M(s_b, \theta_b)$. The angular brackets in the definitions of ξ_b and $c_{b,b'}$ now denote an average over such sequences, where the distribution of initial points (s_1, θ_1) in K is obtained by uniformly filling the energy shell E with particles, then evolving each particle to its first collision with the wall.

Since chaotic mixing exists in the full phase space, it also exists in K: any smooth distribution of initial conditions in K will, with repeated iterations of the mapping M, approach the distribution $f(s, \theta)$ which is invariant under M (within the coarse-graining approximation). This process of mixing occurs over $\sim \nu_L$ iterations of M. Thus, whatever the distribution of first bounces (s_1, θ_1) obtained as per the last sentence of the previous paragraph, this distribution will evolve after approximately ν_L iterations into a distribution $f(s, \theta)$ which then remains unchanged by successive applications of M.

Given these considerations, the quantity ξ_b, for $b > \nu_L$, becomes

$$\xi \equiv \int_0^l ds \int_0^\pi d\theta\, f(s, \theta)\, \dot{n}_\alpha(s) \sin\theta \tag{A5}$$

where $\dot{n}_\alpha(s)$ is the value of $\dot{n}_\alpha$ at the point s on the container wall. Similarly, for b, $b' > \nu_L$, $c_{b,b'}$ depends only on $\Delta b \equiv b' - b$, and is given by

$$c_{\Delta b} = \int_0^l ds \int_0^\pi d\theta\, f(s, \theta) \left[\dot{n}_\alpha(s) \sin\theta - \xi\right] M^{\Delta b} \left[\dot{n}_\alpha(s) \sin\theta - \xi\right], \tag{A6}$$

where $M^{\Delta b}$ operates to the right, mapping the point (s, θ) forward by Δb bounces.

It remains to obtain $f(s, \theta)$. Consider the sequence of points $\{(s_b, \theta_b); b = 1, \cdots, N\}$ corresponding to N consecutive bounces of a sample trajectory (assumed non-periodic) in the frozen container. In the limit $N \to \infty$, the distribution of these points in K is invariant under M, and hence when normalized gives $f(s, \theta)$. The distribution thus reached will not depend on the initial conditions of the trajectory, and so the same distribution may be obtained by using a large number of particles (instead of only one) inside the container; consider such a "sample gas" of particles. $f(s, \theta)\, ds\, d\theta$ then gives the density of bounces, due to all the particles in our sample gas, which have accumulated after an infinite time in the small region $ds\, d\theta$ around (s, θ) in K. This density is, in turn, proportional to the rate at which the particles of this gas strike the small segment between s and $s + ds$ along the wall, coming from an angle between θ and $\theta + d\theta$. Since the distribution of particles and their velocities is uniform and isotropic throughout the container (by chaotic mixing), this rate is independent of s, but contains the flux factor $\sin\theta$. Thus, with normalization (so that $\int ds \int d\theta\, f = 1$), we get

$$f(s, \theta) = \frac{1}{2l} \sin\theta, \tag{A7}$$

from which it follows that

$$\xi = \frac{\pi}{4l} \int_0^l ds\, \dot{n}_\alpha(s) = \frac{\pi \dot{A}}{4l}, \tag{A8}$$

with $\dot{A}$ evaluated at $\epsilon t = \alpha$.

From the discussion of the previous paragraph, it should be clear that ξ, in addition to being equal to $\langle \dot{n}_{\alpha b} \sin\theta_b \rangle$ for $b > \nu_L$, is also equal to the average value of $\dot{n}_\alpha \sin\theta$ sampled by a single particle bouncing around chaotically inside the frozen container:

$$\xi = \lim_{N\to\infty} \frac{1}{N} \sum_{b=1}^{N} \dot{n}_{\alpha b} \sin\theta_b. \tag{A9}$$

We use this result in Sec. V.

In the three-dimensional case, as in two dimensions, each bounce is specified by its location on the surface of the container, along with the direction of its velocity just prior to collision. We denote the former by a vector $\mathbf{s}$ with respect to some fixed origin in space; $\dot{n}_\alpha(\mathbf{s})$ gives the value of the frozen wall velocity field at this point $\mathbf{s}$. We have already defined the angle of collision θ as the angle which the incoming velocity $\mathbf{v}$ makes with a plane tangent to the surface of the container at $\mathbf{s}$. To completely specify the direction of $\mathbf{v}$, we also need an azimuthal angle ϕ which gives the direction of the projection of $\mathbf{v}$ onto this plane. (The direction corresponding to $\phi = 0$ is arbitrary.) Thus the dynamics of a particle moving inside a three-dimensional container may be reduced to a mapping $M : K \to K$, where K is now the space of all possible bounces $(\mathbf{s}, \theta, \phi)$, with $\mathbf{s}$ ranging over the entire surface of the container, θ from 0 to $\pi/2$, and ϕ from 0 to 2π. (The set of all possible incoming velocities $\mathbf{v}$ forms, in velocity space, the surface of a hemisphere whose polar direction is normal to the wall at $\mathbf{s}$, and points outward; note that θ is not the ordinary polar angle on this hemisphere, but rather its complement.) The measure which we use on K is $d\mu = d\sigma \cos\theta \, d\theta \, d\phi$, where $d\sigma$ denotes ordinary surface area on the walls of the container, and $\cos\theta \, d\theta \, d\phi$ gives the solid angle in velocity space.

The arguments concerning chaotic mixing in the two-dimensional case apply in three dimensions as well. Thus, letting $f(\mathbf{s}, \theta, \phi)$ denote the distribution in K which is invariant under M, we have (for b, $b' > \nu_L$):

$$\xi_b \to \xi = \int d\mu \, f(\mathbf{s}, \theta, \phi) \, \dot{n}_\alpha(\mathbf{s}) \sin\theta \tag{A10}$$

$$c_{b,b'} \to c_{\Delta b} = \int d\mu \, f(\mathbf{s}, \theta, \phi) \left[\dot{n}_\alpha(\mathbf{s}) \sin\theta - \xi\right] M^{\Delta b} \left[\dot{n}_\alpha(\mathbf{s}) \sin\theta - \xi\right]. \tag{A11}$$

Here, $\int d\mu \equiv \oint d\sigma \int_0^{\pi/2} \cos\theta \, d\theta \int_0^{2\pi} d\phi$ denotes integration over K ($\oint d\sigma$ denotes integration over the surfaces of the container), and $M^{\Delta b}$ operates to the right, mapping $(\mathbf{s}, \theta, \phi)$ forward by Δb bounces. (For purposes of this mapping, the factor to the right of $M^{\Delta b}$ in Eq. A11 is treated as a function of all of the variables of integration, which just happens to be independent of ϕ.)

To obtain the invariant distribution $f(\mathbf{s}, \theta, \phi)$ we use the same strategy as before, filling the container with a large number of particles, and asking for the rate at which a small area $d\sigma$ around $\mathbf{s}$ is struck by particles coming from a solid angle $\cos\theta \, d\theta \, d\phi$ around (θ, ϕ). As before, this rate is proportional simply to $\sin\theta$. With normalization ($\int d\mu \, f = 1$), we get

$$f(\mathbf{s}, \theta, \phi) = \frac{1}{\pi S} \sin\theta, \tag{A12}$$

and so

$$\xi = \frac{2}{3S} \oint d\sigma\, \dot{n}_\alpha(\mathrm{s}) = \frac{2\dot{V}}{3S}. \tag{A13}$$

APPENDIX B

In this Appendix we solve for τ, the average time between the bounces of a particle of energy E moving chaotically inside a time-independent container. Let $v = (2E/m)^{1/2}$ denote the speed of the particle. If we fill the container with a large number $\mathcal{N}$ of such (noninteracting) particles, then the total rate R at which the walls of the box are being struck is

$$R = \frac{\mathcal{N}}{\tau}. \tag{B1}$$

We now obtain an alternate expression for R, without the appearance of τ.

First, the two-dimensional case. Consider a small segment ds of the wall. The rate at which this segment is being struck by particles making an angle of collision between θ and $\theta + d\theta$ is given by

$$j(\theta, d\theta)\, ds\, \sin\theta, \tag{B2}$$

where j is the current density of particles bombarding ds from this range of angles, and $\sin\theta$ is a flux factor. Now,

$$j = \frac{d\theta}{2\pi} \frac{\mathcal{N}}{A} v. \tag{B3}$$

Plugging this into Eq. B2, and integrating over θ from 0 to π we get

$$\frac{\mathcal{N} v}{\pi A} ds \tag{B4}$$

as the total rate at which ds is being bombarded by particles. Integrating over the entire wall, we get

$$R = \frac{\mathcal{N} v l}{\pi A}, \tag{B5}$$

which, upon comparison with Eq. B1, yields

$$\tau = \frac{\pi A}{l v}. \tag{B6}$$

In the three-dimensional case, consider a small patch $d\sigma$ on the surface of the container. The rate at which this patch is being struck by particles coming from a solid angle $d\Omega$ around the direction (θ, ϕ) (as defined in Appendix A) is

$$j(\theta, \phi, d\Omega)\, d\sigma\, \sin\theta, \tag{B7}$$

where j, the current density of such particles, is

$$j = \frac{d\Omega}{4\pi}\frac{\mathcal{N}}{V}v = \frac{\cos\theta\, d\theta\, d\phi}{4\pi}\frac{\mathcal{N}}{V}v. \tag{B8}$$

Integrating Eq. B7 over θ (0 to $\pi/2$) and ϕ (0 to 2π) to obtain the total rate of particles hitting $d\sigma$, then integrating over the entire wall of the container, we get

$$R = \frac{\mathcal{N}vS}{4V}. \tag{B9}$$

Thus,

$$\tau = \frac{4V}{Sv}. \tag{B10}$$

REFERENCES

[1] E. Ott, Phys. Rev. Lett. **42**, 1628 (1979).

[2] R. Brown, E. Ott, and C. Grebogi, Phys. Rev. Lett. **59**, 1173 (1987).

[3] R. Brown, E. Ott, and C. Grebogi, J. Stat. Phys. **49**, 511 (1987).

[4] C. Jarzynski, Phys. Rev. A **46**, 7498 (1992).

[5] M. Wilkinson, J. Phys. A **23**, 3603 (1990).

[6] J. Błocki *et al.*, Ann. Phys. **113**, 338 (1978).

[7] W.J. Świątecki, in *Semiclassical Descriptions of Atomic and Nuclear Collisions* (Elsevier, 1985), p. 281; J. Błocki, J.-J. Shi, and W.J. Świątecki, "Order, Chaos and Nuclear Dynamics", Lawrence Berkeley Laboratory preprint LBL-31563, November 1991, to be published.

[8] R. Kubo, M. Toda, and N. Hashitsume, *Statistical Physics II* (Springer-Verlag, Berlin, 1985), Chap. 1.

[9] F. Reif, *Fundamentals of Statistical and Thermal Physics* (McGraw-Hill, New York, 1965), Sec. 15.9.

[10] S.E. Koonin and J. Randrup, Nucl. Phys. **A289**,476 (1977).

[11] In Ref. [3], Brown *et al.* define a correlation function $C(s)$ for billiard systems. Integrating this function from $s = -\infty$ to $s = +\infty$ provides an alternative method of obtaining Eq. 5.19.

[12] H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, 1980), second edition, p. 24.

[13] D. Gross, Nucl. Phys. **A240**, 472 (1975).

[14] C. Jarzynski and W.J. Świątecki, "A Universal Asymptotic Velocity Distribution for Independent Particles in a Time-Dependent Irregular Container", Lawrence Berkeley Laboratory preprint LBL-31771, January 1992, to be published in Nucl. Phys.

[15] J. Błocki, F. Brut, and W.J. Świątecki, "A Numerical Verification of the Prediction of an Exponential Velocity Spectrum for a Gas of Particles in a Time-Dependent Potential Well", report ISN 92.25, submitted to Nucl. Phys.

[16] J. Błocki, W.J. Świątecki, and J. Skalski, private comm.

[17] The results which we obtain in the two-dimensional case could have been obtained as easily using the Birkhoff surface-of-section for $2d$ billiard systems. We have instead chosen a derivation which is readily extended to three dimensions.

FIGURES

FIG. 1. Two-dimensional version of a chaotic adiabatic billiard gas. The scalar field $\dot{n}$ gives the rate at which the wall is moving normally outward, as a function of position s along the wall. It is assumed that "freezing" the shape at any instant will produce a time-independent billiard in which all particle trajectories are chaotic.

FIG. 2. Particle bouncing off a small segment of wall in a two-dimensional billiard. The value of θ ranges from 0 to π.

FIG. 3. Particle bouncing off a small patch of wall in a three-dimensional billiard. The dashed line represents the normal projection of the trajectory onto the wall. The value of θ ranges from 0 to $\pi/2$; ϕ ranges from 0 to 2π. (The line representing $\phi = 0$ is arbitrary.)

FIG. 4. The trajectory of a particle bouncing off a wall of finite skin depth. The parallel lines represent the contours of the potential $V(\mathbf{q})$ in the vicinity of the bounce.

FIG. 5. The b-b' plane. The correlation function $c_{b,b'}$ is negligible for $|b' - b| > \nu_L$, i.e. outside of the shaded regions. Furthermore, we show that, except in the darkly-shaded region given by $b, b' < \nu_L$, this function depends on b and b' only through their difference $\Delta b = b' - b$, and the function ξ_b ($\xi_{b'}$) is independent of b (b').

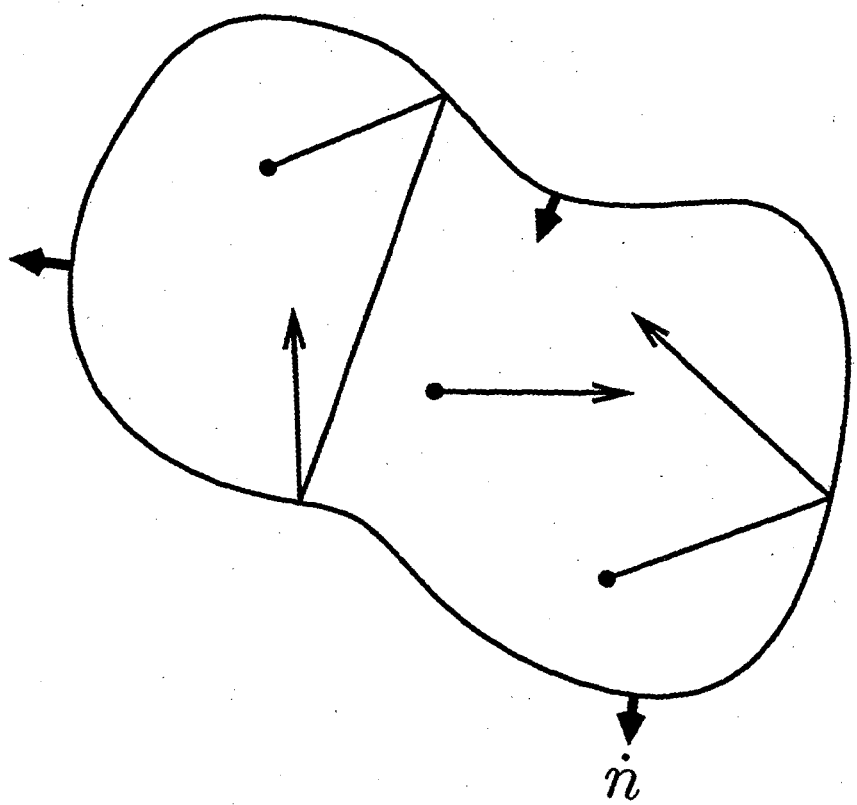

Figure 1

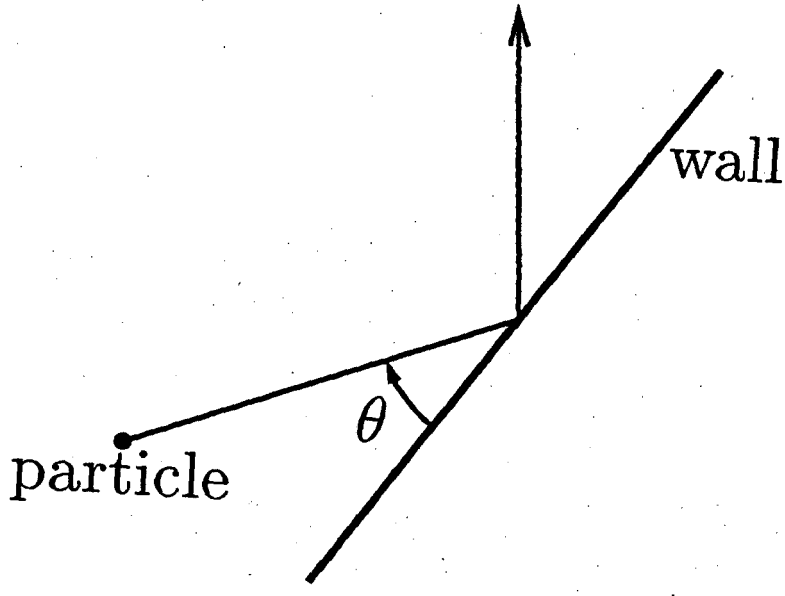

Figure 2

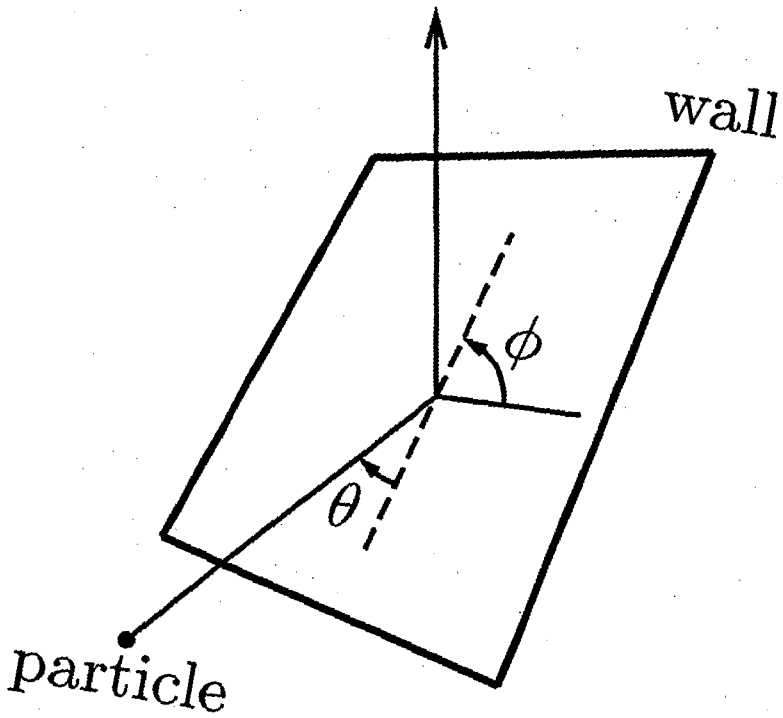

Figure 3

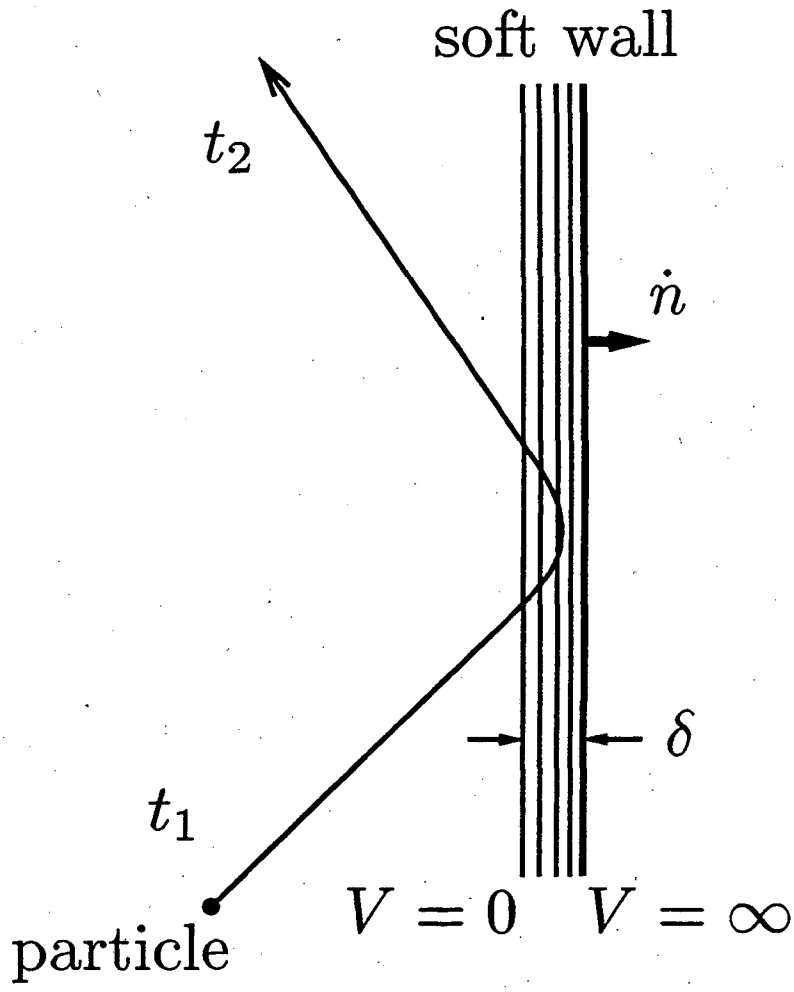

Figure 4

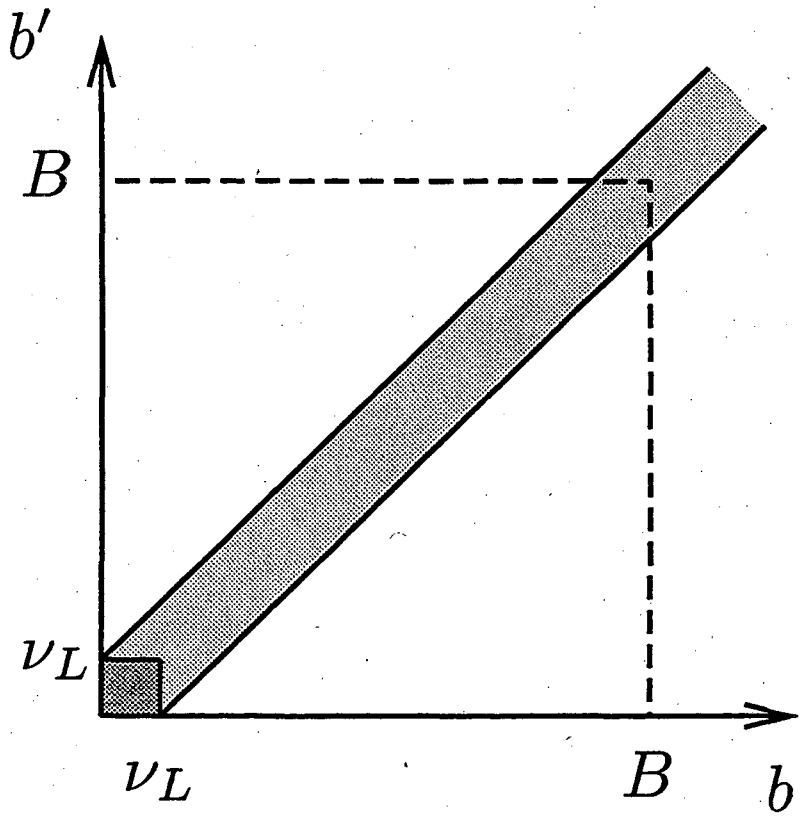

Figure 5

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