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C. Jarzynski
(Ph.D. Thesis)

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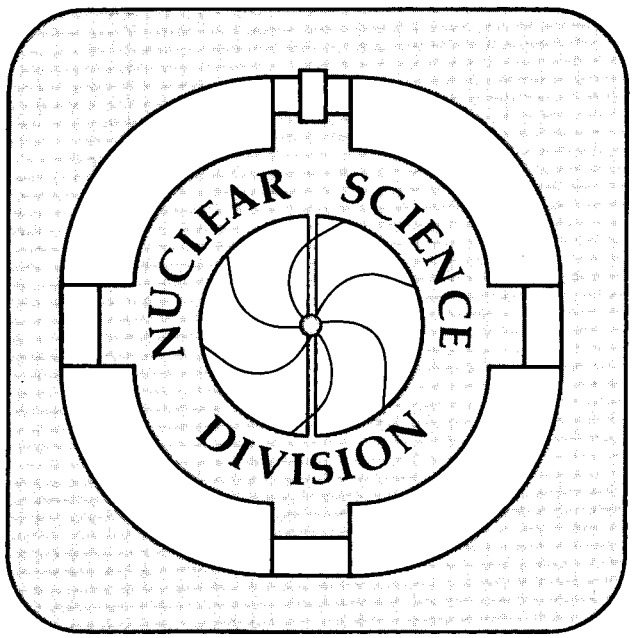

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Studies in Chaotic Adiabatic Dynamics

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Ph.D. Thesis

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January 1994

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Abstract

Studies in Chaotic Adiabatic Dynamics
by

Christopher Jarzynski

Doctor of Philosophy in Physics

University of California at Berkeley

Doctor Władysław J. Świątecki, Co-Chair

Professor Robert G. Littlejohn, Co-Chair

Chaotic adiabatic dynamics refers to the study of systems exhibiting chaotic evolution under slowly time-dependent equations of motion. In this dissertation we restrict our attention to Hamiltonian chaotic adiabatic systems. The results presented are organized around a central theme, namely, that the energies of such systems evolve diffusively. We begin with a general analysis, in which we motivate and derive a Fokker-Planck equation governing this process of energy diffusion. We apply this equation to study the "goodness" of an adiabatic invariant associated with chaotic motion.

We then apply the general formalism to two specific examples. The first is that of a gas of noninteracting point particles inside a hard container that deforms slowly with time. Both the two- and three-dimensional cases are considered. We discuss our results in the context of the Wall Formula for one-body dissipation in nuclear physics, and we show that such a gas approaches, asymptotically with time, an exponential velocity distribution.

The second example involves the Fermi mechanism for the acceleration of cosmic rays. We obtain an explicit evolution equation for the distribution of cosmic ray energies within this model, and we briefly discuss the steady-state energy dis-

tribution that arises when this equation is modified to account for the injection and removal of cosmic rays.

Finally, we re-examine the multiple-time-scale approach as applied to the study of phase space evolution under a chaotic adiabatic Hamiltonian. This leads to a more rigorous derivation of the above-mentioned Fokker-Planck equation, and also to a new term which has relevance to the problem of chaotic adiabatic reaction forces (the forces acting on slow, heavy degrees of freedom due to their coupling to light, fast chaotic degrees).

Co-Chair Date

Contents

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It is both a pleasure and an honor to acknowledge some of those who have made it possible for me to reach this point.

First, my advisors, Władysław J. Świątecki and Robert G. Littlejohn. Władek has had a truly lasting influence on the way that I have come to approach physics. Over countless hours spent discussing a wide range of topics, I have learned the value of his insistence on always seeking a clear and simple understanding of the problem (or solution) at hand. This ability to distill a problem to its essential physics, and the constant stream of creative, original ideas that he offers, invariably stimulate those who have had the very good fortune of working with him. Both my ability to pursue research in physics, and my enthusiasm for the subject, have greatly benefitted from exposure to his unique way of looking at things.

Robert has introduced me to a dimension of theoretical physics that I was, at best, only dimly aware of when I began my doctoral studies. I am referring to his talent and passion for discovering and illuminating the rich mathematical structure underlying physical problems. This pursuit, which pervades so much of his work, lends that work an esthetic appeal that has never failed to inspire me. Furthermore, the clarity of his exposition — both written and spoken — will always be for me the standard by which I will measure my own progress (hopefully!) in that area.

So many others have taught me so much physics during my years here that it is impossible to do justice to them all. Of the graduate students and postdocs that I have come to know and work with at LBL — Steve Creagh, Greg Flynn, Matthias Reinsch, Dan Cook, Stefan Weigert, Mario Feingold, Satoshi Adachi — let me single out Jim Morehead, for the time he has spent with me at the chalkboard, for his mathematical expertise (and his generosity in sharing it), and above all for years of friendship. With time, I honestly believe that Jim would even have coaxed

me out of my irrational fear of Wigner functions.

Let me also mention Allan Kaufman, not only for serving on my thesis and quals committees, but also for his insistence on rigor: it has improved the quality of this Thesis, for which I am grateful indeed.

I also thank Michael Lieberman for serving on my thesis committee, and John Rasmussen and Stuart Freedman for being on my quals committee.

My doctoral research has been enriched by my participation in a Polish-American collaboration investigating aspects of chaos as they relate to nuclear physics. This participation has included two visits to Poland, during which I have met and had stimulating discussions with a great many people. In particular, the interchange of ideas which I have begun with Jan Błocki is something that I hope to continue in the future.

Of course, I have managed to have a personal life at Berkeley as well. Starting with my first days at the International House, many friends — some of whom have already left to continue their lives elsewhere — have made my years here very enjoyable. I will always look back on them fondly. As an undergraduate, I was told by a young professor that graduate school is no fun, that it is simply a time which one must suffer through to obtain a Ph.D. I am glad he was wrong.

I entered Berkeley with a reasonable confidence that I would leave with a Ph.D., but no idea that an even bigger change was in store for me along the way. One of the results of my getting married last June was that I became part of a wonderful family who have been consistently generous in their efforts to make me feel welcome among them. For this, and for all of the support that they have shown me, I am very lucky and very grateful.

This brings me to the enormous debt of gratitude that I owe to my family. For nearly thirty (!) years they have given me love and kindness and guidance. Though separated by geography, they are never far from my thoughts, and the knowledge

that I am not far from theirs has many times been a source of encouragement when I have needed it. My parents have never stopped educating me; in all that I do there is a reflection of their years of dedication and hard work.

Finally, I have come to owe so much to one whom I have known for just two years: my wife, Maire. My debt is not only for the abundance of love, support, happiness, and friendship that she has given me. Beyond these, she has brought something intangible to my life, something which has made it full and rich in a way I had not known. If it is true that my advisors have taught and inspired me, if it is true that without my parents I would never have arrived at Berkeley, then it is equally true that Maire has changed for me the meaning of what I have accomplished here.

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Chapter 1

Introduction

The subject matter of this Thesis is *chaotic adiabatic dynamics*, the dynamics of systems which evolve chaotically under a slowly time-dependent Hamiltonian. Most of the focus will be on *energy diffusion* in ensembles of such systems, although near the end we touch on the closely related topic of *adiabatic reaction forces*.

This introductory chapter is divided into two sections. The first is a thumbnail sketch of concepts related to adiabatic dynamics in general, as well as to chaotic adiabatic dynamics, energy diffusion, and adiabatic reaction forces in particular. The purpose here is to place into context the topics covered in this Thesis, and to introduce notation and terminology. This section is not meant to be comprehensive, only to make the rest of the Thesis comprehensible. References to sources of greater detail and rigor are provided.

The second part of this introduction provides brief outlines of Chapters 2 to 6, the body of the Thesis.

1.1 INTRODUCTORY CONCEPTS

Adiabatic dynamics.

Physical situations arise in which a system evolves in time under equations of motion that are themselves slowly time-dependent. Throughout this Thesis the term *adiabatic dynamics* will denote this general class of problems, and it will be understood that the system is a *classical* one whose evolution is governed by some slowly time-dependent Hamiltonian. For instance, consider a particle evolving inside a slowly time-dependent potential well, although in general the system need not be a particle, nor must the Hamiltonian be of the kinetic + potential form. We will always use the term *trajectory* to denote the *phase space* trajectory describing the evolution of a given system.

For the moment, treat the notion of "slow" time dependence of the Hamiltonian, $H(t)$, heuristically: there exists some characteristic time scale for the evolution of the system, and another for the evolution of H, and these are widely separated. Soon, we will introduce a formalism which quantifies this slowness with a dimensionless parameter, ϵ. Also, assume for now that the time-dependence of H is externally imposed. (Later, when discussing adiabatic reaction forces, we will drop this assumption and let H itself become a dynamical quantity.)

Adiabatic invariants.

Adiabatic invariants play a central role in the study of adiabatic dynamics. An adiabatic invariant is a quantity that is conserved in the limit in which the slow evolution of the equations of motion, or in our case the slow evolution of the Hamiltonian, becomes infinitely slow; we call this the *adiabatic limit.* To illustrate, consider the simple example of a harmonic oscillator whose spring constant k is made to change slowly with time. (For a description of the role that this problem, and the closely related one of a pendulum whose length slowly changes, played in

the early days of quantum mechanics, see Ref.[1].) The adiabatic limit is attained by letting k evolve infinitely slowly — and therefore for an infinite length of time — from an initial value k_i to a final value k_f. (Had we kept the time interval fixed as we let the evolution of k become infinitely slow, then of course the limit which we would approach would be simply that of an oscillator with fixed k.) It is a straightforward calculation to show that, in the adiabatic limit, the energy of the oscillator evolves so that its ratio to the frequency of oscillation $\nu = (1/2\pi)\sqrt{k/m}$ remains constant:

$$\frac{E}{\nu} = \text{const.} \tag{1.1}$$

(Note that the term "frequency of oscillation" is being used somewhat loosely: as k changes with time, the motion of the oscillator is no longer exactly periodic. Thus, $\nu(t)$ as defined above is more precisely the frequency of oscillation associated with holding k fixed at its value at time t.) The ratio E/ν is thus an adiabatic invariant for the harmonic oscillator.

This simple result may be generalized. Consider a one-degree-of-freedom system governed by $H(q,p,t)$, and let a *frozen* Hamiltonian be the time-independent Hamiltonian obtained by arresting ("freezing") the evolution of H at some instant in time. This defines a continuous set of such frozen Hamiltonians, parametrized by the time of freezing. We will use the term *frozen motion*, or *frozen dynamics*, to refer to the evolution of trajectories under any one of these frozen Hamiltonians. Let us assume that the frozen motion is bounded in phase space, and therefore — since we are dealing with one degree of freedom — periodic. Now define the quantity $J(q,p,t)$:

$$J = \oint p'\,dq', \tag{1.2}$$

where $\oint$ denotes an integral over the closed loop in phase space formed by launching a trajectory from (q,p) and letting it evolve under the frozen Hamiltonian, with t the time of freezing. Then for motion under the adiabatic Hamiltonian, J is an

adiabatic invariant. A derivation of this result may be found in Ref.[2].

Note that the closed loop mentioned in the previous paragraph is exactly the *energy shell* — the phase space surface of constant H — containing the point (q,p). (We are assuming that every energy shell is a simply connected surface. Also, throughout this Thesis, the term "energy" is meant to be synonymous with "value of the Hamiltonian", whether or not H is time-dependent.) Even though the trajectory is not periodic when H is time-dependent, the energy shell containing the trajectory is still a well-defined closed surface, at any instant in time. It is with respect to this surface that the integral in Eq. 1.2 is defined.

An interesting question regarding J or any other adiabatic invariant, is, how well is it conserved when the evolution of H is slow, but not infinitely so? To study this problem, it is convenient to introduce a *slowness parameter*, ϵ: let us write the time-dependent Hamiltonian as $H(q,p,\epsilon t)$, where ϵ is dimensionless and formally small. Then $\partial H/\partial t \propto \epsilon$, and the adiabatic limit is defined by $\epsilon \to 0$, with ϵt_i and ϵt_f fixed, where t_i and t_f are the initial and final times over which be observe the system. The convenience of ϵ lies in its use as an expansion parameter, in the regime of slow evolution of H. Let us also at this point introduce the notation H_α, with α a continuous parameter, to denote the sequence of frozen Hamiltonians; the value of α is taken to be the value of ϵt at the time of freezing.

A remarkable result, established by Kruskal[3] (and requiring the added assumption that H is an infinitely differentiable function of time), is that the adiabatic invariant J is good to all orders in ϵ. This does not imply that it is exactly conserved, only that, as we approach the adiabatic limit, the change in J decreases more rapidly than any integer power of ϵ.

The ergodic adiabatic invariant.

So far, we have considered only one degree of freedom. With $N \geq 2$ degrees of freedom, the qualitative behavior of a system evolving under an adiabatic Hamil-

tonian depends on the kind of motion produced by the sequence of frozen Hamiltonians. At one extreme is the *integrable* case: for each frozen Hamiltonian H_α there exist N independent constants of motion that commute with one another under the Poisson bracket. In this case, the frozen motion is equivalent to the independent evolution of N one-degree-of-freedom systems, as is transparent in *action-angle variables.* Correspondingly, the adiabatic evolution exhibits N adiabatic invariants J_i independently conserved to all orders in ϵ (see Section E of Ref.[3]).

At the other extreme is the *chaotic, ergodic* case: the frozen motion is chaotic and ergodic over the *energy shell.* That is, a trajectory evolving under any of the frozen Hamiltonians will ergodically explore the entire phase space surface of constant H_α; furthermore, it will do so chaotically, diverging away from its neighboring trajectories at an exponential rate. Note that this implies *global chaos*: all regions of phase space are filled with chaotically evolving trajectories. We will use the term *chaotic adiabatic Hamiltonian* to describe a slowly-changing H whose associated frozen H_α's produce chaotic and ergodic evolution. A system evolving under H is then a *chaotic adiabatic system*, and the general study of such evolution is *chaotic adiabatic dynamics.*

Hertz[4] seems to have been the first to realize that in this case, an adiabatic invariant is the volume of phase space enclosed by the energy shell on which the trajectory finds itself. Mostly for the purposes of introducing notation, let us formally state Hertz's result. Let $\mathbf{z} = (\mathbf{q}, \mathbf{p})$ denote a point in $2N$-dimensional phase space, and let $\mathbf{z}(t)$ be a trajectory evolving under the chaotic adiabatic Hamiltonian $H(\mathbf{z}, \epsilon t)$. Now define

$$\Omega(E, \epsilon t) = \int dz\, \theta\big[E - H(\mathbf{z}, \epsilon t)\big], \tag{1.3}$$

where θ is the unit step function, and the integral is over all phase space. Geometrically, Ω is the volume of phase space enclosed by the energy shell E at time t; we assume this quantity to be finite. Then in the adiabatic limit, $\Omega(H, \epsilon t)$, with

H evaluated along the trajectory $\mathbf{z}(t)$, is conserved. We call Ω the *chaotic adiabatic invariant.* (Ott[5] and others have used the term *ergodic adiabatic invariant.* However, since it is the chaoticity rather than the ergodicity of the dynamics that is responsible for the diffusive character of energy evolution, described below, we have chosen to stick with the adjective "chaotic".)

For $N = 1$, Ω is exactly the quantity J. This is associated with the fact that in one degree of freedom, motion under a time-independent Hamiltonian is ergodic (though not chaotic) over the energy shell.

Given the result that integrable adiabatic invariants (the J_i's) are conserved to all orders in ϵ, it is natural to wonder how well the chaotic adiabatic invariant is conserved. In other words, what is the "goodness" of the chaotic adiabatic invariant? Ott and coworkers[5–7] have investigated this question: Using multiple-time-scale analysis, Ott[5] has shown that the change in Ω evolves diffusively: the amount by which we may expect Ω to differ from its initial value grows like $\epsilon\sqrt{t}$, where t is the elapsed time. Thus for times over which H changes by order unity — times of order ϵ^{-1} — the change in Ω scales like $\sqrt{\epsilon}$. This makes Ω a considerably poorer invariant than its integrable kin, the J_i's.

Energy diffusion.

While the question of the goodness of the chaotic adiabatic invariant is interesting in its own right, its relevance to a wider range of issues becomes apparent in the context of the following question. How does the *energy* of a chaotic adiabatic system evolve with time? In the adiabatic limit, the answer is straightforward: the energy $E(t)$ evolves so as to preserve the value of Ω:

$$\frac{d}{dt}\Omega\big(E(t), \epsilon t\big) = 0. \tag{1.4}$$

This represents a *reversible* evolution of the energy of the system: by reversing the slow evolution of the Hamiltonian, we exactly reverse that of the energy. For finite

ϵ, on the other hand, this no longer holds. As the change in Ω grows diffusively, so does ΔE, the difference between the actual energy of the system and that predicted by the invariance of Ω. Reversing the evolution of $H(\mathbf{z}, \epsilon t)$ therefore does not reverse that of $E(t)$; rather, ΔE continues to grow diffusively.

The fact that the energy of a chaotic adiabatic system evolves diffusively is a central piece of information regarding chaotic adiabatic dynamics. We will refer to this process as *chaotic adiabatic energy diffusion*, or simply *energy diffusion.*

As is often the case in the study of dynamical systems, we gain significantly more by asking about the behavior of an ensemble of trajectories, than by focusing on a single one. Let *chaotic adiabatic ensemble* denote an ensemble of trajectories evolving under a chaotic adiabatic Hamiltonian. From the discussion of the preceding paragraphs, the distribution of energies of a chaotic adiabatic ensemble ought to evolve under some sort of diffusion equation. Wilkinson[8] has used Ott's result to write down a Fokker-Planck (i.e. drift + diffusion) equation for such a distribution. It is a central theme of this Thesis — emphasized by application to specific problems — that this *energy diffusion equation* represents a very useful tool for the analysis of chaotic adiabatic dynamics.

Adiabatic reaction forces.

So far in this introduction, it has been assumed that the time-dependence of H is externally imposed, and our interest has been devoted exclusively to the trajectory (or trajectories) evolving under this pre-determined, slowly changing Hamiltonian. We now introduce a class of problems for which the Hamiltonian itself becomes a dynamical quantity of interest.

Consider a physical situation in which there exists a natural division of the degrees of freedom into "heavy" degrees which evolve on a slow time scale, and "light" degrees whose time-dependence is rapid. For convenience, we will refer to the heavy degrees as the *slow system*, and the light ones as the *fast system.*

We assume that these are coupled to one another. Often in such situations, it is the motion of the slow system that we are primarily interested in. We now describe a framework which treats the fast and the slow systems on very separate footings, and which provides a solution for the slow motion in a series of successive approximations, ordered in powers of the slowness parameter ϵ. For simplicity, we assume that only the position of the slow system, and not its velocity, is coupled to the fast system.

The equations of motion governing the fast system are slowly time-dependent, owing to the appearance of the slow degrees of freedom in these equations. This suggests treating the position of the slow system as a parameter of the Hamiltonian governing the fast system. Adopting this point of view, we let the term *frozen fast dynamics* indicate the dynamics of the fast system with the slow one held fixed.

In turn, writing the equations of motion for the slow system, we find terms which fluctuate very rapidly. This leads us to replace the exact forces acting on the slow system, with their time-averaged values, where the averaging is done over a time that is short on the scale of the slow motion, but long on that of the fast motion. To solve for the evolution of the slow system, we must solve for these averaged forces, which we call *adiabatic reaction forces.*

Adiabatic reaction forces exist whether the fast motion may be characterized as regular, chaotic, or mixed. We will be assuming that the frozen fast dynamics is ergodic and chaotic over the energy shell. Thus the evolution of the fast system becomes a problem in chaotic adiabatic dynamics.

Without attempting a thorough summary of adiabatic reaction forces, we present a few salient results. First, to leading approximation, adiabatic reaction forces are conservative: the motion of the slow system may be derived from a fictitious potential energy surface, determined by the adiabatic energy of the fast system. This is known as "adiabatic averaging"[9] and is the classical counterpart of the Born-

Oppenheimer approximation. At first order in ϵ, however, the adiabatic reaction forces include velocity-dependent terms, which it is convenient to separate into friction-like and magnetic-like components. The former act opposite to the slow velocity, the latter perpendicular to it.

Deterministic friction, the friction-like component of first-order adiabatic reaction forces, has been recognized for some time, and is in fact the basis of *one-body dissipation* in dynamical nuclear processes.[10–13] (One-body dissipation is the irreversible flow of energy from the collective motion of a nucleus to the individual nucleons, in the approximation where the latter are treated as mutually noninteracting. Here one is really dealing with a single slow system coupled to *many* fast systems, rather than just one, but this does not essentially change the problem.) The *wall formula*,[10–12] which gives the rate of energy absorption by a gas of noninteracting particles inside a slowly time-dependent irregularly shaped container, is an early expression of deterministic friction. The dissipative character of deterministic friction is closely related to the diffusive character of energy evolution under a chaotic adiabatic Hamiltonian. Wilkinson, in fact, has derived a general expression for deterministic friction from the energy diffusion equation mentioned above.[8]

The magnetic-like component of first-order adiabatic reaction forces, *geometric magnetism*, is the classical counterpart of a force which at the quantal level is closely related to Berry's phase.[14] Berry and Robbins, in a recent paper,[15] have presented a systematic derivation of both deterministic friction and geometric magnetism (as well as the leading "Born-Oppenheimer" force) within a single framework.

1.2 OUTLINE OF CHAPTERS

Having briefly summarized a few relevant points concerning chaotic adiabatic dynamics, we outline the individual chapters comprising the main body of this

Thesis. Since each of these chapters is to some extent self-contained, there will be a certain amount of repetition from one to the next.

In Chapter 2, we derive a general *energy diffusion equation* governing the distribution of energies of an ensemble of trajectories evolving under a chaotic adiabatic Hamiltonian. While this result is identical to that obtained by Wilkinson[8] using Ott's results, the derivation presented here is very different, and represents original work.[a] Furthermore, while formally not as rigorous as other derivations (see e.g. Chapter 6), the approach of Chapter 2 provides a clear intuitive understanding of energy diffusion. Also discussed in this chapter are several general aspects of the energy diffusion equation, in particular its application to the goodness of the chaotic adiabatic invariant. It is shown that the predictions of this equation disagree with certain of Ott's results regarding this matter. More will be said on this discrepancy later.

In Chapter 3 the approach developed in Chapter 2 is applied to time-dependent billiard problems, in both two and three dimensions. The result is a diffusion equation governing the distribution of energies of a gas of noninteracting point particles inside a slowly time-dependent, hard-walled cavity. (The sequence of shapes through which the cavity evolves are assumed to produce particle motion which is chaotic and ergodic.) It is shown that the results derived in this chapter may be formally treated as the limiting case of the results of the preceding chapter. Finally, several results pertaining to one-body dissipation are obtained and discussed.

In Chapter 4 the three-dimensional time-dependent billiard problem is again considered, only this time using the "piston approach" that was originally used in the derivation of the wall formula.[10] We show that the gas of particles evolves asymptotically toward an exponential distribution of velocities.

In Chapter 5 the *Fermi mechanism* for the acceleration of cosmic rays is studied

[a] I was not aware of Wilkinson's results until after the publication of my own.

in the context of energy diffusion. The main result here is a relativistic energy diffusion equation. This leads, among other things, to a relativistic version of the wall formula.

In the chapters mentioned up to this point, the focus has been on the distribution of energies of chaotic adiabatic ensembles. In Chapter 6, by contrast, we ask about the evolution of the phase space density describing such ensembles. Ott[5] considered this question using multiple-time-scale analysis, and solved for the phase space density to first order in the slowness parameter ϵ. We re-examine this approach, and discover a first-order term which was missed by Ott. Two consequences follow. First, the inclusion of this extra term resolves the above-mentioned discrepancy between the predictions of the energy diffusion equation and Ott's results concerning the goodness of the chaotic adiabatic invariant. Second, this extra term leads to a velocity-*independent* adiabatic reaction force which is of the same order as deterministic friction and geometric magnetism. Finally, a by-product of this chapter is a derivation of the energy diffusion equation that is more rigorous (if less intuitively clear) than that of Chapter 2.

In Chapter 7, we wrap things up with a brief discussion of several issues related to the topics studied in this Thesis.

Chapter 2

The Energy Diffusion Equation

2.1 INTRODUCTION

In this chapter we consider systems evolving chaotically under a slowly time-dependent Hamiltonian, H. The principal result of the chapter can be stated as follows. If we are given an ensemble of such systems, with initial conditions corresponding to different initial energies, and if we observe these systems as they each evolve chaotically under the slowly changing H, then the distribution of energies $\eta(E,t)$ — defined so that $\eta(E,t)\,dE$ gives the number of systems with energy in an interval dE around E at time t — satisfies the following Fokker-Planck equation:

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

We will refer to this as the *energy diffusion equation.* Here, g_1 and g_2 are functions of E and t for which explicit expressions will be presented entirely in terms of the motion of systems of energy E evolving under the time-*independent* Hamiltonian obtained by "freezing" H at time t. Thus, the time-dependent problem is solved in terms of the solutions of a continuous sequence of time-independent problems.

The problem of systems evolving chaotically under a slowly time-dependent Hamiltonian has been considered by Ott, Brown, and Grebogi.[5–7] Ott has demon-

strated that, to lowest order in the rate of change of the Hamiltonian, the time-dependent energy of such a system is determined by the invariance of a certain quantity — the *chaotic adiabatic invariant*, Ω — discussed below. Thus, an ensemble of such systems, with different initial conditions corresponding to a common initial energy E_0, will — to lowest order — evolve so as to maintain a common energy, $\mathcal{E}(t)$, which is prescribed by the invariance of Ω. Working to next order, Ott *et al.* have studied deviations away from this result, and have derived expressions for the rates at which such an ensemble acquires a first and second moment of energy with respect to $\mathcal{E}(t)$. In this chapter we apply the energy diffusion equation to derive expressions for these rates, and find that the results contain terms which do not appear in those of Ott *et al.* We also derive explicit expressions for $\langle \Delta\Omega \rangle$ and $\langle (\Delta\Omega)^2 \rangle$ as functions of time, where $\Delta\Omega$ is the change in the value of Ω for a given system, and the brackets indicate an average over the ensemble. The quantities $\langle \Delta\Omega \rangle$ and $\langle (\Delta\Omega)^2 \rangle$ are therefore a direct measure of the goodness of the chaotic adiabatic invariant Ω.

The plan of the chapter is as follows. In Section 2.2 we place this problem in its natural context: the study of adiabatic Hamiltonian systems. In Section 2.3 we motivate the diffusion equation given above. In Section 2.4 we obtain explicit expressions for the coefficients g_1 and g_2 that appear in Eq. 2.1. In Section 2.5 we compare the predictions of Eq. 2.1 with those of Ott *et al.* In Section 2.6 we evaluate directly the extent to which the invariance of Ω is violated. Finally, in Section 2.7 we demonstrate that the energy diffusion equation makes the correct predictions for two simple cases.

2.2 ADIABATIC HAMILTONIAN SYSTEMS

In adiabatic Hamiltonian problems, one considers a system whose evolution in phase space is governed by a slowly time-varying Hamiltonian. A classic example

is that of a pendulum whose length is made to change slowly with time. The study of such systems has been primarily concerned with adiabatic invariants, quantities that stay constant in the adiabatic limit, defined as the limit in which the Hamiltonian evolves infinitely slowly from its initial configuration to its final configuration.

It is conventional to incorporate the adiabaticity directly into the definition of the Hamiltonian itself, by use of a dimensionless parameter ϵ:

$$H = H(\mathbf{z}, \epsilon t) \quad , \tag{2.2}$$

where $\mathbf{z} = (\mathbf{q}, \mathbf{p})$ denotes a point in $2N$-dimensional phase space, and t denotes time. The parameter ϵ is then proportional to the rate at which H evolves ($\partial H/\partial t \sim \epsilon$) and is formally taken to be small. The adiabatic limit is obtained by letting ϵ approach zero while holding ϵt_i and ϵt_f fixed, where t_i and t_f are initial and final times. Thus, one always starts with the same initial Hamiltonian, and ends with the same final Hamiltonian, but the rate at which H evolves from the one to the other is decreased as ϵ approaches zero; the time interval involved, $t_f - t_i$, scales like ϵ^{-1}.

Adiabatic invariants and related quantities are often expressed in terms of motion governed by the "frozen" Hamiltonian, defined as the time-*independent* Hamiltonian obtained by arresting the evolution of the adiabatic Hamiltonian, H, at some instant in time. The evolution of H therefore defines, over time, a continuous set of such frozen Hamiltonians; we will use the notation $H_\alpha(\mathbf{z})$, where $\alpha = \epsilon t$, to denote the Hamiltonian frozen at time t.

In adiabatic systems with one degree of freedom, the frozen Hamiltonian H_α always gives rise to periodic motion, the trajectories $q(t), p(t)$ forming closed orbits in phase space. The quantity $J = \oint p\, dq$, where the integral is over one period of this motion, is then an adiabatic invariant of the time-dependent Hamiltonian.[2] This result is easily generalized to systems with N degrees of freedom, for the special case in which H_α is always integrable: with action-angle variables, one separates

the motion under H_α into that of N independent one-degree-of-freedom systems; this yields N different adiabatic invariants, one associated with each action-angle pair.

In a series of papers,[5–7] Ott, Brown, and Grebogi have studied *chaotic adiabatic* Hamiltonian systems, defined by the property that a trajectory evolving under any of the associated frozen Hamiltonians H_α will ergodically and chaotically explore the entire energy shell — the surface of constant energy — to which its motion in phase space is, by conservation of energy, confined. (This case represents the extreme opposite of the integrable case.) The assumption of chaoticity — exponential divergence of neighboring trajectories — implies that the number of degrees of freedom, N, is at least two. Furthermore, the combination of exponential divergence of trajectories and ergodic exploration of the energy shell gives H_α the property of *mixing*: any smooth distribution of initial conditions over an energy shell will eventually evolve into a uniform distribution over that shell, to an arbitrary degree of fineness (i.e. the "coarse-grained" distribution will become uniform). For such systems, the volume of phase space enclosed by the instantaneous energy shell on which a trajectory evolving under H finds itself, is an adiabatic invariant.[4,5] That is, if we denote the energy of a system evolving under $H(\mathbf{z}, \epsilon t)$ by

$$E(t) \equiv H(\mathbf{z}(t), \epsilon t) \quad , \tag{2.3}$$

where $\mathbf{z}(t)$ represents the evolution of that system in phase space, then the quantity

$$\Omega(E, \epsilon t) \equiv \int d\mathbf{z}\ \theta\big[E - H(\mathbf{z}, \epsilon t)\big] \quad , \tag{2.4}$$

where θ is the ordinary step function, is an adiabatic invariant: $\Omega(E(t), \epsilon t)$ is conserved in the adiabatic limit. We call this quantity the *chaotic adiabatic invariant.* Ott *et al.* investigate deviations away from its exact conservation, for a slow but finite time-dependence of H. Specifically, they consider an ensemble of systems defined by a uniform distribution of initial conditions over a single energy shell. In

the case of infinitely slow evolution of H (the adiabatic limit), the quantity Ω is conserved for each of these systems, and so the ensemble evolves into one that is distributed over a single final energy shell that encloses the same volume of phase space as the initial shell. For the case of slow but finite evolution of H, Ott *et al.* consider the rates at which deviations from this result — in the form of a first and second moment of energy of the ensemble with respect to the originally predicted final energy — are acquired. Using multiple-time-scale analysis, expressions for these rates are derived entirely in terms of motion under the set of frozen Hamiltonians H_α. The authors point out that their results indicate that the change in the chaotic adiabatic invariant grows *diffusively.*

2.3 THE DIFFUSION EQUATION

In the present chapter, we take a different approach to the study of systems evolving under a chaotic adiabatic Hamiltonian. We consider an arbitrary ensemble of such systems, all subject to the same H — let the term *chaotic adiabatic ensemble* denote such an ensemble — and we argue from the outset that the corresponding distribution of energies will evolve by a process of diffusion. This will lead us to postulate a Fokker-Planck equation to govern this evolution (Eq. 2.6 below); we will derive expressions for the drift and diffusion coefficients in terms of motion governed by the set of frozen Hamiltonians H_α.

Since $H(\mathbf{z}, \epsilon t)$ is assumed to evolve slowly, we will be interested in small values of the parameter ϵ. We will therefore order terms in our evolution equation according to powers of ϵ, making the assumption that integral powers suffice. As will be shown below, keeping only terms of $O(\epsilon^1)$ corresponds to the adiabatic limit. Since we will be interested in the lowest-order deviations from this limit, we will want an equation that is good to $O(\epsilon^2)$.

By concentrating on the distribution of energies, $\eta(E,t)$, rather than on the distribution of the ensemble in phase space, we have projected out all but one dimension of the $2N$-dimensional space in which each of the systems evolves. Thus, rather than viewing each member of the ensemble as a trajectory evolving deterministically in $2N$-dimensional phase space, we picture each system performing one-dimensional motion along the energy axis. Furthermore, this motion is stochastic, in the sense that the initial energy of a system does not determine the subsequent evolution of its energy. We will now consider this point more closely, to motivate our attempt to describe the evolution of η by a diffusion equation.

Let us introduce the time-dependent phase space function $\dot{H}(\mathbf{z},\epsilon t)$, defined by differentiating $H(\mathbf{z},\epsilon t)$ with respect to the t in its final argument: $\dot{H} \equiv \partial H/\partial t$. By Hamilton's equations, the energy of a trajectory $\mathbf{z}(t)$ changes according to the value of $\dot{H}$ along its path in phase space:

$$\frac{d}{dt}E(t) = \dot{H}(\mathbf{z}(t),\epsilon t) \quad , \tag{2.5}$$

This "velocity" along the energy axis scales like the first power of ϵ. It will prove convenient to define the "frozen" function $\dot{H}_\alpha(\mathbf{z})$ obtained by holding fixed the final argument of $\dot{H}(\mathbf{z},\epsilon t)$ at the value α, just as $H_\alpha(\mathbf{z})$ was defined in relation to $H(\mathbf{z},\epsilon t)$. Now, for sufficiently small ϵ, a typical trajectory will wander significantly over the energy shell on which it finds itself, long before straying significantly away from it. In doing so, it will chaotically sample the distribution of values of $\dot{H}$ over that shell. When projected onto the energy axis, this motion appears as the one-dimensional wandering of a system whose velocity along that axis (dE/dt) is small, and fluctuates stochastically.

As with any stochastic motion, an important quantity is the correlation time, t_c, associated with the fluctuations in velocity. This measures a typical amount of time over which a given system "remembers" its velocity, and is determined by the decay of the correlation function associated with that velocity. In our case,

the decay of the correlation function associated with dE/dt results from the mixing property of the Hamiltonian, and we expect that $t_c \sim 1/\lambda$, where λ is the Lyapunov exponent (see Appendix A of this chapter). For sufficiently small ϵ, the change in energy that takes place over this correlation time t_c is small. Thus, the motion of a given system along the energy axis is characterized by small, rapid (on the time scale over which H changes) stochastic fluctuations. This consideration suggests that an ensemble of such systems will evolve diffusively along the energy axis.[16]

If we accept that η evolves by a process of diffusion, then it is natural to make the Ansatz that this process is governed by a Fokker-Planck equation,[17]

$$\frac{\partial \eta}{\partial t} = -\frac{\partial}{\partial E}(g_1 \eta) + \frac{1}{2}\frac{\partial^2}{\partial E^2}(g_2 \eta) \quad , \tag{2.6}$$

where the drift coefficient g_1 and the diffusion coefficient g_2 are functions of both energy and time. Specifically, we will write $g_1(E, \epsilon t)$ and $g_2(E, \epsilon t)$; the explicit dependence on ϵt rather that t arises because we expect the drift and diffusion coefficients to be determined by the instantaneous Hamiltonian (and the manner in which it is instantaneously changing), which depends explicitly on ϵt.

In attempting to describe the evolution of η as a process of diffusion, we must keep in mind that diffusion arises as the cumulative result, over time, of many fluctuations in the stochastic motion. It will therefore manifest itself only on time scales significantly longer than the correlation time t_c characterizing these fluctuations. Thus, we expect Eq. 2.6 to be valid only over time scales Δt much longer than t_c.

2.4 DRIFT AND DIFFUSION COEFFICIENTS

Under the assumption that the logic of the preceding section is sound, and that the distribution of energies, η, indeed evolves under an equation of the form given by Eq. 2.6, we now proceed to solve for the coefficients g_1 and g_2.

Note first that the drift coefficient $g_1(E, \epsilon t)$ gives the rate of change of the average energy, while the diffusion coefficient $g_2(E, \epsilon t)$ gives the rate of growth of the variance in the energies, for an ensemble of systems that share a common initial energy E at time t. This means that, if we start at time t_0 with an ensemble of systems distributed uniformly over an energy shell E_0 in phase space, and if we allow these to evolve under H for a time Δt which is long in comparison with t_c, but short on the time scale over which H changes, then after this time Δt the distribution of energies will have acquired a second moment relative to E_0 given by:

$$\left\langle (E - E_0)^2 \right\rangle = g_1^2 (\Delta t)^2 + g_2 \Delta t, \tag{2.7}$$

with g_1 and g_2 evaluated at $(E_0, \epsilon t_0)$. Therefore, we begin by solving — in terms of the phase space evolution of the trajectories representing this ensemble — for $\langle (E - E_0)^2 \rangle$, with the aim of extracting g_1 and g_2 from this result. *We will work to leading non-vanishing order in ϵ.*

Consider first a single trajectory $\mathbf{z}(t)$ which is a member of this ensemble, i.e.

$$H(\mathbf{z}(t_0), \epsilon t_0) = E_0 \quad . \tag{2.8}$$

The change in energy of this system, between times t_0 and $t_0 + \Delta t$, is given by an integral of the function $\dot{H} = \partial H / \partial t$ along the trajectory. Thus, defining

$$u(t) \equiv \dot{H}(\mathbf{z}(t), \epsilon t) \quad , \tag{2.9}$$

we have

$$E - E_0 = \int_{t_0}^{t_0 + \Delta t} dt\, u(t) \quad . \tag{2.10}$$

The function $u(t)$ is determined by the trajectory $\mathbf{z}(t)$. Thus, the ensemble of trajectories defined by a uniform distribution over the energy shell E_0 at time t_0 determines an associated ensemble of functions $u(t)$. Letting brackets denote an

average over this ensemble, we have

$$\begin{aligned}\left\langle (E-E_0)^2 \right\rangle &= \left\langle \left[\int_{t_0}^{t_0+\Delta t} dt\, u(t) \right]^2 \right\rangle \\ &= \int_{t_0}^{t_0+\Delta t} dt' \int_{t_0}^{t_0+\Delta t} dt'' \left\langle u(t')\, u(t'') \right\rangle \quad . \end{aligned} \tag{2.11}$$

To leading order, this quantity scales like ϵ^2 (since $u(t) \sim \epsilon$). Now, in the limit $\epsilon \to 0$, with ϵt_0 and Δt held fixed, H becomes the time-independent H_α, where α is fixed at ϵt_0. Therefore, to evaluate $\langle (E-E_0)^2 \rangle$ to lowest order, we replace the trajectories $\mathbf{z}(t)$ evolving under H, by trajectories $\mathbf{z}_\alpha(t)$ evolving under H_α, with α fixed at ϵt_0 (the condition which this places on ϵ is discussed below); we also hold the argument ϵt of $\dot{H}$ fixed at ϵt_0 in Eq. 2.9. Thus, to lowest order, we have

$$u(t) = \dot{H}(\mathbf{z}_\alpha(t), \epsilon t_0) = \dot{H}_\alpha(\mathbf{z}_\alpha(t)) \quad . \tag{2.12}$$

Our ensemble of trajectories $\mathbf{z}_\alpha(t)$ evolving under the time-dependent H_α remains uniformly distributed over the energy shell E_0 for all times t, and so the associated ensemble of functions $u(t)$ defines a stationary stochastic process. We may write

$$\left\langle u(t')\, u(t'') \right\rangle = \bar{u}^2 + \left\langle [u(t') - \bar{u}]\, [u(t'') - \bar{u}] \right\rangle \quad , \tag{2.13}$$

where $\bar{u} \equiv \langle u(t) \rangle$ is independent of t and is equal to the average value of $\dot{H}_\alpha$ over the energy shell E_0 of H_α. The second quantity on the right hand side is a correlation function (see Appendix A of this chapter); since we have a stationary stochastic process, this quantity depends on t' and t'' only through their difference $s \equiv t'' - t'$, and will be denoted by $C(s)$. We may express this correlation function as a phase space average:

$$C(s) = \left\{ \left[\dot{H}_\alpha(\mathbf{z}) - \bar{u} \right] \mathcal{O}_\alpha(s) \left[\dot{H}_\alpha(\mathbf{z}) - \bar{u} \right] \right\}_{E_0,\alpha} \quad , \tag{2.14}$$

where the operator $\mathcal{O}_\alpha(s)$ acting on a point $\mathbf{z}$ evolves it for a time s under the frozen Hamiltonian H_α, and the braces denote a phase space average over the energy shell

E_0 of H_α. The quantities $\bar{u}$ and $C(s)$ both depend on E_0 and ϵt_0 (since α is fixed at ϵt_0).

We now have

$$\begin{aligned}\left\langle (E-E_0)^2 \right\rangle &= \int_{t_0}^{t_0+\Delta t} dt' \int_{t_0}^{t_0+\Delta t} dt'' \left[\bar{u}^2 + C(s)\right] \\ &= \bar{u}^2(\Delta t)^2 + \Delta t \int_{-\Delta t}^{\Delta t} ds \left(1 - \frac{|s|}{\Delta t}\right) C(s) \quad . \end{aligned} \tag{2.15}$$

Since $\Delta t \gg t_c$, the integral in this expression may be replaced by

$$\int_{-\infty}^{+\infty} ds\, C(s) \quad , \tag{2.16}$$

provided that the latter converges; this is a standard result for stationary stochastic process.[18] We then have

$$\left\langle (E-E_0)^2 \right\rangle = \bar{u}^2(\Delta t)^2 + \Delta t \int_{-\infty}^{+\infty} ds\, C(s) \quad . \tag{2.17}$$

We point out that, in the case of a Hamiltonian H_α for which the integral appearing here diverges, our approach clearly does not work. Generally, if the integral of the correlation function of some stochastic process diverges, then the correlation time t_c associated with that process is taken to be infinite.[19] In such a case, our approach, motivated by the assumption of a correlation time much shorter than a typical time over which the distribution of energies changes significantly, cannot be expected to hold.

We now confront a seemingly serious objection to our derivation of the above results. In evaluating $\langle (E-E_0)^2 \rangle$ to lowest order in ϵ, we replaced the ensemble $\{\mathbf{z}(t)\}$ of trajectories evolving under the slowly time-dependent H, with the ensemble $\{\mathbf{z}_\alpha(t)\}$ evolving under the frozen H_α. Now, if these ensembles are nearly identical — in the sense that corresponding members sharing a common initial condition at time t_0 will have diverged only slightly after time Δt — then our evaluation of $\langle (E-E_0)^2 \rangle$ will be valid. However, this places an unrealistically stringent condition on ϵ: if we imagine the time-dependence of H as introducing perturbations

proportional to ϵ to motion under H_α, then two corresponding trajectories $\mathbf{z}(t)$ and $\mathbf{z}_\alpha(t)$ will diverge exponentially in time, with Lyapunov exponent $\lambda \cong 1/t_c$; only if ϵ is exceedingly small will motion under H be similar to that under H_α, over a time $\Delta t \gg t_c$. In the following paragraph we argue that this view is too pessimistic, that in fact as long as a far less restrictive condition on ϵ — namely, that motion under H is similar to that under H_α over times on the order of t_c (rather than Δt) — holds, we can expect Eq. 2.17 to be valid.

In deriving Eq. 2.17, we are dealing with the diffusive spreading of energies. The rate of diffusion for an ensemble of systems undergoing stochastic motion is determined by the velocity correlations characterizing this motion. Therefore, as long as the velocity correlations $\langle [u(t') - \bar{u}]\,[u(t'') - \bar{u}] \rangle$ associated with the ensembles $\{\mathbf{z}(t)\}$ and $\{\mathbf{z}_\alpha(t)\}$ are similar (in the time interval t_0 to $t_0 + \Delta t$), we can expect our results for $\langle (E - E_0)^2 \rangle$ to be valid. Now, let us assume that ϵ is small enough that evolution under H is nearly identical to that under H_α, for times on the order of t_c. Since mixing occurs over times on this order, and since we have assumed that H changes negligibly over time Δt, we expect that our ensemble of trajectories will — to a good approximation — remain uniform over the energy shell E_0, between times t_0 and $t_0 + \Delta t$. (The fact that H changes negligibly guarantees that the trajectories stay very close to the energy shell E_0; the continual process of mixing maintains uniformity, within a coarse-graining approximation.) This implies that the stochastic process defined by the ensemble of functions $u(t)$ is approximately stationary. Combining this with the fact that, over times on the order of the correlation time, evolution under H is nearly identical to that under H_α, we conclude that the correlations $\langle [u(t') - \bar{u}]\,[u(t'') - \bar{u}] \rangle$ associated with the ensemble $\{\mathbf{z}(t)\}$ are nearly identical to those associated with $\{\mathbf{z}_\alpha(t)\}$, with α fixed at ϵt_0. Thus, Eq. 2.17 should be valid.

Both terms on the right hand side of Eq. 2.17 scale like ϵ^2. Comparing this

equation with Eq. 2.7, we find the leading terms of g_1 and g_2 to scale like ϵ and ϵ^2, respectively. Letting g_{12} denote the (as yet undetermined) $O(\epsilon^2)$ term of g_1, and henceforth ignoring all quantities of $O(\epsilon^3)$ or smaller, we have:

$$g_1(E,\epsilon t) = \bar{u}(E,\epsilon t) + g_{12}(E,\epsilon t) \tag{2.18}$$

$$g_2(E,\epsilon t) = \int_{-\infty}^{+\infty} ds\; C(s;E,\epsilon t) \quad . \tag{2.19}$$

It now remains to obtain the $O(\epsilon^2)$ term of g_1. To accomplish this, we will make use of Liouville's theorem. We begin by rewriting Eq. 2.6 in terms of the distribution of "enclosed phase space volumes", $\zeta(\Omega,t)$, rather than the distribution of energies $\eta(E,t)$. That is, define ζ so that $\zeta(\Omega,t)\,d\Omega$ gives, at time t, the number of systems found on energy shells enclosing a volume of phase space between Ω and $\Omega + d\Omega$. Then, as shown in Appendix B of this chapter, ζ satisfies

$$\frac{\partial\zeta}{\partial t} = -\frac{\partial}{\partial\Omega}\big(G_1\zeta\big) + \frac{1}{2}\frac{\partial^2}{\partial\Omega^2}\big(G_2\zeta\big) \quad , \tag{2.20}$$

where

$$G_1(\Omega,\epsilon t) = \Sigma\Big(g_{12} + \frac{1}{2\Sigma}\frac{\partial\Sigma}{\partial E}g_2\Big) \tag{2.21}$$

$$G_2(\Omega,\epsilon t) = \Sigma^2 g_2, \tag{2.22}$$

and

$$\Sigma(E,t) \equiv \frac{\partial}{\partial E}\Omega(E,t) = \int dz\,\delta\big[E - H(z,\epsilon t)\big]. \tag{2.23}$$

(In the equations for G_1 and G_2, the quantities g_{12}, g_2, and Σ are evaluated at the energy E corresponding to the shell enclosing phase space volume Ω.) Eq. 2.20 immediately gives an expression for the current $J_\Omega(\Omega,t)$ along the Ω axis, associated with any normalizable distribution $\zeta(\Omega,t)$:

$$\begin{aligned} J_\Omega &= G_1\zeta - \frac{1}{2}\frac{\partial}{\partial\Omega}\big(G_2\zeta\big) \\ &= \Big(G_1 - \frac{1}{2}\frac{\partial G_2}{\partial\Omega}\Big)\zeta - \frac{1}{2}G_2\frac{\partial\zeta}{\partial\Omega}. \end{aligned} \tag{2.24}$$

Now, suppose we start with a distribution of initial conditions that is uniform in phase space up to some cutoff energy E_c, and zero beyond. This corresponds to

$$\zeta(\Omega, t_0) = \theta(\Omega_c - \Omega), \tag{2.25}$$

Ω_c being the volume enclosed by the energy shell E_c. Thus,

$$J_\Omega(\Omega, t_0) = \Big(G_1 - \frac{1}{2}\frac{\partial G_2}{\partial \Omega}\Big)\theta(\Omega_c - \Omega) + \frac{1}{2}G_2\delta(\Omega_c - \Omega). \tag{2.26}$$

Then, since Liouville's theorem tells us that a phase space density evolves as an incompressible fluid, we know that initially our density will be changing only at the cutoff energy shell E_c itself, hence we demand that at time t_0, $J_\Omega = 0$ everywhere except at Ω_c. From Eq. 2.26, this gives

$$G_1 - \frac{1}{2}\frac{\partial G_2}{\partial \Omega} = 0, \tag{2.27}$$

for $\Omega < \Omega_c$. However, Ω_c was chosen arbitrarily, hence we conclude that Eq. 2.27 holds for all Ω. Combining this with Eqs. 2.21 and 2.22, and using Eq. 2.23, we get

$$g_{12} = \frac{1}{2\Sigma}\frac{\partial}{\partial E}(g_2\Sigma). \tag{2.28}$$

We now have our final equation of motion for $\eta(E,t)$, good to $O(\epsilon^2)$:

$$\frac{\partial \eta}{\partial t} = -\frac{\partial}{\partial E}\big[(\bar{u} + g_{12})\eta\big] + \frac{1}{2}\frac{\partial^2}{\partial E^2}(g_2\eta) \quad , \tag{2.29}$$

where the various coefficients, and how they scale with ϵ, are given by:

$$\bar{u}(E, \epsilon t) = \big\{\dot{H}_\alpha(\mathbf{z})\big\}_{E,\alpha} \sim \epsilon \tag{2.30}$$

$$g_2(E, \epsilon t) = \int_{-\infty}^{+\infty} ds \Big\{\big[\dot{H}_\alpha(\mathbf{z}) - \bar{u}\big]\mathcal{O}_\alpha(s)\big[\dot{H}_\alpha(\mathbf{z}) - \bar{u}\big]\Big\}_{E,\alpha} \sim \epsilon^2 \tag{2.31}$$

$$g_{12}(E, \epsilon t) = \frac{1}{2\Sigma}\frac{\partial}{\partial E}(g_2\Sigma) \sim \epsilon^2 \quad , \tag{2.32}$$

with α evaluated at ϵt, and $\Sigma(E, \epsilon t) = \int d\mathbf{z}\, \delta[E - H(\mathbf{z}, \epsilon t)]$. The braces indicate a phase space average over the energy shell E of H_α. The term involving $\bar{u}$ is

responsible for the $O(\epsilon^1)$ drift in the average energy of the systems in the ensemble; as discussed below, this is the drift prescribed by the adiabatic invariance of Ω. The term with g_2 gives rise to the diffusion of energies, at $O(\epsilon^2)$; in order to satisfy Liouville's equation, this diffusion must be accompanied by an $O(\epsilon^2)$ correction to the drift, given by the g_{12} term. We will refer to Eq. 2.29 — the central result of this chapter — as the *energy diffusion equation.* Using Eq. 2.32, we can rewrite this result in an alternative form, without the explicit appearance of g_{12}:

$$\frac{\partial \eta}{\partial t} = -\frac{\partial}{\partial E}(\bar{u}\eta) + \frac{1}{2}\frac{\partial}{\partial E}\Big[g_2 \Sigma \frac{\partial}{\partial E}\Big(\frac{\eta}{\Sigma}\Big)\Big] \quad . \tag{2.33}$$

2.5 COMPARISON OF RESULTS

In this section, we compare our results with those of Refs.[5–7].

We begin by showing that, in the adiabatic limit, there is agreement: the energy diffusion equation describes an ensemble of systems, the energy of each of which evolves so as to keep the chaotic adiabatic invariant, Ω, constant.

In the adiabatic limit, the $O(\epsilon^2)$ terms of this diffusion equation make no contribution to the change in η, so we have

$$\frac{\partial \eta}{\partial t} = -\frac{\partial}{\partial E}(\bar{u}\eta) \quad . \tag{2.34}$$

This is simply a continuity equation describing an ensemble of systems moving under a "velocity" field $\bar{u}(E, \epsilon t)$ along the E-axis. Thus,

$$\frac{d}{dt}E(t) = \bar{u}(E(t), \epsilon t) \quad , \tag{2.35}$$

where $E(t)$ is the energy of a given member of the ensemble. To prove that this agrees with the adiabatic invariance of Ω, we need to show that the velocity field $\bar{u}(E, \epsilon t)$ is such that $\Omega(E(t), \epsilon t)$ is constant in time. We take the total time derivative:

$$\frac{d}{dt}\Omega(E(t), \epsilon t) = \frac{\partial \Omega}{\partial E}(E, \epsilon t)\, \bar{u}(E, \epsilon t) + \frac{\partial \Omega}{\partial t}(E, \epsilon t) \quad , \tag{2.36}$$

with the right hand sided evaluated at $E = E(t)$. Using the identities $\Sigma = \partial\Omega/\partial E$ and $\bar{u} = (-1/\Sigma)(\partial\Omega/\partial t)$ — both of which follow from the definitions of Σ, Ω, and $\bar{u}$ (see Eqs. 2.23, 2.4, and 2.30) — the right hand side vanishes, completing our proof.

Now, for slow but finite time-dependence of H, the quantity Ω is not an exact invariant. In studying the goodness of the chaotic adiabatic invariant, Ott *et al.* consider the evolution of a normalized ensemble whose distribution at initial time t_0 is uniform over an energy shell E_0. From the preceding paragraph, we know that, to lowest order in ϵ (i.e. in the adiabatic limit), we have:

$$\eta(E,t) = \delta(E - \mathcal{E}(t)) \quad , \tag{2.37}$$

where

$$\frac{d}{dt}\mathcal{E}(t) = \bar{u}(\mathcal{E}(t), \epsilon t) \quad , \tag{2.38}$$

and $\mathcal{E}(t_0) = E_0$. Ott *et al.* investigate deviations from this result by considering the moments of the distribution of energies at time t, with respect to $\mathcal{E}(t)$:

$$M_n(t) \equiv \int dE\, \eta(E,t) \left[E - \mathcal{E}(t)\right]^n \quad , \quad n = 1, 2, \cdots . \tag{2.39}$$

They obtain expressions for the rates at which these moments are acquired. For times that scale like ϵ^{-1}, their results (in the notation of this Thesis) are:

$$\frac{dM_1}{dt} = g_{12}(\mathcal{E}(t), \epsilon t) + O(\epsilon^3) \tag{2.40}$$

$$\frac{dM_2}{dt} = g_2(\mathcal{E}(t), \epsilon t) + O(\epsilon^3) \tag{2.41}$$

$$\frac{dM_n}{dt} = O(\epsilon^3) \quad , \quad n \geq 3 \quad . \tag{2.42}$$

As discussed below, these are the results that one would expect from the energy diffusion equation, if the distribution at time t could be well approximated by $\delta(E - \mathcal{E}(t))$. However, since first and second moments with respect to $\mathcal{E}(t)$ are — by the above equations — acquired at rates of $O(\epsilon^2)$, we expect that, after times

like ϵ^{-1}, these deviations will be $O(\epsilon^1)$. As the following analysis will reveal, when these moments are combined with the dependence of $\bar{u}$ on E, we get additional terms of $O(\epsilon^2)$ in Eqs. 2.40 and2.41.

We now solve for dM_n/dt, $n = 1, 2, 3, \cdots$, using the energy diffusion equation. We start by differentiating Eq. 2.39 with respect to time:

$$\begin{aligned} \frac{dM_n}{dt} &= \int dE \left\{ -\frac{\partial}{\partial E}\left[(\bar{u} + g_{12})\eta\right] + \frac{1}{2}\frac{\partial^2}{\partial E^2}(g_2\eta) \right\} \left[E - \mathcal{E}(t)\right]^n \\ &\quad - n \int dE\, \eta \left[E - \mathcal{E}(t)\right]^{n-1} \frac{d}{dt}\mathcal{E}(t) \quad , \end{aligned} \tag{2.43}$$

where $\bar{u}$, g_{12}, and g_2 are functions of E and ϵt, and $\eta = \eta(E, t)$. After differentiating by parts the term involving $\bar{u}$ in the first integral, rewriting the second integral using Eq. 2.38, and combining the two, we get

$$\begin{aligned} \frac{dM_n}{dt} &= n \int dE \left[\bar{u}(E, \epsilon t) - \bar{u}(\mathcal{E}(t), \epsilon t)\right] \eta \left[E - \mathcal{E}(t)\right]^{n-1} \\ &\quad - \int dE \frac{\partial}{\partial E}(g_{12}\eta) \left[E - \mathcal{E}(t)\right]^n \\ &\quad + \int dE \frac{1}{2}\frac{\partial^2}{\partial E^2}(g_2\eta) \left[E - \mathcal{E}(t)\right]^n \quad . \end{aligned} \tag{2.44}$$

Since we require this to be good only to $O(\epsilon^2)$, and since $g_{12}, g_2 \sim \epsilon^2$, we can replace η in the second and third integrals by its leading term, which is $\delta(E - \mathcal{E}(t))$, as per the adiabatic invariance of Ω. Then, after integration by parts, the second integral reduces to $g_{12}(\mathcal{E}(t), \epsilon t)\, \delta_{n,1}$, while the third reduces to $g_2(\mathcal{E}(t), \epsilon t)\, \delta_{n,2}$, where $\delta_{i,j}$ is the Kronecker delta function. We rewrite the first integral by Taylor-expanding $\bar{u}(E, \epsilon t)$ around $E = \mathcal{E}(t)$. This yields, to $O(\epsilon^2)$, the following set of equations:

$$\begin{aligned} \frac{dM_n}{dt} &= n \sum_{k=1}^{\infty} \frac{1}{k!}\, \bar{u}^{(k)}(\mathcal{E}(t), \epsilon t)\, M_{n-1+k} \\ &\quad + g_{12}(\mathcal{E}(t), \epsilon t)\, \delta_{n,1} + g_2(\mathcal{E}(t), \epsilon t)\, \delta_{n,2} \quad , \end{aligned} \tag{2.45}$$

where $\bar{u}^{(k)}(\mathcal{E}(t); \epsilon t)$ denotes the kth derivative of $\bar{u}$ with respect to energy, evaluated at energy $\mathcal{E}(t)$ and time t. By considering the subset of these equations for which $n \geq 3$, one can establish that all moments other than the first and second grow at

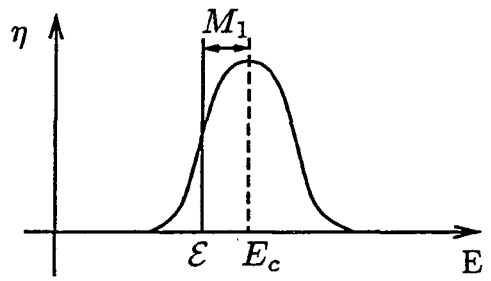

Figure 2.1: Distribution of energies at time t, for an ensemble of systems which was distributed uniformly over the energy shell E_0 at time t_0.

rates that scale like ϵ^3, and therefore, after times like ϵ^{-1}, these moments scale like ϵ^2. Since, on the right hand side of the above equations, these moments are always multiplied by a quantity proportional to ϵ — namely, $\bar{u}^{(k)}$ — we conclude that their contribution there is $O(\epsilon^3)$. This agrees with Eq. 2.42, and leaves us with:

$$\frac{dM_1}{dt} = g_{12} + \bar{u}^{(1)} M_1 + \frac{1}{2}\bar{u}^{(2)} M_2 + O(\epsilon^3) \tag{2.46}$$

$$\frac{dM_2}{dt} = g_2 + 2\,\bar{u}^{(1)} M_2 + O(\epsilon^3) \quad , \tag{2.47}$$

where g_{12}, g_2, $\bar{u}^{(1)}$, and $\bar{u}^{(2)}$ are all evaluated at $\mathcal{E}(t)$, ϵt. Since g_{12}, $g_2 \sim \epsilon^2$, we conclude that the first and second moments M_1 and M_2 grow at rates that scale like ϵ^2. After times on the order of ϵ^{-1}, these moments scale like ϵ^1; therefore, the terms which involve the product of these moments with derivatives of $\bar{u}$ are $O(\epsilon^2)$, and must be kept.

The terms in Eqs. 2.46 and 2.47 offer an easy interpretation. The distribution $\eta(E,t)$ is shown schematically in Fig.2.1, for $t - t_0 \sim \epsilon^{-1}$. Instead of a δ-function at $\mathcal{E}(t)$ — which would occur if the adiabatic invariant were conserved exactly — the distribution is a peak of finite width, with an average at some energy E_c. The difference between E_c and $\mathcal{E}(t)$ is the previously defined moment M_1, an $O(\epsilon^1)$ quantity. Thus, dM_1/dt is given by the difference between the rate at which the centroid E_c moves along the energy axis, and the rate at which the energy $\mathcal{E}(t)$ changes. Now, if we imagine "slicing up" the distribution $\eta(E,t)$ into a continuous

set of δ-functions, then the slice located at E will drift along the energy axis with an instantaneous velocity given by the drift coefficient g_1, evaluated at E. Therefore, the velocity of the centroid E_c is equal to the average value of g_1 over the distribution $\eta(E,t)$. The rate of change of $\mathcal{E}(t)$, on the other hand, is given exactly by $\bar{u}$, evaluated at $\mathcal{E}(t)$. The term g_{12} in Eq. 2.46 therefore comes from approximating the distribution at time t as a δ-function at $\mathcal{E}(t)$: in this approximation, the instantaneous velocity of the centroid is $g_1(\mathcal{E}(t), \epsilon t)$, and so

$$\frac{dM_1}{dt} = g_1 - \bar{u} = g_{12} \quad , \tag{2.48}$$

evaluated at $\mathcal{E}(t)$. The next term in Eq. 2.46 is due to the $O(\epsilon^1)$ displacement of the distribution away from $\mathcal{E}(t)$: the difference between the drift coefficient g_1 at E_c and at $\mathcal{E}(t)$ is, to $O(\epsilon^2)$, equal to $\bar{u}^{(1)}M_1$. Finally, there is a contribution to dE_c/dt due to the finite width of $\eta(E,t)$: since g_1 depends on energy, the slices into which the distribution is divided drift at different rates. With a linear expansion of g_1 around E_c, the faster-moving slices on one side of E_c are balanced by the slower-moving ones on the other, and no new contribution to dM_1/dt results; however, going to a quadratic expansion, we get an additional term which works out to be $\frac{1}{2}\bar{u}^{(2)}M_2$, to $O(\epsilon^2)$. All other additional terms are $O(\epsilon^3)$ or smaller.

The terms in Eq. 2.47 may be interpreted similarly. The first term on the right hand side is obtained by approximating the distribution at time t as a δ-function at energy $\mathcal{E}(t)$; dM_2/dt is then simply the diffusion coefficient, g_2, evaluated at $\mathcal{E}(t)$. The second term is due to the finite width of the distribution η: if we again imagine slicing this peak into a continuous set of δ-functions, then, as a function of E, there will be a gradient in the rates at which these slices drift along the E axis. The resulting contribution to dM_2/dt is $2\bar{u}^{(1)}M_2$ (to $O(\epsilon^2)$). All other additional terms, whether due to the displacement of E_c away from $\mathcal{E}(t)$, or to the finite width of η, are $O(\epsilon^3)$ or smaller.

The three terms in Eqs. 2.46 and 2.47 which involve the derivatives of $\bar{u}$ — and

which arise from the fact that, after times that scale like ϵ^{-1}, one must take into account the fact that η is not exactly a δ-function at $\mathcal{E}(t)$ — do not appear in the results of Ott *et al.* The source of this discrepancy will be made clear in Chapter 6.

2.6 GOODNESS OF THE CHAOTIC ADIABATIC INVARIANT

Since, in the adiabatic limit, the conservation of Ω determines the energy of a given system, the rates at which the moments M_1 and M_2 grow indicate how well Ω is being conserved (more precisely, the extent to which the invariance of Ω is violated) for a chaotic adiabatic ensemble defined by a common initial energy. However, the goodness of the chaotic adiabatic invariant may be studied more directly by considering $\Delta\Omega$, the change in Ω for a system evolving under a chaotic adiabatic Hamiltonian. Specifically, consider once again an ensemble of initial conditions distributed uniformly over a given energy shell E_0, which encloses a volume of phase space Ω_0. Thus, representing this ensemble as a distribution over the Ω-axis, we have

$$\zeta(\Omega, t_0) = \delta(\Omega - \Omega_0). \tag{2.49}$$

By the adiabatic invariance of Ω, this distribution ζ will remain unchanged in the adiabatic limit. Now consider the moments

$$\begin{aligned} \left\langle \Delta\Omega \right\rangle &= \int d\Omega\, (\Omega - \Omega_0)\, \zeta(\Omega, t) \\ \left\langle (\Delta\Omega)^2 \right\rangle &= \int d\Omega\, (\Omega - \Omega_0)^2 \zeta(\Omega, t) \quad , \end{aligned} \tag{2.50}$$

i.e. the ensemble averages of $\Delta\Omega$ and $(\Delta\Omega)^2$, as functions of time. These measure — more directly than M_1 and M_2 — the deviations away from the exact invariance

of Ω. Using Eq. 2.20, an analysis identical to the one performed in Section 2.5 gives, to $O(\epsilon^2)$,

$$\begin{aligned} \frac{d}{dt}\langle \Delta\Omega \rangle &= G_1(\Omega_0, \epsilon t) \\ \frac{d}{dt}\langle (\Delta\Omega)^2 \rangle &= G_2(\Omega_0, \epsilon t) \quad . \end{aligned} \tag{2.51}$$

(All higher moments, e.g. $\langle (\Delta\Omega)^3 \rangle$, grow at rates that scale like ϵ^3 or smaller.) The above results may be integrated to yield explicit lowest-order expressions for $\langle \Delta\Omega \rangle$ and $\langle (\Delta\Omega)^2 \rangle$ as functions of time:

$$\begin{aligned} \langle \Delta\Omega \rangle &= \int_{t_0}^{t} G_1(\Omega_0, \epsilon t')\, dt' \\ \langle (\Delta\Omega)^2 \rangle &= \int_{t_0}^{t} G_2(\Omega_0, \epsilon t')\, dt' \quad . \end{aligned} \tag{2.52}$$

For times $(t - t_0)$ that scale like ϵ^{-1}, these moments will be $O(\epsilon^1)$.

2.7 SPECIAL CASES

As a final exercise, we consider two particularly simple examples of chaotic adiabatic systems. We start with a three-dimensional potential well $V_0(\mathbf{r})$ such that the Hamiltonian $H_0 = p^2/2m + V_0(\mathbf{r})$ gives rise to ergodic and chaotic motion over any energy shell. Now consider the time-dependent Hamiltonians:

$$\begin{aligned} H^{tr}(\mathbf{z}, \epsilon t) &\equiv \frac{p^2}{2m} + V_0(\mathbf{r} - \epsilon \mathbf{u} t) \\ \text{and} \quad H^{rot}(\mathbf{z}, \epsilon t) &\equiv \frac{p^2}{2m} + V_0(\mathcal{R}_{\hat{\mathbf{n}}}(-\epsilon\omega t)\mathbf{r}) \quad , \end{aligned} \tag{2.53}$$

where the operator $\mathcal{R}_{\hat{\mathbf{n}}}(\theta)$ performs a rotation by an angle θ about a unit vector $\hat{\mathbf{n}}$ through the origin. Thus, H^{tr} is obtained by endowing the potential well $V_0(\mathbf{r})$ with translational motion at a small, uniform velocity $\epsilon\mathbf{u}$, H^{rot} by letting the well rotate about $\hat{\mathbf{n}}$ at a small angular speed $\epsilon\omega$. Both cases are examples of chaotic adiabatic systems, and in both cases we expect there to be no diffusion of energies, since in the

co-moving or co-rotating frame the effective Hamiltonian is time-independent. We now demonstrate that the energy diffusion equation confirms these expectations.[20]

Begin with the rigidly translating well. Since the Hamiltonian at one instant in time is related to that at any other instant by a simple translation of the potential well, it is clear that the volume of phase space enclosed by a given energy shell is independent of time: $\partial\Omega/\partial t = 0$. Since $\bar{u}$ may be expressed as $(1/\Sigma)\partial\Omega/\partial t$, this means that $\bar{u}(E, \epsilon t) = 0$. To solve for $g_2(E, \epsilon t)$, we start with the correlation function $C(s; E, \epsilon t)$. Like Ω, this quantity is easily seen to be independent of time, and so we may evaluate it at $\epsilon t = 0$, for which we have

$$\dot{H}_\alpha(\mathbf{z}) = -\epsilon \mathbf{u} \cdot \nabla V_0(\mathbf{r}) \quad . \tag{2.54}$$

Thus,

$$C(s; E, \epsilon t) = \left\{ \left[-\epsilon \mathbf{u} \cdot \nabla V_0(\mathbf{r}) \right] \mathcal{O}_\alpha(s) \left[-\epsilon \mathbf{u} \cdot \nabla V_0(\mathbf{r}) \right] \right\}_{E,\alpha} \quad , \tag{2.55}$$

where $\mathcal{O}_\alpha(s)$ is the time-evolution operator associated with $H_\alpha = p^2/2m + V_0(\mathbf{r})$, and the braces indicate an average over the energy shell E of this Hamiltonian. Letting $(\mathbf{R}, \mathbf{P})$ denote the point in phase space reached by evolving a trajectory from $(\mathbf{r}, \mathbf{p})$ for a time s under H_α, we have

$$\begin{aligned} C(s; E, \epsilon t) &= \epsilon^2 \left\{ \left[\mathbf{u} \cdot \nabla V_0(\mathbf{r}) \right] \left[\mathbf{u} \cdot \nabla V_0(\mathbf{R}) \right] \right\}_{E,\alpha} \\ &= \epsilon^2 \left\{ \left[\mathbf{u} \cdot \nabla V_0(\mathbf{r}) \right] \left[\mathbf{u} \cdot \left(-\frac{\partial \mathbf{P}}{\partial s} \right) \right] \right\}_{E,\alpha} \quad , \end{aligned} \tag{2.56}$$

since $-\nabla V_0(\mathbf{R})$ is the force acting on the trajectory at point $\mathbf{R}$, and is equal to the rate of change of $\mathbf{P}$ with respect to s. We now pull $\partial/\partial s$ outside of the braces and integrate to get g_2:

$$\begin{aligned} g_2(E, \epsilon t) &= \int_{-\infty}^{+\infty} ds\, C(s; E, \epsilon t) \\ &= -\epsilon^2 \left\{ \left[\mathbf{u} \cdot \nabla V_0(\mathbf{r}) \right] \left[\mathbf{u} \cdot \mathbf{P} \right] \right\}_{E,\alpha} \Big|_{s=-\infty}^{s=+\infty} \quad . \end{aligned} \tag{2.57}$$

Since motion under H_α is mixing, all correlations vanish in the limits $s \to \pm\infty$;

thus,

$$\lim_{s\to\pm\infty}\Big\{\big[\mathbf{u}\cdot\nabla V_0(\mathbf{r})\big]\,\big[\mathbf{u}\cdot\mathbf{P}\big]\Big\}_{E,\alpha} = \Big\{\mathbf{u}\cdot\nabla V_0(\mathbf{r})\Big\}_{E,\alpha}\Big\{\mathbf{u}\cdot\mathbf{p}\Big\}_{E,\alpha} = 0 \quad , \tag{2.58}$$

and so $g_2(E,\epsilon t)=0$. From Eq. 2.32, it immediately follows that $g_{12}(E,\epsilon t)=0$, and so we finally obtain $\partial\eta/\partial t = 0$. The distribution of energies is therefore constant in time, i.e. there is no diffusion of energies.

For the case of a rotating potential well, we begin by noting that, as in the case of a rigidly translating well, $\Omega(E;\epsilon t)$ is constant in time, and so $\bar{u}(E,\epsilon t)=0$. The correlation function, too, is independent of time, and therefore we evaluate it at $\epsilon t = 0$, where we have

$$\begin{aligned}\dot{H}_\alpha(\mathbf{z}) &= -\epsilon\omega\hat{\mathbf{n}}\times\mathbf{r}\cdot\nabla V_0(\mathbf{r}) \\ &= -\epsilon\omega\hat{\mathbf{n}}\cdot\mathbf{r}\times\nabla V_0(\mathbf{r}) \quad .\end{aligned} \tag{2.59}$$

Thus,

$$\begin{aligned}C(s;E,\epsilon t) &= \Big\{\big[-\epsilon\omega\hat{\mathbf{n}}\cdot\mathbf{r}\times\nabla V_0(\mathbf{r})\big]\mathcal{O}_\alpha(s)\big[-\epsilon\omega\hat{\mathbf{n}}\cdot\mathbf{r}\times\nabla V_0(\mathbf{r})\big]\Big\}_{E,\alpha} \\ &= \epsilon^2\omega^2\Big\{\big[\hat{\mathbf{n}}\cdot\mathbf{r}\times\nabla V_0(\mathbf{r})\big]\,\big[\hat{\mathbf{n}}\cdot\mathbf{R}\times\nabla V_0(\mathbf{R})\big]\Big\}_{E,\alpha} \\ &= -\epsilon^2\omega^2\Big\{\big[\hat{\mathbf{n}}\cdot\mathbf{r}\times\nabla V_0(\mathbf{r})\big]\,\big[\hat{\mathbf{n}}\cdot\frac{\partial}{\partial s}(\mathbf{R}\times\mathbf{P})\big]\Big\}_{E,\alpha} \quad ,\end{aligned} \tag{2.60}$$

with notation as before. Thus,

$$\begin{aligned}g_2(E,\epsilon t) &= \int_{-\infty}^{+\infty} ds\, C(s;E,\epsilon t) \\ &= -\epsilon^2\omega^2\Big\{\big[\hat{\mathbf{n}}\cdot\mathbf{r}\times\nabla V_0(\mathbf{r})\big]\,\big[\hat{\mathbf{n}}\cdot\mathbf{R}\times\mathbf{P}\big]\Big\}_{E,\alpha}\Big|_{s=-\infty}^{s=+\infty} \quad .\end{aligned} \tag{2.61}$$

As before, correlations vanish for $s\to\pm\infty$, so

$$\lim_{s\to\pm\infty}\Big\{\big[\hat{\mathbf{n}}\cdot\mathbf{r}\times\nabla V_0(\mathbf{r})\big]\,\big[\hat{\mathbf{n}}\cdot\mathbf{R}\times\mathbf{P}\big]\Big\}_{E,\alpha} = \Big\{\hat{\mathbf{n}}\cdot\mathbf{r}\times\nabla V_0(\mathbf{r})\Big\}_{E,\alpha}\Big\{\hat{\mathbf{n}}\cdot\mathbf{r}\times\mathbf{p}\Big\}_{E,\alpha} = 0 \quad . \tag{2.62}$$

Thus, $g_2 = 0$, and so $g_{12} = 0$, and so we end up with $\partial\eta/\partial t = 0$, which again confirms expectations.

We have therefore shown that, for the two special cases considered in this Section, the energy diffusion equation agrees with what we expect from simple physical arguments.

2.8 APPENDIX A

This appendix concerns correlation functions and some associated concepts. Suppose that we have some stochastic process, i.e. an ensemble of functions $u(t)$ which represent the possible samplings of a process considered to be "random". Letting angular brackets denote an average over this ensemble, we define the correlation function

$$\begin{aligned} C(t',t'') &\equiv \Big\langle \big[u(t') - \big\langle u(t')\big\rangle\big]\big[u(t'') - \big\langle u(t'')\big\rangle\big]\Big\rangle \\ &= \big\langle u(t')u(t'')\big\rangle - \big\langle u(t')\big\rangle\big\langle u(t'')\big\rangle \quad . \end{aligned} \tag{2.63}$$

This function reveals the length of time over which a member of the ensemble remembers its value, in the following sense. If the process $u(t)$ is chaotic, we expect that, when the magnitude of the separation time $s \equiv t'' - t'$ is large enough, the values of $u(t')$ and $u(t'')$ will be uncorrelated:

$$\big\langle u(t')u(t'')\big\rangle = \big\langle u(t')\big\rangle\big\langle u(t'')\big\rangle \quad . \tag{2.64}$$

In other words, the value of $u(t')$ for a particular member of the ensemble tells us nothing about $u(t'')$. In this limit, we get $C(t',t'') = 0$. On the other hand, for short separation times, there may exist correlations between $u(t')$ and $u(t'')$, i.e. the ensemble average of the product does not necessarily equal the product of the averages, and so $C(t',t'') \neq 0$. (In particular, for $t' = t''$, the correlation function is simply the mean square deviation of $u(t')$ from the average value $\langle u(t')\rangle$.) The span

of time $t'' - t'$ over which significant correlations exist is a measure of the amount of time for which a member of the ensemble will carry some memory of its value at t'.

Ordinarily, the correlation function depends on both t' and t'' (although it is symmetric with respect to exchange of these two arguments). However, if the stochastic process is stationary — i.e. if the characteristics of the ensemble do not change with time — then $C(t', t'')$ depends on t' and t'' only through the separation time s, and may be written simply as $C(s)$.

To illustrate a stationary stochastic process, consider a time-independent Hamiltonian $H_0(\mathbf{z})$, along with some other time-independent function on phase space $A(\mathbf{z})$. Assume that evolution under H_0 is chaotic and ergodic over the energy shell, hence H_0 has the property of mixing. Suppose further that we have an ensemble of trajectories $\mathbf{z}(t)$ distributed uniformly over an energy shell E of H_0, and evolving under H_0; such an ensemble will remain uniform over the energy shell for all t. The associated ensemble of functions

$$a(t) \equiv A(\mathbf{z}(t)) \tag{2.65}$$

then defines a stationary stochastic process. The ensemble average $\bar{a} \equiv \langle a(t) \rangle$ is independent of t, and is simply the average value of A over the energy shell E. The correlation function $C(s)$ is defined by

$$C(s) \equiv \Big\langle \big[a(t) - \bar{a}\big] \big[a(t+s) - \bar{a}\big] \Big\rangle \quad , \tag{2.66}$$

where the brackets denote an ensemble average. Since the ensemble remains distributed uniformly over the energy shell E for all times t, we may alternatively express this correlation function as

$$C(s) = \Big\{ \big[A(\mathbf{z}) - \bar{a}\big] O(s) \big[A(\mathbf{z}) - \bar{a}\big] \Big\}_E \quad , \tag{2.67}$$

where the operator $O(s)$ evolves a point $\mathbf{z}$ forward by a time s, and the braces denote an average over points $\mathbf{z}$ on the energy shell E.

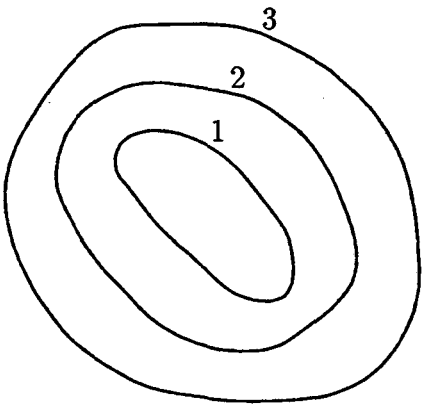

Figure 2.2: Level surfaces of $A'(\mathbf{z}) \equiv A(\mathbf{z}) - \bar{a}$, on the energy shell E of $H_0(\mathbf{z})$.

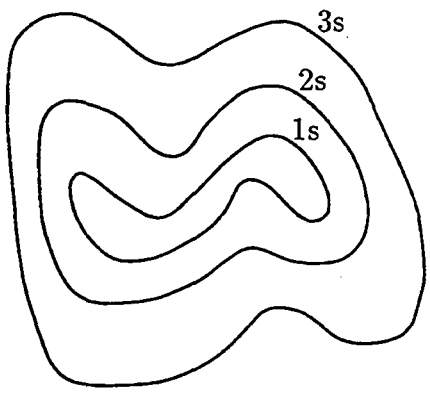

Figure 2.3: Surfaces to which the level surfaces of $A'(\mathbf{z})$ have evolved, after time s. These can be thought of as the level surfaces of a new function, $A'_s(\mathbf{z})$.

We can picture the construction of $C(s)$ as follows. First, consider the function $A'(\mathbf{z})$, which one gets by subtracting, from $A(\mathbf{z})$, its average value over the energy shell E:

$$A'(\mathbf{z}) = A(\mathbf{z}) - \bar{a} \quad . \tag{2.68}$$

Let Fig.2.2 represent, schematically, the energy shell; the three closed curves represent level surfaces of $A'(\mathbf{z})$. Let these surfaces evolve under H_0 for some time s, to the surfaces shown in Fig.2.3. These new surfaces can be thought of as the level surfaces of a new function $A'_s(\mathbf{z})$ over the energy shell. Now take the product of these two functions $A'(\mathbf{z})$ and $A'_s(\mathbf{z})$, and compute the average value of this product over the energy shell; this average is the correlation function. For sufficiently short times s, the surfaces will have evolved only slightly, i.e. $A'_s(\mathbf{z}) \cong A'(\mathbf{z})$, and so the correlation function is approximately the average value of A'^2 over the energy shell. On the other hand, in the limit $s \to \infty$, the mixing property of H_0 guarantees

that any enclosed area of the energy shell — for instance, the area between two of the original level surfaces — will have undergone enough stretching and folding to become distributed uniformly (to an arbitrary degree of fineness) over the energy shell. It follows that, in this limit, $C(s)$ is the product of the averages of A' and A'_s, and hence is equal to zero. We can define the correlation time t_c as the separation time s over which $C(s)$ decays to zero. Since the mechanism underlying this decay is the process of mixing — which follows from the exponential divergence of trajectories — we expect that the correlation time will be on the order of $1/\lambda$, where λ is the Lyapunov exponent associated with the divergence of trajectories under this Hamiltonian.

2.9 APPENDIX B

In this Appendix we derive Eq. 2.20 for the evolution of $\zeta(\Omega, t)$, the distribution of "enclosed phase space volumes".

ζ is defined so that the number of systems whose energy shells enclose volumes of phase space between Ω and $\Omega + d\Omega$, at time t, is given by $\zeta(\Omega, t)\, d\Omega$, for small $d\Omega$. Although we have written ζ as a function of (Ω, t), in contrast to η, which has been written as a function of (E, t), it will prove convenient in this Appendix to avoid speicifying a particular set of independent variables. Rather, we will think of both η and ζ as time-dependent functions of *energy shell*, where either E or Ω may be chosen to label the different shells at any instant in time.

Since η and ζ describe the same ensemble of systems, we have

$$\eta\, dE = \zeta\, d\Omega, \tag{2.69}$$

where dE and $d\Omega$ correspond to the same increment in energy shell. From this, we get

$$\eta = \Sigma\zeta, \tag{2.70}$$

where $\Sigma = \partial\Omega/\partial E$.

Now consider the quantities J_E and J_Ω defined by the continuity equations

$$\frac{\partial \eta}{\partial t} + \frac{\partial J_E}{\partial E} = 0 \quad , \quad \frac{\partial \zeta}{\partial t} + \frac{\partial J_\Omega}{\partial \Omega} = 0. \tag{2.71}$$

Physically, these describe "currents" along the E- and Ω-axes, respectively. We may picture this by drawing the energy axis, and placing a "hash mark" at the energy E corresponding to the energy shell at which we wish to evaluate J_E. Then J_E measures the net flow of systems across this hash mark. To picture J_Ω on the same axis, imagine another hash mark at the same energy, but endow this hash mark with a velocity dE/dt which is chosen so that the associated value of Ω is stationary; J_Ω measures the net instantaneous flow across this moving hash mark. From this picture it is clear that these two currents are related by:

$$J_\Omega = J_E - \frac{dE}{dt}\Big)_\Omega \eta, \tag{2.72}$$

where $dE/dt)_\Omega$ denotes the rate of change of E with Ω fixed.

Since η evolves under Eq. 2.6, it follows immediately that

$$J_E = g_1\eta - \frac{1}{2}\frac{\partial}{\partial E}(g_2\eta) \quad . \tag{2.73}$$

In Section 2.5, it was shown that

$$\frac{dE}{dt}\Big)_\Omega = \bar{u}. \tag{2.74}$$

Combining these results with Eq. 2.72, and with Eq. 2.18 ($g_1 = \bar{u} + g_{12}$), we get:

$$\begin{aligned} J_\Omega &= g_{12}\eta - \frac{1}{2}\frac{\partial}{\partial E}(g_2\eta) \\ &= \Sigma g_{12}\zeta - \frac{1}{2}\Sigma\frac{\partial}{\partial \Omega}(\Sigma g_2\zeta) \\ &= G_1\zeta - \frac{1}{2}\frac{\partial}{\partial \Omega}(G_2\zeta), \end{aligned} \tag{2.75}$$

where

$$\begin{aligned} G_1 &= \Sigma\Big(g_{12} + \frac{1}{2}\frac{\partial \Sigma}{\partial \Omega}g_2\Big) \\ G_2 &= \Sigma^2 g_2. \end{aligned} \tag{2.76}$$

From these results we immediately get (see Eq. 2.71):

$$\frac{\partial \zeta}{\partial t} = -\frac{\partial}{\partial \Omega}\big(G_1 \zeta\big) + \frac{1}{2}\frac{\partial^2}{\partial \Omega^2}\big(G_2 \zeta\big). \tag{2.77}$$

Chapter 3

Energy Diffusion in a Chaotic Adiabatic Billiard Gas

3.1 INTRODUCTION

This chapter 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. 3.1.) 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 chapter 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.

Section 3.2 of this chapter specifies the problem precisely, and introduces notation. In Section 3.3 we argue that the distribution of particle energies of a chaotic adiabatic billiard gas evolves diffusively; this suggests a Fokker-Planck equation for

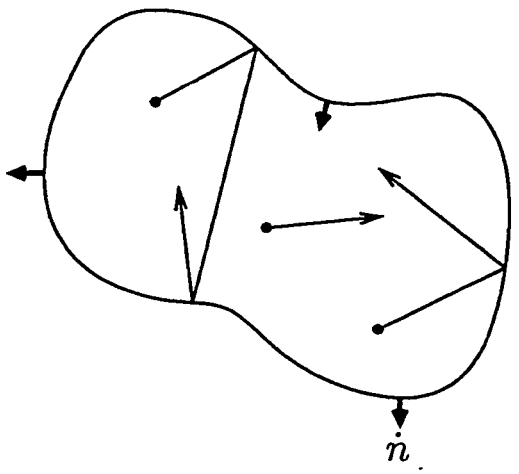

Figure 3.1: Two-dimensional version of a chaotic adiabatic billiard gas. The scalar field $\dot{n}$ gives the rate at which the wall is moving normally outward, as a function of position s along the wall. It is assumed that "freezing" the shape at any instant will produce a time-independent billiard in which all particle trajectories are chaotic.

the evolution of $\eta(E,t)$. In Section 3.4 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 Section 3.5 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 Section 3.6, a chaotic adiabatic billiard gas can be treated as the limiting case of a *chaotic adiabatic ensemble.* (See Chapter 2.) This chapter thus represents an application of the general approach of Chapter 2 to a specific class of problems.

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 time-dependent container filled with a gas of independent point particles. 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*,[10–12] an expression for the rate at which one-body dissipation transfers energy from the collective degrees of freedom of the idealized nucleus to the individual nucleons. In Section 3.7, we discuss the wall formula in the context of the general problem considered in this chapter, and we derive a few new, related results.

3.2 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 *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 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 mixing in a *frozen* container, to the problem of a gas of particles in a slowly time-dependent one. 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

$$T \gtrsim t_L. \tag{3.1}$$

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, mixing occurs before the particles "realize" that the shape is changing; as the container slowly evolves, the continual process of mixing tends to maintain a uniform distribution of particles throughout the container, and an isotropic distribution of velocities.

One more assumption needs to be made in order for the central result of this chapter to be valid. Since this assumption involves a correlation sum to be defined below, we postpone its explicit statement to Section 3.4, where it is italicized.

We will use the term *chaotic adiabatic billiard gas* to describe a gas of non-interacting particles inside a container whose slowly evolving shape satisfies the assumptions discussed above. For a specific example (in two dimensions) of such a container, see the "three-leaf clover" (or "Philips electric razor"[21]) billiard in Appendix C of this chapter. Our goal is an evolution equation for the distribution of particle energies, $\eta(E,t)$.

3.3 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[16] 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, as in Chapter 2, the following Fokker-Planck equation for the time-dependent distribution of energies, $\eta(E,t)$:

$$\frac{\partial \eta}{\partial t} = -\frac{\partial}{\partial E}(g_1 \eta) + \frac{1}{2}\frac{\partial^2}{\partial E^2}(g_2 \eta). \tag{3.2}$$

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 in the previous chapter, we 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. 3.2 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.

3.4 DRIFT AND DIFFUSION COEFFICIENTS

To derive expressions for g_1 and g_2, we start as in Chapter 2 with an initial distribution of energies described by a delta-function:

$$\eta(E,t_0) = \delta(E - E_0). \tag{3.3}$$

Letting η evolve under Eq. 3.2 for a short time Δt, we then have

$$\begin{aligned} \left\langle (E - E_0)^2 \right\rangle &\equiv \int dE\, \eta(E, t_0 + \Delta t)\, (E - E_0)^2 \\ &= (g_1 \Delta t)^2 + g_2 \Delta t. \end{aligned} \tag{3.4}$$

By considering a gas of particles sharing a common energy E_0 at time t_0, then by solving, in terms of quantities characterizing the subsequent motion of these particles, for $\langle (E - E_0)^2 \rangle$, and finally by comparing the result with Eq. 3.4, we will obtain expressions for g_1 and g_2. We will solve only for the leading term of $\langle (E - E_0)^2 \rangle$, 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, as in Chapter 2.

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. 3.1; 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. 3.2 and 3.3.) 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

$$B \cong \Delta t/\tau, \tag{3.5}$$

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, to leading order,

$$E - E_0 = -2mv \sum_{b=1}^{B} \dot{n}_b \sin\theta_b, \tag{3.6}$$

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 $\langle (E - E_0)^2 \rangle$, 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:

$$\left\langle (E - E_0)^2 \right\rangle = 4m^2v^2 \sum_{b=1}^{B} \sum_{b'=1}^{B} \left\langle \dot{n}_b \sin\theta_b \, \dot{n}_{b'} \sin\theta_{b'} \right\rangle. \tag{3.7}$$

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. 3.7, 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. 3.7 becomes

$$\left\langle (E - E_0)^2 \right\rangle = 4m^2v^2 \sum_{b=1}^{B} \sum_{b'=1}^{B} \left\langle \dot{n}_{\alpha b} \sin\theta_b \, \dot{n}_{\alpha b'} \sin\theta_{b'} \right\rangle_{\alpha}, \tag{3.8}$$

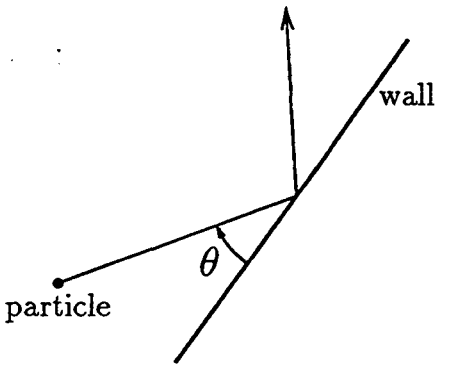

Figure 3.2: Particle bouncing off a small segment of wall in a two-dimensional billiard. The value of θ ranges from 0 to π.

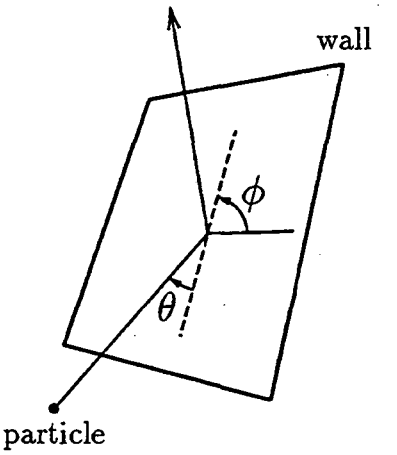

Figure 3.3: Particle bouncing off a small patch of wall in a three-dimensional billiard. The dashed line represents the normal projection of the trajectory onto the wall. The value of θ ranges from 0 to $\pi/2$; ϕ ranges from 0 to 2π. The line representing $\phi = 0$ is arbitrary.

where the angular brackets $\langle \cdots \rangle_\alpha$ indicate an average over an ensemble of trajectories evolving inside the *frozen* Sh_α, with $\alpha = \epsilon t_0$, 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. 3.8 as

$$\left\langle (\dot{n}_{\alpha b} \sin\theta_b - \xi_b)\,(\dot{n}_{\alpha b'} \sin\theta_{b'} - \xi_{b'}) \right\rangle_\alpha + \xi_b \xi_{b'} \equiv c_{b,b'} + \xi_b \xi_{b'}, \qquad (3.9)$$

where $\xi_b \equiv \langle \dot{n}_{\alpha b} \sin\theta_b \rangle_\alpha$ is the value of $\dot{n}_\alpha \sin\theta$ at the bth bounce, averaged over the ensemble of trajectories in the frozen container. Since the distribution of this ensemble is invariant with time (by virtue of uniform distribution over the energy shell E_0), ξ_b is in fact independent of b. We will therefore write it simply as ξ.

Similarly, $c_{b,b'}$, which measures correlations in $\dot{n}_\alpha \sin\theta$ between the bth and b'th bounces, depends on b and b' only through the difference $\Delta b \equiv b' - b$, and so will be written as $c_{\Delta b}$. The double sum in Eq. 3.8 then becomes

$$\sum_{b=1}^{B}\sum_{b'=1}^{B}(c_{\Delta b}+\xi^2) = B^2\xi^2 + B\sum_{\Delta b=-B}^{B}\left(1-\frac{|\Delta b|}{B}\right)c_{\Delta b}. \tag{3.10}$$

Because of the property of mixing, $c_{\Delta b} \cong 0$ for $|\Delta b| > \nu_L$, where $\nu_L \cong t_L/\tau$. 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 Eq. 2.16. *We assume that this sum converges.* We now have, to $O(\epsilon^2)$,

$$\begin{aligned}\left\langle (E-E_0)^2\right\rangle &= 4m^2v^2\left(B^2\xi^2 + B\sum_{\Delta b=-\infty}^{+\infty} c_{\Delta b}\right)\\ &= \left(\frac{2mv}{\tau}\xi\Delta t\right)^2 + \frac{4m^2v^2}{\tau}\Delta t\sum_{\Delta b=-\infty}^{+\infty} c_{\Delta b}.\end{aligned} \tag{3.11}$$

Comparison with Eq. 3.4 yields, to $O(\epsilon^2)$,

$$g_1 = \pm\frac{2mv}{\tau}\xi + O(\epsilon^2) \tag{3.12}$$

$$g_2 = \frac{4m^2v^2}{\tau}D, \tag{3.13}$$

where

$$D \equiv \sum_{\Delta b=-\infty}^{+\infty} c_{\Delta b}. \tag{3.14}$$

We now relax the assumption made immediately after Eq. 3.7, 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. 3.12 and 3.13 will remain valid. (We have already assumed, in Section 3.2, that this more relaxed condition holds.) The justification for this assertion is similar to that presented in Chapter 2 (see the paragraph following Eq. 2.19).

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. 3.12 to

$$g_1(E, \epsilon t) = -\beta(\epsilon t)\, E + O(\epsilon^2), \tag{3.15}$$

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

$$\beta = \dot{A}/A \qquad (2d \text{ container}) \tag{3.16}$$

$$2\dot{V}/3V \qquad (3d \text{ container}), \tag{3.17}$$

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. 3.12 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. 3.13, 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 of this chapter, we get, to $O(\epsilon^2)$,

$$g_2(E, \epsilon t) = \gamma(\epsilon t)\, E^{3/2}, \tag{3.18}$$

with

$$\gamma = (8l/\pi A)\,(2m)^{1/2}\, D \qquad (2d) \tag{3.19}$$

$$(2S/V)\,(2m)^{1/2}\, D \qquad (3d), \tag{3.20}$$

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 was detailed in Section 2.4. There we found

$$g_1 = g_{11} + \frac{1}{2\Sigma}\frac{\partial}{\partial E}(g_2\Sigma), \tag{3.21}$$

where g_{11} is the $O(\epsilon^1)$ term of g_1 (given above by Eq. 3.15), and

$$\Sigma(E,\epsilon t) \equiv \frac{\partial}{\partial E}\Omega(E,\epsilon t), \tag{3.22}$$

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,

$$\Omega = 2\pi mAE \quad , \quad \Sigma = 2\pi mA. \tag{3.23}$$

In three dimensions, we get

$$\Omega = \frac{4}{3}\pi(2m)^{3/2}VE^{3/2} \quad , \quad \Sigma = 2\pi(2m)^{3/2}VE^{1/2}. \tag{3.24}$$

Using Eq. 3.21 we rewrite Eq. 3.2 as

$$\frac{\partial\eta}{\partial t} = -\frac{\partial}{\partial E}(g_{11}\eta) + \frac{1}{2}\frac{\partial}{\partial E}\Big[g_2\Sigma\frac{\partial}{\partial E}\Big(\frac{\eta}{\Sigma}\Big)\Big]. \tag{3.25}$$

Combining our results for g_{11}, g_2, and Σ with Eq. 3.25, we finally write the evolution equation for η, to $O(\epsilon^2)$, as

$$\frac{\partial\eta}{\partial t} = \beta\frac{\partial}{\partial E}(E\eta) + \frac{\gamma}{2}\frac{\partial}{\partial E}\Big(E^{3/2}\frac{\partial\eta}{\partial E}\Big) \qquad (2d) \tag{3.26}$$

or

$$\frac{\partial\eta}{\partial t} = \beta\frac{\partial}{\partial E}(E\eta) + \frac{\gamma}{2}\frac{\partial}{\partial E}\Big[E^2\frac{\partial}{\partial E}\Big(E^{-1/2}\eta\Big)\Big] \qquad (3d). \tag{3.27}$$

Eqs. 3.26 and 3.27 represent the central result of this chapter. The coefficients β and γ are given (Eqs. 3.16 and 3.19, or 3.17 and 3.20) 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, in a certain approximation, 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 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. 3.26 or 3.27 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,

$$\frac{\partial \eta}{\partial t} = \beta \frac{\partial}{\partial E}\big(E\eta\big), \tag{3.28}$$

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

$$\frac{d}{dt}\mathcal{E}(t) = -\beta(\epsilon t)\,\mathcal{E}(t) = \begin{cases} -(\dot{A}/A)\,\mathcal{E}(t) & (2d) \qquad (3.29) \\ -(2\dot{V}/3V)\,\mathcal{E}(t) & (3d). \qquad (3.30) \end{cases}$$

From this, we get $(d/dt)\,\Omega(\mathcal{E}(t), \epsilon t) = 0$ (see Eqs. 3.23 and 3.24). Eqs. 3.26 and 3.27 are therefore consistent with the adiabatic invariance of Ω.

3.5 THE QUASILINEAR APPROXIMATION

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:

$$D \cong c_0. \tag{3.31}$$

We denote this the *quasilinear approximation*, following standard usage.[22] 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. 3.31 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.

Take Eq. 3.31 to be valid. In Appendix A of this chapter we solve for c_0, obtaining

$$\begin{aligned} c_0 = \ & \tfrac{2}{3l} \oint ds \left[\dot{n}^2 - \tfrac{3\pi^2}{32}\bar{\dot{n}}^2\right] \ \equiv \frac{2}{3l} I_2(\epsilon t) \qquad (2d) \\ c_0 = \ & \tfrac{1}{2S} \oint d\sigma \left[\dot{n}^2 - \tfrac{8}{9}\bar{\dot{n}}^2\right] \ \equiv \frac{1}{2S} I_3(\epsilon t) \qquad (3d). \end{aligned} \tag{3.32}$$

Here, $\oint ds$ and $\oint d\sigma$ indicate integrals over the entire wall of the container, and $\bar{\dot{n}}$ is the average value of $\dot{n} = \dot{n}(\epsilon t)$ over the wall. Combining these results with Eqs. 3.16, 3.19, and 3.26, or Eqs. 3.17, 3.20, and 3.27, we have the simplified results

$$\frac{\partial \eta}{\partial t} = \frac{\dot{A}}{A}\frac{\partial}{\partial E}(E\eta) + \frac{8\sqrt{2m}}{3\pi A} I_2 \frac{\partial}{\partial E}\Big(E^{3/2}\frac{\partial \eta}{\partial E}\Big) \qquad (2d) \tag{3.33}$$

and

$$\frac{\partial \eta}{\partial t} = \frac{2\dot{V}}{3V}\frac{\partial}{\partial E}(E\eta) + \frac{\sqrt{2m}}{2V} I_3 \frac{\partial}{\partial E}\Big[E^2\frac{\partial}{\partial E}\Big(E^{-1/2}\eta\Big)\Big] \qquad (3d). \tag{3.34}$$

3.6 RELATION TO PREVIOUS RESULTS

In this section we show that one can consistently treat a chaotic adiabatic billiard gas as an example of a chaotic adiabatic ensemble, by treating the container as the limiting case of a smooth potential well. In Chapter 2, we obtained the following expressions for the drift and diffusion coefficients g_1 and g_2

$$g_1(E,\epsilon t) = \bar{u} + \frac{1}{2\Sigma}\frac{\partial}{\partial E}\left(\Sigma g_2\right) \tag{3.35}$$

$$g_2(E,\epsilon t) = \int_{-\infty}^{+\infty} ds\, C(s), \tag{3.36}$$

We now show that these expressions reduce, in the limit of an infinitely hard wall, to the corresponding expressions derived in Section 3.4 for the billiard gas.

We begin by recalling the definitions of $\bar{u}$ and $C(s)$. Let $\dot{H}(\mathbf{z},\epsilon t)$ be the slowly time-dependent function obtained by differentiating the Hamiltonian $H(\mathbf{z},\epsilon t)$ 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

$$\bar{u} \equiv \left\{\dot{H}_\alpha(\mathbf{z})\right\} \tag{3.37}$$

$$C(s) \equiv \left\{\left[\dot{H}_\alpha(\mathbf{z}) - \bar{u}\right] O_\alpha(s) \left[\dot{H}_\alpha(\mathbf{z}) - \bar{u}\right]\right\}, \tag{3.38}$$

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 in Chapter 2. 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. 3.4. 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

$$\dot{H} = -\dot{n}\,\hat{\mathbf{n}} \cdot \nabla V(\mathbf{q}) = -\dot{n}\,|\nabla V(\mathbf{q})|, \tag{3.39}$$

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

$$\dot{H}_\alpha = -\dot{n}_\alpha\,\hat{\mathbf{n}} \cdot \nabla V(\mathbf{q}). \tag{3.40}$$

By the assumed ergodicity of motion inside the hard-walled container (and by extension in the soft-walled container, for infinitesimal 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:

$$\bar{u} = \left\{\dot{H}_\alpha\right\} = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt\, \dot{H}_\alpha(\mathbf{z}(t)). \tag{3.41}$$

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. 3.4, is, by Eq. 3.40,

$$\int_{t_1}^{t_2} dt\, \dot{H}_\alpha(\mathbf{z}(t)) = -\dot{n}_\alpha\,\hat{\mathbf{n}} \cdot \int_{t_1}^{t_2} dt\, \nabla V(\mathbf{q}(t)). \tag{3.42}$$

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

$$\int_{t_1}^{t_2} dt\, \dot{H}_\alpha(\mathbf{z}(t)) = \dot{n}_\alpha\,\hat{\mathbf{n}} \cdot \left[\mathbf{p}(t_2) - \mathbf{p}(t_1)\right] = -2mv\dot{n}_\alpha \sin\theta. \tag{3.43}$$

Thus, Eq. 3.41 becomes

$$\bar{u} = -\frac{2mv}{\tau} \lim_{N\to\infty} \frac{1}{N} \sum_{b=1}^{N} \dot{n}_{\alpha b} \sin\theta_b, \tag{3.44}$$

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

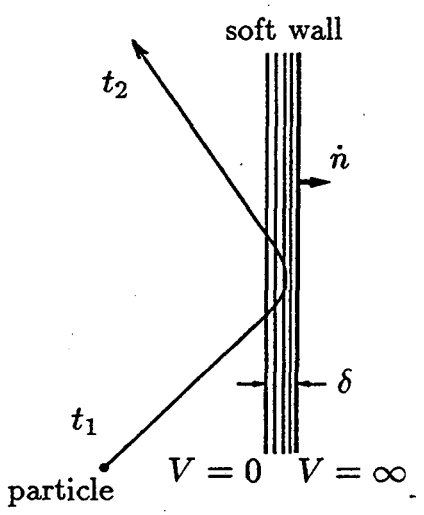

Figure 3.4: The trajectory of a particle bouncing off a wall of finite skin depth. The parallel lines represent the contours of the potential $V(\mathbf{q})$ in the vicinity of the bounce.

bouncing forever off the walls of the frozen container, which, by ergodicity, is equal to the previously defined ξ. Thus,

$$\bar{u} = -\frac{2mv}{\tau}\xi = -\beta E. \tag{3.45}$$

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

$$\left\langle \left[\dot{H}_\alpha(\mathbf{z}(t)) - \bar{u}\right]\left[\dot{H}_\alpha(\mathbf{z}(t+s)) - \bar{u}\right]\right\rangle_\alpha, \tag{3.46}$$

where $\mathbf{z}(t)$ is a trajectory evolving under H_α, and the angular brackets denote an average over a uniform distribution of such trajectories over the energy shell E. (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

$$\int_{-\infty}^{+\infty} ds\, C(s) = \lim_{T\to\infty} \frac{1}{T}\left\langle \left(\int_0^T dt \left[\dot{H}_\alpha(\mathbf{z}(t)) - \bar{u}\right]\right)^2\right\rangle. \tag{3.47}$$

Using Eqs. 3.43 and 3.45, we have

$$\int_0^T dt \left[\dot{H}_\alpha(\mathbf{z}(t)) - \bar{u}\right] = -2mv \sum_{b=1}^{N} (\dot{n}_{\alpha b} \sin\theta_b - \xi), \tag{3.48}$$

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

$$\int_{-\infty}^{+\infty} ds\, C(s) = \lim_{T\to\infty} \frac{1}{T}\left\langle \left[-2mv \sum_{b=1}^{N} (\dot{n}_{\alpha b} \sin\theta_b - \xi)\right]^2\right\rangle \tag{3.49}$$

$$= \frac{4m^2v^2}{\tau} \lim_{N\to\infty} \frac{1}{N} \sum_{b=1}^{N} \sum_{b'=1}^{N} c_{b'-b} \tag{3.50}$$

$$= \frac{4m^2v^2}{\tau} D = \gamma E^{3/2}, \tag{3.51}$$

where the steps taken are similar to those of Section 3.4.

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

$$\bar{u} \rightarrow -\beta E \tag{3.52}$$

$$\int_{-\infty}^{+\infty} ds\, C(s) \rightarrow \gamma E^{3/2}. \tag{3.53}$$

When these expressions are plugged into Eqs. 3.35 and 3.36, they give an evolution equation for $\eta(E,t)$ identical to that obtained in Section 3.4. This shows that a chaotic adiabatic billiard gas can be consistently treated as an example of a chaotic adiabatic ensemble.

(In Ref.[7], 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. 3.53.)

3.7 ONE-BODY DISSIPATION

As discussed in Refs.[10–12], 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 chapter.

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.[10,23] As pointed out in Ref.[10], 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 (perhaps the first) of deterministic friction, in which the energy of "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.[10], the wall formula is derived for this rate:

$$\frac{dE_T}{dt} = \rho\bar{v} \oint d\sigma\, \dot{n}^2. \tag{3.54}$$

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, $\bar{v}$ 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. 3.54. We will refer to this derivation as the "piston approach" to one-body dissipation.[47]

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 chapter. 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, we use the quasilinear approximation of Section 3.5. 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. 3.34 (with $\dot{V} = 0$), we have

$$\frac{dE_T}{dt} = \frac{\sqrt{2m}}{2V} I_3 \int dE \frac{\partial}{\partial E}\Big[E^2 \frac{\partial}{\partial E}\big(E^{-1/2}\eta\big)\Big]\, E, \tag{3.55}$$

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

$$\frac{dE_T}{dt} = \frac{\sqrt{2m}}{V} I_3 \int dE\ \eta\ E^{1/2}. \tag{3.56}$$

The average speed of the particles is given by

$$\overline{v} = \frac{1}{\mathcal{N}} \int dE\ \eta\ (2E/m)^{1/2}, \tag{3.57}$$

where $\mathcal{N} = \int dE\ \eta$ is the total number of particles. This enables us to rewrite Eq. 3.56 as

$$\frac{dE_T}{dt} = \frac{m\mathcal{N}}{V} \overline{v} \oint \dot{n}^2\, d\sigma, \tag{3.58}$$

which is the wall formula.

Having demonstrated that the results of the present chapter (in the simplified form of Section 3.5) agree with the wall formula, we now consider the factor $\overline{v}$ which appears in the latter. Differentiating both sides of Eq. 3.57 with respect to time, then applying Eq. 3.34, then integrating by parts twice, we obtain

$$\frac{d\overline{v}}{dt} = \frac{3}{4V} \oint \dot{n}^2\, d\sigma. \tag{3.59}$$

Eqs. 3.58 and 3.59 constitute a closed set of equations, in the sense that, if we know how the shape of the container evolves with time, then Eq. 3.59 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. 3.59, 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.

We now consider a generalization of Eqs. 3.58 and 3.59. First, note that Eq. 3.58 may be rewritten as

$$\frac{d}{dt}\overline{v^2} = \frac{2}{V}\overline{v} \oint d\sigma\, \dot{n}^2, \tag{3.60}$$

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:

$$\overline{v^n}(t) = \int dE\ \eta(E,t)\ (2E/m)^{n/2}. \tag{3.61}$$

Differentiating both sides with respect to time, applying Eq. 3.34, and integrating twice by parts yields

$$\frac{d}{dt}\overline{v^n} = \frac{n(n+2)}{4V}\overline{v^{n-1}} \oint d\sigma\, \dot{n}^2; \tag{3.62}$$

Eqs. 3.59 and 3.60 are specific examples of this general formula.

In Chapter 4, Eq. 3.62 is obtained using a generalization of the piston approach described above. A consequence of Eq. 3.62, as shown in Chapter 4, and supported by numerical simulations,[25] is that, asymptotically with time, a chaotic adiabatic billiard gas will achieve a distribution of particle velocities which has a universal form:

$$f(\mathbf{v}) \propto \exp(-v/c), \tag{3.63}$$

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.

We conclude this section by drawing attention to the fact that, elsewhere in this chapter, we have treated the changing shape of the container as externally imposed, whereas in the nuclear context it is a dynamical quantity. This calls into question the validity of applying Eq. 3.34 to the problem considered here; might not the evolution of η be affected significantly by allowing the walls to recoil? To answer briefly, we point out that the inertia associated with the collective degrees of freedom of the nucleus, while not infinite, is still much greater than that of an individual nucleon. Therefore the effects of recoil on the evolution of η should constitute a small correction, and Eq. 3.34 should remain valid to leading order. Of course, a proper treatment of this issue belongs to the study of adiabatic reaction forces; see Chapter 6 and Ref.[15].

3.8 APPENDIX A

In this Appendix we evaluate the quantities ξ and c_0, both functions of ϵt. These quantities are defined with respect to a gas of noninteracting particles evolving inside the frozen shape Sh_α, with $\alpha = \epsilon t$. The particles are assumed to share a common energy, and to be distributed uniformly within the container, with an isotropic distribution of velocities. While the definitions of ξ and c_0 involve the dynamics of these particles, our final expressions will be given solely in terms of quantities characterizing the shape of the container and its instantaneous wall velocity field. We use the following notation. $\mathcal{N}$ is the number of particles in our gas ($\mathcal{N} \gg 1$), and v is their common speed. A and l, both functions of ϵt, refer to the area and perimeter of the two-dimensional container; $\oint ds$ denotes a line integral over the entire wall. Similarly, in three dimensions, V and S refer to the volume and surface area of the container, and $\oint d\sigma$ denotes a surface integral over the wall.

Note that

$$\dot{A} \equiv dA/dt = \oint ds\, \dot{n} \qquad (2d)$$
$$\dot{V} \equiv dV/dt = \oint d\sigma\, \dot{n} \qquad (3d), \tag{3.64}$$

where $\dot{n} = \dot{n}(\epsilon t)$ is the wall velocity field describing the evolution of $\mathrm{Sh}(\epsilon t)$.

The quantity ξ was defined in Section 3.4 as

$$\xi = \xi_b = \left\langle \dot{n}_{\alpha b} \sin\theta_b \right\rangle, \tag{3.65}$$

the average value of $\dot{n}_\alpha \sin\theta$ over the bth bounce of all particles in the gas. As mentioned, the invariance with time of the distribution of these particles implies that ξ is independent of b, and therefore we may alternatively write it as

$$\xi = \left\langle\left\langle \dot{n}_\alpha \sin\theta \right\rangle\right\rangle, \tag{3.66}$$

where the double angular brackets denote an average over *all* bounces of all the particles of the gas. In this form, ξ becomes easy to evaluate.

To evaluate ξ in two dimensions, first consider a small segment ds of the wall of the container. The rate r at which this segment is being struck by particles making an angle of collision between θ and $\theta + d\theta$ is given by

$$r = j\, ds\, \sin\theta, \tag{3.67}$$

where $j = (d\theta/2\pi)(\mathcal{N}v/A)$ is the current density of particles bombarding ds from this range of angles, and $\sin\theta$ is a flux factor. The quantity $\xi = \langle\langle \dot{n}_\alpha \sin\theta \rangle\rangle$ is then the weighted average $\int r\,(\dot{n}_\alpha \sin\theta)\,/\,\int r$, where the integral is over the entire wall, and over θ from 0 to π. This yields

$$\xi = \frac{\pi \dot{A}}{4l}. \tag{3.68}$$

The quantity $c_0 = c_{b,b} = \langle(\dot{n}_{\alpha b} \sin\theta_b - \xi_b)^2\rangle$ is, like ξ, independent of b, and may be written as

$$c_0 = \left\langle\left\langle (\dot{n}_\alpha \sin\theta - \xi)^2 \right\rangle\right\rangle$$

$$= \int r\,(\dot{n}_\alpha \sin\theta - \xi)^2 \Big/ \int r, \tag{3.69}$$

which reduces to

$$c_0 = \frac{2}{3l} \oint ds \left[\dot{n}^2 - \frac{3\pi^2}{32}\bar{\dot{n}}^2\right], \tag{3.70}$$

where $\bar{\dot{n}} \equiv (1/l) \oint ds\, \dot{n} = \dot{A}/l$ is the average value of $\dot{n} = \dot{n}(\epsilon t)$ over the wall of the container. (Since the final expression for c_0 no longer involves the dynamics of particles in the frozen container, our notation has reverted from $\dot{n}_\alpha$ to $\dot{n}(\epsilon t)$.)

In three dimensions, consider a small patch $d\sigma$ on the surface of the container. Let r be 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 by Fig. 3.3. This rate is given by $r = j\, d\sigma\, \sin\theta$, where

$$j = \frac{d\Omega}{4\pi}\frac{\mathcal{N}}{V}v = \frac{\cos\theta\, d\theta\, d\phi}{4\pi}\frac{\mathcal{N}}{V}v. \tag{3.71}$$

$\xi = \langle\langle \dot{n}_\alpha \sin\theta \rangle\rangle$ is again equal to $\int r\,(\dot{n}_\alpha \sin\theta)/\int r$, only now the integral is over the entire surface area of the wall, θ from 0 to $\pi/2$, and ϕ from 0 to 2π. This yields

$$\xi = \frac{2\dot{V}}{3S}. \tag{3.72}$$

Similarly,

$$\begin{aligned} c_0 &= \int r\,(\dot{n}_\alpha \sin\theta - \xi)^2 \Big/ \int r \\ &= \frac{1}{2S} \oint d\sigma \left[\dot{n}^2 - \frac{8}{9}\bar{\dot{n}}^2\right], \end{aligned} \tag{3.73}$$

where $\bar{\dot{n}} = (1/S) \oint d\sigma\, \dot{n} = \dot{V}/S$ is again the average of $\dot{n}(\epsilon t)$ over the wall.

3.9 APPENDIX B

In this Appendix we solve for τ, the average time between the bounces of a particle of speed v moving chaotically inside a frozen container. Filling the container with a large number $\mathcal{N}$ of such particles, the total rate at which the walls of the

container are being struck is $R = \mathcal{N}/\tau$. Alternatively, $R = \int r$, in the notation of Appendix A. Setting these two equal yields

$$\begin{aligned} \tau &= \frac{\pi A}{lv} \qquad (2d) \\ \tau &= \frac{4V}{Sv} \qquad (3d). \end{aligned} \tag{3.74}$$

3.10 APPENDIX C

In this Appendix we consider an example of a time-dependent billiard satisfying the various conditions of the present chapter.

It is possible to rigorously establish the property of global chaos for certain two-dimensional billiard systems.[26] Two of the best-known examples are the Sinai billiard[27] and the Bunimovich stadium.[28] However, in both of these cases there exists a continuous family of periodic trajectories, which, as argued in Ref.[7] (see also references therein, and Ref.[29]), implies that the sum $\sum_{-\infty}^{+\infty} c_{\Delta b}$ diverges. These systems therefore violate the added assumption made in Section 3.4 of this chapter.

We now propose the "three-leaf clover", shown in Fig. 3.5, as a family of billiard systems satisfying all the conditions of the present chapter. Varying the parameter $\alpha = R/r$ gives a continuous family of shapes Sh_α. By direct application of Theorem 1 of Ref.[26], one can establish the property of global chaos for any of these shapes. Furthermore, it is fairly straightforward to prove that, for $\alpha \geq 1$, all periodic orbits inside Sh_α are isolated, i.e. no continuous families exist. Thus, by filling such a clover with a gas of noninteracting particles, then allowing R and r to change slowly with time, always maintaining $\alpha \geq 1$, one has an example of a two-dimensional chaotic adiabatic billiard gas. (For another example, see the modified Sinai billiard in Ref.[7].)

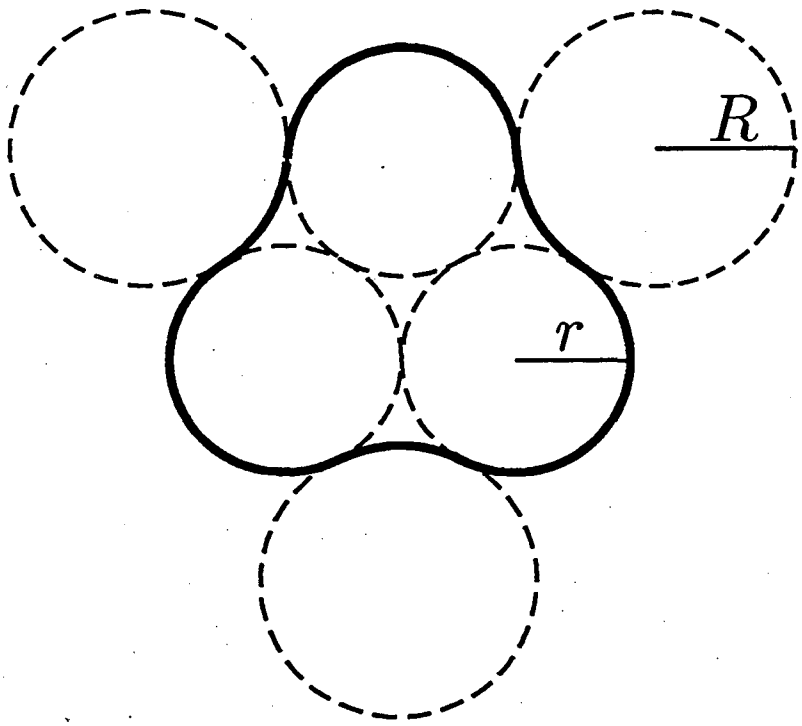

Figure 3.5: The three-leaf clover (heavy outline), a two-dimensional billiard system whose boundary consists of the arcs of six circles. The common radius of the outer circles is R; that of the inner ones is r. By varying $\alpha = R/r$, one has a continuous family of such shapes, all globally chaotic. For $\alpha \geq 1$, all periodic orbits are isolated.

Chapter 4

A Universal Asymptotic Velocity Distribution for a Three-Dimensional Billiard Gas

4.1 INTRODUCTION

In Chapter 3 we obtained a diffusion equation for energy evolution in a chaotic adiabatic billiard gas. In the present chapter we study the same problem from a different point of view. The approach which we adopt here is the one originally used in deriving the *wall formula*[10] for one-body dissipation in nuclear dynamics. One-body dissipation arises in the *independent particle model* of nuclear dynamics, which is based on an explicit separation between the collective degrees of freedom of a nucleus, and the degrees of freedom of the individual nucleons. Investigations into one-body dissipation[10,11,30–46] have accumulated evidence that a transition from ordered to chaotic nucleonic motion is accompanied by a transition in the collective properties of nuclei from those of an elastic solid to those of a very viscous fluid (hence the interest that simple models like the chaotic adiabatic billiard gas hold

for nuclear dynamics). As in previous studies involving the wall formula, we restrict ourselves to three dimensions.

The two primary results of this chapter are, first, an extension of the validity of the wall formula to the long-time regime, and second, a prediction regarding the asymptotic distribution of velocities for a three-dimensional chaotic adiabatic billiard gas.

4.2 THE WALL FORMULA

It was shown in Ref.[10] that, under certain assumptions, the rate of change of the energy E of such a gas is given by the *wall formula* for nuclear dissipation:

$$\frac{dE}{dt} = \rho\overline{v} \oint \dot{n}^2 \, d\sigma, \tag{4.1}$$

where ρ is the mass density of the gas, $\overline{v}$ the mean speed of the gas particles and $\dot{n}$ 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 v^2, Eq. 4.1 may be re-written as

$$\frac{d\overline{v^2}}{dt} = \frac{2\overline{v}}{V} \oint \dot{n}^2 \, d\sigma, \tag{4.2}$$

where V is the volume of the container, equal to M/ρ. 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. 4.2 by itself is not able to predict the long term evolution of the energy. However, in Chapter 3 we were able to derive a "second wall formula",

$$\frac{d\overline{v}}{dt} = \frac{3}{4V} \oint \dot{n}^2 \, d\sigma, \tag{4.3}$$

from which we get

$$\overline{v} = \overline{v}_0\Big(1 + \frac{3}{4}I(t)\Big), \tag{4.4}$$

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

$$I(t) = \frac{1}{\overline{v}_0 V} \int_0^t dt' \oint \dot{n}^2 \, d\sigma, \tag{4.5}$$

and where the subscript 0 denotes initial value.

Multiplying Eq. 4.3 by $2\overline{v}$ we also find

$$2\overline{v}\frac{d\overline{v}}{dt} \equiv \frac{d\overline{v}^2}{dt} = \frac{3\overline{v}}{2V} \oint \dot{n}^2 \, d\sigma, \tag{4.6}$$

so that, using Eq. 4.2 we obtain

$$\frac{d\overline{v^2}}{dt} = \frac{4}{3}\frac{d\overline{v}^2}{dt}, \tag{4.7}$$

i.e.

$$\overline{v^2} - \overline{v_0^2} = \frac{4}{3}\left(\overline{v}^2 - \overline{v}_0^2\right). \tag{4.8}$$

It follows that the time evolution of the relative energy is given, for arbitrarily long times, by the following closed formula (consistent with Ref.[12]):

$$\begin{aligned} \frac{E}{E_0} &= \frac{\overline{v^2}}{\overline{v_0^2}} = 1 + \frac{4}{3}\left[\overline{v}_0^2\left(1 + \frac{3}{4}I\right)^2 - \overline{v}_0^2\right]/\overline{v_0^2} \\ &= 1 + C\left(I + \frac{3}{8}I^2\right), \end{aligned} \tag{4.9}$$

where C is a constant given by $2\overline{v}_0^2/\overline{v_0^2}$. From Eq. 4.8 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:

$$\overline{v^2} \to \frac{4}{3}\overline{v}^2. \tag{4.10}$$

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 proceed to generalize the wall formula, obtaining an expression for the rate

of change of an arbitrary moment $\overline{v^n}$. We then deduce that, asymptotically, all the resulting moments agree with the moments of an exponential function!

The derivation of the generalized wall formula for $\overline{v^n}$ proceeds along the lines of the derivation of $\overline{v^2}$ in Ref.[10]. Consider a gas of non-interacting particles characterized by an initial isotropic velocity distribution $f(v)$, normalized so that

$$\int_0^\infty 4\pi\, dv\, v^2 f(v) = 1. \tag{4.11}$$

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. Fig.4.1 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 Δt 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 ν is the number density of the undisturbed gas. Hence the number of particles colliding

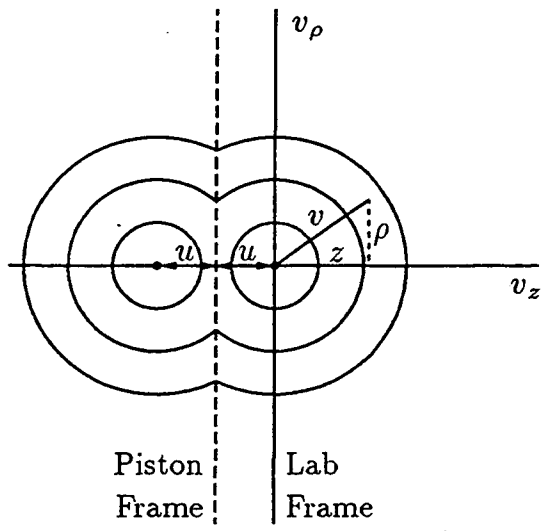

Figure 4.1: The appearance of contour lines of the velocity distribution function for a gas in the vicinity of a piston moving with speed u towards the gas. Here z and ρ stand for v_z and v_ρ, the components of the particle's velocity $\mathbf{v}$ along the $z-$ and $\rho-$directions, ρ being the radial distance from the axis of the axially symmetric velocity-space distribution.

with the piston in time Δt, whose velocity components are restricted to lie between ρ 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

$$\nu\Delta\sigma\Delta t(u+z)f(v)2\pi\rho\, d\rho\, dz. \tag{4.12}$$

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

$$\Delta v = v_{\text{new}} - v_{\text{old}} = \sqrt{\rho^2 + (z+2u)^2} - \sqrt{\rho^2 + z^2}, \tag{4.13}$$

and the effect on the nth power of the speed is

$$\begin{aligned} \Delta v^n &= v_{\text{new}}^n - v_{\text{old}}^n = \left[\rho^2 + (z+2u)^2\right]^{n/2} - \left[\rho^2 + z^2\right]^{n/2} \\ &= 2nv^{n-2}zu + 2\left[nv^{n-2} + n(n-2)v^{n-4}z^2\right]u^2 + \cdots, \end{aligned} \tag{4.14}$$

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 Δv^n by Eq. 4.12, integrating over ρ from 0 to ∞,

over z from $-u$ to ∞, and dividing by Δt gives the rate of increase of the summed nth powers of v for the particles in the cylinder: (the sum is over particles, not n)

$$\frac{d}{dt}\sum v^n = \nu \quad \Delta\sigma \int_{z=-u}^{\infty} dz \int_{\rho=0}^{\infty} d\rho\, \rho 4\pi f(v) \\ \times \quad \left[nv^{n-2}z^2u + \left(2nv^{n-2}z + n(n-2)v^{n-4}z^3\right)u^2 + \cdots\right]. \quad (4.15)$$

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

$$\frac{d}{dt}\sum v^n = \quad \nu \quad \Delta\sigma \int_{z=-u}^{\infty} dz \int_{v=|z|}^{\infty} dv\, v 4\pi f(v) \\ \times \quad \left[nv^{n-2}z^2u + \left(2nv^{n-2}z + n(n-2)v^{n-4}z^3\right)u^2\right]. \quad (4.16)$$

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^2. This leaves an expression for $(d/dt)\sum v^n$ identical with Eq. 4.16, 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

$$\frac{d}{dt}\sum v^n = \nu\Delta\sigma \int_{z=0}^{\infty} dz\, z 4\pi f(z)\left[nz^{n-2}\frac{z^3}{3}u + \left(2nz^{n-2}\frac{z^2}{2} + n(n-2)z^{n-4}\frac{z^4}{4}\right)u^2\right]. \quad (4.17)$$

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:

$$\begin{aligned}\frac{d}{dt}\sum v^n &= \nu\Delta\sigma\left[\frac{1}{3}nu\overline{v^n} + \left(n\overline{v^{n-1}} + \frac{1}{4}n(n-2)\overline{v^{n-1}}\right)u^2\right] \\ &= \nu\Delta\sigma\left[\frac{1}{3}n\overline{v^n}u + \frac{1}{4}n(n+2)\overline{v^{n+1}}u^2\right], \end{aligned} \quad (4.18)$$

where

$$\overline{v^n} = \int_0^{\infty} 4\pi\, dv\, v^2 v^n\, f(v). \quad (4.19)$$

We now apply this "piston formula" to the case of a container whose surface elements $d\sigma$ 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 nth power 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^n, i.e. $d\overline{v^n}/dt$, is obtained by dividing Eq. 4.18 by N. Since $N/\nu = V$, the container's volume, we find

$$\frac{d\overline{v^n}}{dt} = \frac{1}{V}\oint d\sigma \left[-\frac{1}{3}n\overline{v^n}\dot{n} + \frac{1}{4}n(n+2)\overline{v^{n-1}\dot{n}^2}\right]. \tag{4.20}$$

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

$$\frac{d\overline{v^n}}{dt} = \frac{1}{4}n(n+2)\overline{v^{n-1}}\frac{1}{V}\oint \dot{n}^2 d\sigma. \tag{4.21}$$

For $n = 2$ we obtain the standard wall formula in the form of Eq. 4.2. For $n = 1$ we recover the "second wall formula" of Chapter 3 (or Eq. 4.3), derived here in a different way. We now proceed to use Eq. 4.21 to derive the asymptotic form of the velocity distribution $f(v)$.

4.3 ASYMPTOTIC VELOCITY DISTRIBUTION

Combining Eqs. 4.3 and 4.21 we have

$$\frac{d\overline{v^n}}{dt} = \frac{1}{3}n(n+2)\overline{v^{n-1}}\frac{d\overline{v}}{dt}. \tag{4.22}$$

For $n = 2$ we find

$$\frac{d\overline{v^2}}{dt} = \frac{4\times 2}{3}\overline{v}\frac{d\overline{v}}{dt} = \frac{4\times 2}{3}\frac{1}{2}\frac{d\overline{v}^2}{dt}, \tag{4.23}$$

which is the same as Eq. 4.7 and which leads asymptotically to

$$\overline{v^2} \to \frac{4\times 2}{3}\frac{1}{2}\overline{v}^2. \tag{4.24}$$

For $n = 3$ we have

$$\frac{d\overline{v^3}}{dt} = \frac{5\times 3}{3}\overline{v^2}\frac{d\overline{v}}{dt} \rightarrow \frac{5\times 3}{3}\frac{4\times 2}{3}\frac{1}{2}\overline{v}^2\frac{d\overline{v}}{dt} = \frac{5\times 3}{3}\times\frac{4\times 2}{3}\times\frac{1}{2}\times\frac{1}{3}\frac{d\overline{v}^3}{dt}, \quad (4.25)$$

thus

$$\overline{v^3} \rightarrow \frac{5\times 3}{3}\times\frac{4\times 2}{3}\times\frac{1}{2}\times\frac{1}{3}\overline{v}^3. \quad (4.26)$$

For general n we have, by induction,

$$\overline{v^n} \rightarrow \frac{(n+2)n}{3}\frac{(n+1)(n-1)}{3}\frac{n(n-2)}{3}\cdots\frac{4\times 2}{3}\times\frac{1}{2}\times\frac{1}{3}\times\frac{1}{4}\cdots\frac{1}{n}\overline{v}^n. \quad (4.27)$$

It follows that

$$\frac{\overline{v^n}}{\overline{v}^n} \rightarrow \frac{(n+2)!}{2\times 3^n}. \quad (4.28)$$

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

$$\frac{\overline{v^n}}{\overline{v}^n} = \frac{\int_0^\infty dv\, v^{n+2}e^{-v/c}/\int_0^\infty dv\, v^2e^{-v/c}}{(\int_0^\infty dv\, v^3e^{-v/c}/\int_0^\infty dv\, v^2e^{-v/c})^n} = \frac{(n+2)!}{2\times 3^n}. \quad (4.29)$$

This shows that, under the explicit and implicit assumptions made in arriving at Eq. 4.28, the asymptotic velocity distribution $f(v)$ for particles bouncing about in an irregular, volume-conserving, time-dependent three-dimensional container is an exponential. The time dependence of the range c of the exponential, related to $\overline{v}$ by $c = \frac{1}{3}\overline{v}$, is given by Eq. 4.4.

4.4 DISCUSSION

We end with a few brief comments regarding two of the assumptions that went into deriving the results of this chapter. The first concerns the slowness of the wall velocity $\dot{n}$ compared to the particle speeds. This is not as serious a limitation as it may at first seem, since as long as the particle velocities increase monotonically with time, they will eventually become larger than the wall velocities and the approximation $|\dot{n}| \ll \overline{v}$ will automatically continue to improve with time, becoming virtually perfect asymptotically.

A statistical argument may be made for the assumption that the particle speeds do indeed increase monotonically: we may think of the walls of the container as being a dynamical quantity (following some unspecified set of equations of motion) whose evolution has been coupled to the degrees of freedom of the particles. Since, however, we are ignoring the recoil of the walls at collisions with the particles, effectively the inertia of the walls is infinite, and hence the energy content of the moving walls is infinite. Thinking in terms of the particles striving to attain thermal equilibrium with the walls, we conclude that they will never do so, and will continue to gain energy monotonically.

The assumption that the average particle speed grows monotonically is supported as well by a consideration of the limit of very *large* piston speeds. Suppose the speed of a piston is greater than that of any of the particles. Then 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. Hence the average particle speed certainly increases in this limit.

(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, as well as contrived situations where the container's deformations are continuously speeded up so that the approximation $\overline{v} \gg |\dot{n}|$ is never satisfied.)

The other assumption underlying the present analysis concerns the application of the piston formula, Eq. 4.18, derived for a semi-infinite volume of gas, with the particles initially isotropic in velocity space, to the surface elements of a finite container. (For the derivation of the original piston formula see Ref.[47].) 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 with an isotropic velocity dis-

tribution. Formally, this assumption is equivalent to the *quasilinear approximation* of Chapter 3. More intuitively, the assumption demands that somehow the shape of the container and the way in which it is changing combine to very effectively randomize the motion of the particles. It is not enough to simply assume that the frozen dynamics is chaotic, since even in that case if we endow the container with purely translational motion, there will be no continual gain in the energies of the particles. The precise, mathematically rigorous specification of when this hypothesis holds and when it fails could turn out to be a difficult problem in theoretical dynamics.

Finally, 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 result concerning the asymptotic distribution of particle speeds 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 (Ref.[43]).

Chapter 5

Chaotic Adiabatic Energy Diffusion and the Fermi Mechanism

5.1 INTRODUCTION

In Chapters 2 and 3 we developed the Fokker-Planck approach to the study of energy diffusion in chaotic adiabatic systems. In this chapter we apply this approach to a model which depicts the mechanism proposed by Fermi[48] to explain the origin of cosmic ray energies. The *Fermi mechanism* posits that cosmic rays — protons, alpha particles, and heavier nuclei which exist in the interstellar regions of the galaxy — are accelerated to tremendous energies by repeated scattering off slowly moving magnetic clouds which also inhabit the interstellar space. In the model which we will study here, the cosmic rays are an ensemble of particles evolving under a slowly time-dependent Hamiltonian created by the magnetic clouds. The goal of our analysis is an evolution equation for the cosmic ray energy spectrum.

This chapter is organized as follows. In Section 5.2, we review the Fermi mech-

anism, then we introduce a specific model depicting this mechanism in Section 5.3. We analyze this model in Section 5.4, obtaining a general equation governing the cosmic ray energy spectrum. In Section 5.5, we briefly discuss what happens if we allow for the injection and removal of particles. In Section 5.6, we consider in some detail a particular version of our model, which ties in with previous work. Finally, we discuss in Section 5.7 how the analysis in this chapter fits into the more general framework developed in Chapter 2, and in Section 5.8 we end with some general remarks regarding the Fermi mechanism.

5.2 THE FERMI ACCELERATION MECHANISM

Cosmic rays are observed to have very high energies — up to 10^{20}eV — with a spectrum roughly obeying an inverse power law. To account for the origin of cosmic ray energies, Fermi[48] proposed a mechanism by which

> "the main process of acceleration is due to the interaction of cosmic particles with wandering magnetic fields which ... occupy the interstellar spaces."

Fermi's simple and ingenious idea was to treat the wandering magnetic clouds as large, slowly moving objects off which the cosmic rays scatter elastically, as in Fig.5.1. (Collisions between the particles themselves are rare enough to be ignored.) This picture immediately suggests an explanation for the huge energies achieved by cosmic rays:

> "ultimately statistical equilibrium should be established between the degrees of freedom of the wandering fields and the degrees of freedom of the particle[s]. Equipartition evidently corresponds to an unbelievably high energy."

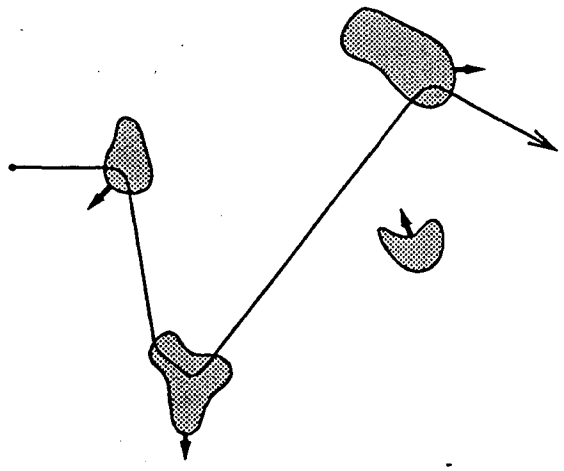

Figure 5.1: The Fermi mechanism: a cosmic particle (bullet) scattering elastically off slowly moving magnetic clouds (shaded). The particle accelerates as it tries to achieve equipartition of energy with the clouds.

Thus, the process of cosmic ray acceleration is essentially that of a system persistently striving toward statistical equilibrium. However, since the system is not closed — new cosmic rays are constantly being produced, and existing ones removed (e.g. by absorption processes) — what results is not a true equipartition of energy, but rather a steady-state situation, in which the production, acceleration, and removal of particles balance to give a time-independent spectrum of energies.

Fermi went on to perform a back-of-the-envelope evaluation of the proposed scenario. First, picturing the scatterers as "reflecting obstacles" (for purposes of a simple estimate), he argued that the average energy gained during a collision will be proportional to the energy of the particle at the time of collision. This results in a particle energy which, on average, grows exponentially with number of collisions, and therefore, in the case of ultra-relativistic (UR) particles, exponentially with time. Next, Fermi assumed that the principal mechanism for the removal of a particle from the system is its eventual absorption by other nuclear matter in the galaxy. For UR particles, the probability per unit time for such an event is independent of particle energy, implying exponential decay of these particles from the system. Fermi finally showed that the combination of these two factors —

exponential growth of energy and exponential decay of particles — produces an inverse power law spectrum of particle energies.

Davis[49] later argued that, alongside the average *drift* (growth) in particle energies studied by Fermi, one ought also to include the effect of the *diffusion* of particle energies, since during collision with a scatterer a particle may either gain or lose energy, albeit with a preference for the former. Davis considered a general diffusion (Fokker-Planck) equation for the distribution of particle energies, using a logarithmic-energy axis, then examined the consequences of various choices for the values of the drift and diffusion coefficients, D_ϵ and $D_{\epsilon\epsilon}$, respectively. In the case when both coefficients are constant, a power law spectrum emerges. (It is simple to show that a constant drift coefficient on a $\log E$ axis translates into a drift which is proportional to energy on an energy axis; a constant diffusion coefficient becomes one proportional to E^2. The case considered by Fermi — drift $\propto E$, no diffusion — therefore corresponds to $D_\epsilon = \text{const.}$, $D_{\epsilon\epsilon} = 0$, in Davis's formulation.)

Like Davis, we will use a Fokker-Planck equation to describe the acceleration of particles by the magnetic clouds (although we will employ an ordinary energy axis rather than a $\log E$ axis). We will derive both the drift and diffusion coefficients which specify this equation. Our result will be an explicit description of the acceleration process.

5.3 A SIMPLE MODEL

The model which we will analyze in detail is a fairly literal depiction of Fermi's original suggestion: the cosmic rays are a gas of relativistic particles sharing space with a collection of slowly moving, massive scatterers (the wandering magnetic fields). The particles do not interact with one another, but bounce off the moving scatterers; the latter therefore act simply as agents which continually "stir up" the

gas of cosmic rays, to ever higher energies. The collisions are elastic, but otherwise quite general; in particular, we are not assuming (as did Fermi in deriving an inverse power law spectrum) that they may be approximated as reflections off hard surfaces, although we will investigate this special case.

As mentioned, the evolution of cosmic ray energies can be discussed in terms of a continual approach toward statistical equilibrium, with the particles accelerating as they strive for equipartition of energy with the magnetic clouds. We want to obtain as explicit a description as possible of this process, within the framework of a statistical treatment. Thus, without requiring the exact trajectories of individual scatterers, we aim to describe the evolution of cosmic ray energies in terms of *average* quantities associated with the motion of the scatterers and with the collision mechanism.

In the spirit of a statistical treatment, we assume a great number of scatterers (not necessarily identical), distributed uniformly throughout a closed volume V, with an isotropic distribution of slow velocities. Assume that the positions, orientations, and velocities of the scatterers are assigned randomly, with no correlations between different scatterers, or among the position, orientation, and velocity of a single scatterer.

The assumption of no correlations between scatterers implies that none exist in the sequence of incremental energy changes suffered by a particle as it bounces among the scatterers. In other words, the energy shift at a particular collision is independent of the ones that came before, except insofar as it is a function of the particle energy itself.

The picture of a great many scatterers, distributed throughout the entire volume and moving in all directions, strongly suggests that the distribution of the cosmic particles themselves, at least in a steady-state situation, will also be uniform throughout the empty space between the scatterers, and that their velocities

will be distributed isotropically. We assume this to be the case.

Finally, we assume that the collisions are essentially instantaneous: the duration of interaction is negligible in comparison with the time between collisions. For the case of reflection off hard-walled scatterers, this is automatically satisfied. Since, however, we are considering more general elastic collisions, we explicitly assume that only a negligible fraction of space is occupied by the scatterers.

5.4 ANALYSIS — A DIFFUSION EQUATION

In a steady-state situation, the continual stirring up of the particles coexists with a mechanism for inserting particles into the system, and another for their removal, the three processes balancing to maintain a time-independent spectrum of energies. In our analysis of the simple model described above, we will first consider only the acceleration mechanism, i.e. the scattering of the particles off the moving fields, without creation and destruction of particles. We will derive an evolution equation for the spectrum of particle energies. This will be a relativistic equation, with well-defined ultra- and non-relativistic limits. We will then add terms to this equation to account for the addition and removal of particles.

We thus begin by posing the following question. Given a gas of mutually non-interacting relativistic particles sharing a finite volume of space with a collection of slowly moving scatterers, how does the distribution of particle energies, $\eta(E,t)$, evolve with time?

We analyze this question within the formalism of Hamiltonian dynamics, with the scatterers creating a time-dependent potential. This can be pictured by imagining that the potential energy is zero nearly everywhere in space, with the exceptions being small "pockets" of non-zero potential, independently undergoing translational motion at slow, constant velocities. We ignore the recoil of the scatterers during

their collisions with the particles. The Hamiltonian itself (Eq. 5.1 below) governs the motion of a single relativistic particle within this field of scatterers; thus our gas of cosmic rays is an ensemble of trajectories evolving under a common, time-dependent Hamiltonian. (In the Appendix of this chapter we generalize this model in two ways: first, we do not restrict the interaction Hamiltonian to be of the kinetic + potential form; second, we allow for the rotation of scatterers.)

The Hamiltonian governing the trajectories in relativistic phase space is given by

$$H(\mathbf{r}, \mathbf{p}, t) = (p^2 + m^2)^{1/2} + U(\mathbf{r}, \epsilon t). \tag{5.1}$$

m is the particle mass, U is the time-dependent potential created by the collection of slowly moving scatterers, ϵ is, as throughout this Thesis, a formally small dimensionless parameter emphasizing this slowness, and we are using units in which $c = 1$. We will work to leading non-zero order in ϵ.

Consider now a single particle whose trajectory in relativistic phase space we denote by $\mathbf{z}(t)$, where $\mathbf{z} = (\mathbf{r}, \mathbf{p})$. We are interested in the evolution of this particle's energy. By Hamilton's equations, the rate of change of this energy, dH/dt, is given by the function $\partial H/\partial t$, evaluated along the trajectory $\mathbf{z}(t)$. Since the particle spends most of its existence in the empty space between scatterers, this function will have, roughly, the appearance shown in Fig.5.2, with the "blips", where the energy of the cosmic ray changes, corresponding to collisions with the magnetic clouds. We picture this process in terms of the particle performing a random walk along the energy axis, with steps determined by the sequence of collisions with the scatterers. As in Chapters 2 and 3, the notion of a random walk along the energy axis suggests a Fokker-Planck equation for the distribution of energies, $\eta(E, t)$, of an ensemble of such particles:

$$\frac{\partial \eta}{\partial t} = -\frac{\partial}{\partial E}(g_1 \eta) + \frac{1}{2}\frac{\partial^2}{\partial E^2}(g_2 \eta). \tag{5.2}$$

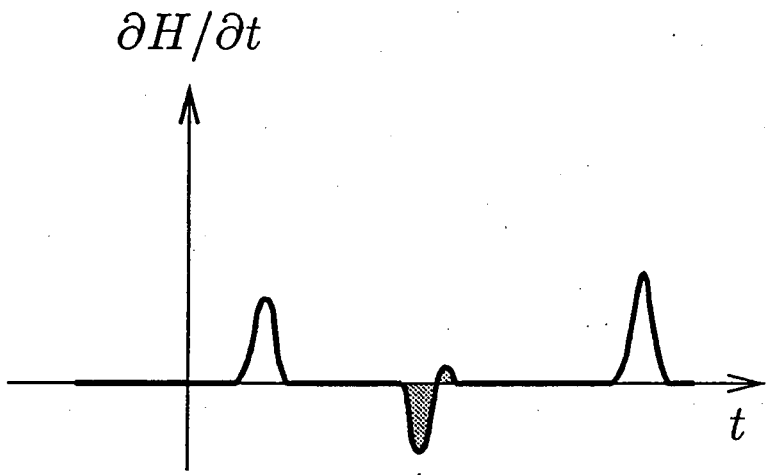

Figure 5.2: The rate of change of a particle's energy as it collides with the slowly moving scatterers, given by the value of $\partial H/\partial t$ along the phase space trajectory. The "blips" in this function occur at the collisions. (The width of these blips has been exaggerated.) The area under a blip (shaded) gives the net change in energy at a single collision.

We first solve for the diffusion coefficient g_2, then use that result to obtain the drift coefficient g_1.

Because we have assumed no correlations between successive collisions of the cosmic rays off the magnetic clouds, the diffusion coefficient is simply

$$g_2 = \langle (\Delta H)^2 \rangle / \tau, \tag{5.3}$$

where $\langle (\Delta H)^2 \rangle$ is the mean square value of the change in particle energy during a collision with a scatterer, and τ is the average time between collisions. (Strictly speaking, we should use the variance in ΔH rather than simply the mean square. However, while in Eqs. 5.4 to 5.7 below we find $\langle (\Delta H)^2 \rangle \sim \epsilon^2$, a similar analysis shows that $\langle \Delta H \rangle^2$ is zero at order ϵ^2, hence to leading order the variance and the mean square are the same.) Both $\langle (\Delta H)^2 \rangle$ and τ are functions of the energy of the

particle. Let us solve for these quantities.

The change in particle energy during a collision occurring between times t_1 and t_2 is given by

$$\Delta H = \int_{t_1}^{t_2} dt \, \frac{\partial H}{\partial t}(\mathbf{z}(t), t). \tag{5.4}$$

The local time-dependent potential created by the scatterer in question has the form $\tilde{U}(\mathbf{r} - \mathbf{R}(\epsilon t))$, where $\tilde{U}$ gives the shape of the potential associated with this scatterer, and $\mathbf{R}(\epsilon t)$ is its slowly time-dependent position: the scatterer moves at a constant velocity $\mathbf{W}$, proportional to ϵ. Thus, Eq. 5.4 becomes

$$\Delta H = -\mathbf{W} \cdot \int_{t_1}^{t_2} dt \, \nabla \tilde{U}(\mathbf{r} - \mathbf{R}), \tag{5.5}$$

where $\mathbf{r} = \mathbf{r}(t)$ is now the path followed by the particle during the collision. Since we are working to leading order in ϵ, we may treat $\mathbf{R}$ as constant during the collision, replacing the true trajectory of the particle bouncing off the slowly moving scatterer with the "frozen" trajectory obtained by holding the scatterer fixed during the collision. (This is not to say that a particle changes its energy during a collision with an immobile scatterer — it does not — but the path taken is nearly identical to the true one, for ϵ sufficiently small, and thus may be used in evaluating the above integral.)

Now, the time integral of $-\nabla \tilde{U}$ over the collision is equal to the net change in the relativistic momentum $\mathbf{p}$ suffered by the particle. Hence, letting $\Delta \mathbf{p} = \mathbf{p}(t_2) - \mathbf{p}(t_1)$ denote this change, we have

$$\begin{aligned} \Delta H &= \mathbf{W} \cdot \Delta \mathbf{p} \\ &= 2Wp \cos\beta \sin\frac{\alpha}{2}, \end{aligned} \tag{5.6}$$

where $p = |\mathbf{p}(t_1)| = |\mathbf{p}(t_2)|$ (using the frozen trajectory), α is the angle between the initial and final momenta, and β is the angle between $\mathbf{W}$ and $\Delta \mathbf{p}$. Squaring this term and averaging gives

$$\langle (\Delta H)^2 \rangle = 4p^2 \langle W^2 \cos^2\beta \sin^2\frac{\alpha}{2} \rangle. \tag{5.7}$$

The average here is over all possible collisions occurring at the given energy, $E = (p^2 + m^2)^{1/2}$ (that is, over the distribution of collisions obtained by immersing the *immobile* scatterers in a uniform, isotropic sea of monoenergetic particles.)

From our assumption that the scatterers' velocities are assigned randomly, uncorrelated with their positions and orientations, it follows that the angle by which a particle is deflected during a particular collision, calculated under the approximation that the scatterer is essentially immobile, will be independent of the velocity assigned to the scatterer; that is, α is uncorrelated with $\mathbf{W}$ and β. With the further assumption that the distribution of velocities $\mathbf{W}$ is isotropic, we get

$$\langle W^2 \cos^2\beta \sin^2\frac{\alpha}{2}\rangle = \langle W^2\rangle\langle\cos^2\beta\rangle\langle\sin^2\frac{\alpha}{2}\rangle = \frac{1}{3}\langle W^2\rangle K, \tag{5.8}$$

where $\cos^2\beta$ has been averaged over the entire 4π of solid angle, and $K = \langle\sin^2\alpha/2\rangle$ is simply the average value of $\sin^2\alpha/2$ over all possible collisions for a particle of energy E. Note that K is generally a function of particle energy, $K = K(E)$, although later we will consider two examples for which K is independent of E.

The quantity τ, the average time between collisions, may be written as

$$\tau = L/v = LE/p, \tag{5.9}$$

where L is the average distance traversed between collisions, and $v = p/E$ is the speed of a particle with relativistic momentum p and energy E. Eq. 5.3 thus becomes

$$g_2(E) = \frac{4}{3}\frac{\langle W^2\rangle}{L}K\frac{p^3}{E}, \tag{5.10}$$

with $p^2 = E^2 - m^2$.

It remains to calculate the drift coefficient g_1. From Chapter 2,

$$g_1 = \bar{u} + \frac{1}{2\Sigma}\frac{\partial}{\partial E}(\Sigma g_2), \tag{5.11}$$

where the leading term, $\bar{u}$, is proportional to ϵ, while the second term is, like g_2, proportional to ϵ^2 (since $W \sim \epsilon$). The quantities $\bar{u}$ and Σ are obtained from $\Omega(E,t)$,

the volume of phase space enclosed by the energy shell $H(\mathbf{z},t) = E$; from Section 2.4,

$$\Sigma = \frac{\partial \Omega}{\partial E} \tag{5.12}$$

$$\bar{u} = -\frac{1}{\Sigma}\frac{\partial \Omega}{\partial t}. \tag{5.13}$$

In our case, ignoring the small fraction of space occupied by the scatterers themselves, the volume of phase space enclosed by the energy shell E is simply the product of the volume of ordinary space available to the particles, V, with the volume of a sphere in momentum space of radius p: $\Omega = \frac{4}{3}\pi V p^3$. This gives

$$\Sigma = 4\pi V p^2 \frac{dp}{dE} = 4\pi V p E \tag{5.14}$$

$$\bar{u} = 0. \tag{5.15}$$

Eqs. 5.2 and 5.11 may be combined:

$$\frac{\partial \eta}{\partial t} = -\frac{\partial}{\partial E}(\bar{u}\eta) + \frac{1}{2}\frac{\partial}{\partial E}\Big[g_2 \Sigma \frac{\partial}{\partial E}\Big(\frac{\eta}{\Sigma}\Big)\Big]. \tag{5.16}$$

Our results for g_2, $\bar{u}$, and Σ then give, finally,

$$\frac{\partial \eta}{\partial t} = \frac{2}{3}\frac{\langle W^2 \rangle}{L}\frac{\partial}{\partial E}\Big[K p^4 \frac{\partial}{\partial E}\Big(\frac{\eta}{pE}\Big)\Big]. \tag{5.17}$$

This is our diffusion equation for the distribution of cosmic ray energies, due to their interactions with the magnetic clouds. Note that this equation is relativistic, but not necessarily ultra-relativistic; the UR limit is obtained with the replacement $p \rightarrow E$. For the sake of completeness, we present the non-relativistic limit as well:

$$\frac{\partial \eta}{\partial t} = \frac{4}{3}\frac{\langle W^2 \rangle}{L}(2m)^{1/2}\frac{\partial}{\partial E}\Big[K E^2 \frac{\partial}{\partial E}\Big(E^{-1/2}\eta\Big)\Big], \tag{5.18}$$

where E now refers to the non-relativistic energy, $p^2/2m$.

To end this section, we consider two idealized examples of scatterers. The first is that of *isotropic scatterers*[50]: in the rest frame of a scatterer, particles impinging

from any direction emerge with an isotropic distribution of momenta. In this case, K is independent of E, and is simply the average of $\sin^2\alpha/2$ over 4π of solid angle:

$$K = \frac{1}{2}\int_{-1}^{+1} d(\cos\alpha)\,\sin^2\frac{\alpha}{2} = \frac{1}{2}. \tag{5.19}$$

Thus,

$$\frac{\partial\eta}{\partial t} = \frac{1}{3}\frac{\langle W^2\rangle}{L}\frac{\partial}{\partial E}\Big[p^4\frac{\partial}{\partial E}\Big(\frac{\eta}{pE}\Big)\Big]. \tag{5.20}$$

As the second example, we consider *hard-walled scatterers*, off which the particles are reflected specularly (angle of incidence = angle of reflection in the scatterer's rest frame). For specular reflection, the angle between initial and final momentum, α, is twice the angle of incidence (or reflection), θ.

To calculate $K = \langle\sin^2\alpha/2\rangle = \langle\sin^2\theta\rangle$, we perform a weighted integral of $\sin^2\theta$ over the range of angles of incidence ($\theta = 0$ to $\pi/2$), throwing in a factor $\cos\theta$ to account for solid angle in velocity space, and a flux factor $\sin\theta$ (see Appendix A of Chapter 3 for elaboration):

$$\langle\sin^2\theta\rangle = \int_0^{\pi/2} d\theta\,\cos\theta\sin^3\theta \Big/ \int_0^{\pi/2} d\theta\,\cos\theta\sin\theta = 1/2. \tag{5.21}$$

This yields a result identical to that for isotropic scatterers,

$$\frac{\partial\eta}{\partial t} = \frac{1}{3}\frac{\langle W^2\rangle}{L}\frac{\partial}{\partial E}\Big[p^4\frac{\partial}{\partial E}\Big(\frac{\eta}{pE}\Big)\Big], \tag{5.22}$$

although the mechanism is somewhat different in the two cases.

5.5 INJECTION AND REMOVAL OF PARTICLES

Eq. 5.17 is really the central result of this chapter. It describes the acceleration of cosmic rays — essentially an ongoing evolution toward statistical equilibrium — within the framework of a simple model. For the sake of continuing in the spirit of Refs.[48,49], we now add to our equation two terms, accounting for the continual production of cosmic rays, and their continual escape from the system.

Without specifying precisely what the injection mechanism may be, assume that it is constant in time, and that no particles are injected above some maximum energy E_m. As for the removal mechanism, we will assume, as in Ref.[48], that it is dominated by absorption of the cosmic particles by other nuclear matter, which implies a rate of disappearance proportional to particle speed, p/E.

Thus, our equation for the evolution of η is modified:

$$\frac{\partial \eta}{\partial t} = a\frac{\partial}{\partial E}\Big[Kp^4\frac{\partial}{\partial E}\Big(\frac{\eta}{pE}\Big)\Big] + I(E) - b\frac{p}{E}\eta, \tag{5.23}$$

where $a = 2\langle W^2\rangle/3L$, $I(E)$ is the particle injection term ($I = 0$ for $E > E_m$), and bp/E (with b a constant) is the differential rate at which a particle of speed p/E is removed from the system. To study the UR tail (presumably beyond E_m) of the steady-state spectrum reached under the above equation, we drop $I(E)$, let $p \to E$, and set $\partial\eta/\partial t$ equal to zero:

$$0 = a\frac{\partial}{\partial E}\Big[KE^4\frac{\partial}{\partial E}\Big(\frac{\eta}{E^2}\Big)\Big] - b\eta. \tag{5.24}$$

If K is independent of energy, as in the two idealized cases considered at the end of Section 5.4, then this equation is satisfied by an inverse power law spectrum, $\eta \propto E^{-s}$, where $(s-1)(s+2) = b/aK$. On the other hand, for K a general function of E, Eq. 5.24 is not satisfied by an inverse power law steady state.

5.6 HARD-WALLED SCATTERERS, AGAIN

In Section 5.4, we applied Eq. 5.17 to the example of hard-walled scatterers. In the present section, we take a slightly different approach to this example, one that will allow for an easy extension of the range of validity of the final result. We then discuss the relation of this result to that of Chapter 3.

Starting with Eq. 5.6, note that, in the case of a hard-walled scatterer, we can rewrite this as

$$\Delta H = 2p\,\mathbf{W}\cdot\hat{\mathbf{n}}\sin\theta, \tag{5.25}$$

where $\hat{\mathbf{n}}$ is a unit vector normal to the surface of the scatterer at the point of collision. As before, $\theta = 2\alpha$ is the angle of incidence. Defining $\dot{n} = \mathbf{W} \cdot \hat{\mathbf{n}}$, we proceed:

$$\begin{aligned} \langle (\Delta H)^2 \rangle &= 4p^2 \langle \dot{n}^2 \sin^2\theta \rangle \\ &= 4p^2 \langle \dot{n}^2 \rangle \langle \sin^2\theta \rangle \\ &= 2p^2 \frac{1}{S} \oint d\sigma\, \dot{n}^2. \end{aligned} \tag{5.26}$$

Here, S is the total surface area of all scatterers combined, and the integral of $\dot{n}^2$ is over this entire area. We have made use of the fact that all scatterers are being bombarded uniformly from all directions; we have also used $\langle \sin^2\theta \rangle = 1/2$, from Section 5.4. Next, using $\tau = LE/p$, and $4V/SL = 1$ (from Appendix B of Chapter 3), we get

$$g_2 = \frac{\langle (\Delta H)^2 \rangle}{\tau} = \frac{1}{2V} \frac{p^3}{E} \oint d\sigma\, \dot{n}^2, \tag{5.27}$$

whence (using Eqs. 5.14 - 5.16)

$$\frac{\partial \eta}{\partial t} = \frac{1}{4V} \oint d\sigma\, \dot{n}^2 \frac{\partial}{\partial E} \Big[p^4 \frac{\partial}{\partial E} \Big(\frac{\eta}{pE} \Big) \Big]. \tag{5.28}$$

So far, Eq. 5.28 is simply Eq. 5.22 in another form. (This is easily verified by expressing $\oint d\sigma\, \dot{n}^2$ as

$$\oint d\sigma\, W^2 \cos^2\beta = \langle W^2 \cos^2\beta \rangle\, S = \langle W^2 \rangle S/3, \tag{5.29}$$

then by using $4V/SL = 1$.) However, take a closer look at the (lowest-order) expression for the change in energy at a collision:

$$\Delta H = 2p\dot{n} \sin\theta. \tag{5.30}$$

The factor $\dot{n}$ appearing here was defined originally as $\mathbf{W} \cdot \hat{\mathbf{n}}$, under the assumption that the motion of the wall at the point of collision is due entirely to the translation of the scatterer. Let us now consider a more general situation: the scatterer,

in addition to undergoing slow translational motion, may also be slowly rotating about its center of mass, and may even be slowly changing its shape (at constant volume). In this situation, let $\dot{n}$, at a given point on the surface of the scatterer, denote the *normal wall velocity* there, that is, the component of the wall's velocity normal to the surface. This reduces to $\mathbf{W} \cdot \hat{\mathbf{n}}$ for purely translational motion. A straightforward relativistic calculation shows that, with this definition of $\dot{n}$, Eq. 5.30 holds even when the motion of the scatterer is no longer just translational. (This reflects the fact that ΔH can depend only on how the wall of the scatterer is moving *at the point of collision*, and not on what the scatterer's surface is doing elsewhere.) This leads to a broader range of validity of Eq. 5.28: it now describes the interaction of a gas of relativistic particles with a collection of hard-walled scatterers, where the latter are allowed to: move through space, rotate about their centers of mass, and change their shapes (at fixed volume).

Note that Eq. 5.28 is an example of Eq. 5.17 with constant K, hence combining it with the injection and removal of particles (as per Section 5.5) will result in a steady-state spectrum with a tail obeying an inverse power law.

In Chapter 3, we derived an evolution equation for the distribution of energies of an ensemble of non-relativistic (NR) particles inside a slowly time-dependent, irregularly shaped, hard-walled container. In the case when the volume of the container (V) is constant, and correlations between collisions off the walls are neglected, we obtained:

$$\frac{\partial \eta}{\partial t} = \frac{(2m)^{1/2}}{2V} \oint d\sigma\, \dot{n}^2 \frac{\partial}{\partial E}\Big[E^2 \frac{\partial}{\partial E}(E^{-1/2}\eta)\Big], \tag{5.31}$$

where $\oint d\sigma\, \dot{n}^2$ is the square of the normal wall velocity, integrated over the surface of the container, and E is the NR particle energy. It is a straightforward exercise to show that Eq. 5.31 is the NR limit of Eq. 5.28. This result should not surprise us: the two problems are essentially the same, except that in one case the moving surfaces off which the particles are reflected are the walls of the container, and in

the other case they are provided by hard scatterers drifting, rotating, and deforming within the enclosed volume.

We conclude this section by mentioning again the *wall formula*,[10–12] which gives the rate of change of the total energy of a gas of non-interacting NR particles inside a slowly time-dependent irregular container:

$$\dot{E}_T = \frac{N\bar{p}}{V} \oint d\sigma\, \dot{n}^2. \tag{5.32}$$

($\bar{p}$ is the average magnitude of momentum of the particles; N is the number of particles.) As discussed in Chapter 3, the wall formula can be shown to follow directly from Eq. 5.31. This suggests an easy generalization: use Eq. 5.28 to derive a relativistically correct wall formula. Thus, letting

$$E_T = \int dE\, E\, \eta, \tag{5.33}$$

we differentiate each side with respect to time, then apply Eq. 5.28. After two integrations by parts, we are left with:

$$\dot{E}_T = \frac{1}{V} \oint d\sigma\, \dot{n}^2 \int dE\, p\, \eta = \frac{N\bar{p}}{V} \oint d\sigma\, \dot{n}^2. \tag{5.34}$$

This establishes that the wall formula, in the form given by Eq. 5.32, is in fact already relativistically correct.

5.7 RELATION TO PREVIOUS RESULTS

We now discuss how the analysis of this chapter fits into the more general framework developed in Chapter 2.

First, as in Chapter 2, we postulated a Fokker-Planck equation to govern the distribution of energies, η. In both cases, the motivation for this *ansatz* is the idea that the energy of a single system or particle can be pictured as performing a kind of random walk, a Brownian motion of sorts along the energy axis. In other

words, the "velocity" dH/dt on that axis — given by the value of $\partial H/\partial t$ along the phase space trajectory representing the system or particle — is treated as a *stochastic process.* We now bring to attention a significant difference between the two derivations.

This difference involves the justification for treating this dH/dt as a stochastic process. In Chapter 2 we appealed to the chaoticity of the underlying trajectory On the other hand, in the present chapter we have not formally assumed chaotic evolution of the particles; rather, we have used statistical arguments — based on assuming a large number of randomly distributed scatterers — to exclude correlations between consecutive steps along the energy axis. Thus in the former case it is a property of the trajectory, and in the latter case a property of the Hamiltonian, that allows us our random walk hypothesis.

These two seemingly different arguments are perhaps not completely unrelated (after all, it is the Hamiltonian which determines the trajectory). For instance, we have a strong intuitive prejudice that a particle bouncing around among very many randomly distributed scatterers will in fact do so chaotically. On the other hand, pathological counterexamples may be found for which the frozen dynamics is not chaotic, yet the random walk treatment may still be valid. (For instance, suppose the scatterers are all hard-walled cubes. Then, since all collisions are simply reflections off flat surfaces, the particles' trajectories are not chaotic, at least not in the standard sense of the term. However, as long as we retain the assumption of randomly assigned scatterer velocities and orientations, the energy changes at consecutive collisions will remain uncorrelated, hence the random walk is still justified.) Therefore, instead of trying to force the model considered in this chapter into the chaotic-adiabatic mold of Chapter 2, we will think of it as an example which illustrates both the approach developed in that chapter, and how that approach may be extended beyond the strict confines of the assumptions made

therein.

Another feature that the analysis presented here shares with the more general one of Chapter 2, is that the drift and diffusion coefficients are given in terms of the frozen dynamics. In the general case, these coefficients are functions not only of energy, but of time as well: the expressions for g_1 and g_2 in terms of the frozen dynamics are parametrized by the time of freezing. In the case considered here, the time-dependence of g_1 and g_2 is null, since only the positions of the scatterers change with time, and the coefficients are independent of these.

5.8 THE FERMI MECHANISM, AGAIN

A central theme of this Thesis is that the Fokker-Planck approach provides a useful framework for the study of energy diffusion in chaotic adiabatic systems. In this chapter we have illustrated this approach by applying it to a model depicting the Fermi mechanism of cosmic ray acceleration. We end with a few brief comments regarding this model.

First, it has been well established that the Fermi mechanism (in the form described herein) is *not* the primary source of cosmic ray acceleration.[50] (Fermi himself was aware of difficulties with his suggestion). However, even if other acceleration mechanisms dominate, interactions with wandering magnetic fields may still represent a relevant factor in the evolution of cosmic ray energies.

Furthermore, the model may be interesting to study in its own right, from the point of view of statistical mechanics; this goes back to Fermi's insight that the acceleration process may be understood as an attempt at equipartition of energies.

Finally, the model presented in this chapter is not the only version of the Fermi mechanism to have been studied. A seemingly much simpler, essentially one-dimensional model, in which the cosmic rays bounce back and forth between

two oscillating parallel plates, has been an impressive source of insight regarding non-linear maps.[22]

5.9 APPENDIX

In this Appendix we consider two generalizations of our model. The first involves the Hamiltonian describing the particle-scatterer interaction: we no longer assume it to have a kinetic + potential form (although we still take $H = (p^2+m^2)^{1/2}$ in the empty space between scatterers). We will show that this does not affect the final result: Eq. 5.17 still holds. The second generalization we shall make is to allow the scatterers to have not only translational, but also rotational degrees of freedom. This will modify Eq. 5.17 without changing its basic form.

To implement the first generalization, we start with the fact that the change in particle energy during a single collision, ΔH, is the time integral of $\partial H/\partial t$ along the particle's trajectory, Eq. 5.4. The scatterer is now described by a local Hamiltonian of the form

$$\tilde{H}(\mathbf{z},t) \;=\; \tilde{h}(\mathbf{r}-\mathbf{R}(\epsilon t),\mathbf{p}), \tag{5.35}$$

where $\tilde{h} = (p^2+m^2)^{1/2}$ outside some finite region. We thus have

$$\Delta H \;=\; -\mathbf{W}\cdot\int_{t_1}^{t_2} dt\,\frac{\partial\tilde{h}}{\partial\mathbf{r}}(\mathbf{r}-\mathbf{R},\mathbf{p}), \tag{5.36}$$

where $\mathbf{W}$, as before, is the slow velocity of this scatterer, and the integral is along the trajectory $(\mathbf{r}(t),\mathbf{p}(t))$. Again, working to leading order in ϵ, we treat $\mathbf{R}$ as constant in this integral, and use the frozen trajectory. The latter satisfies

$$\frac{d\mathbf{r}}{dt} = \frac{\partial\tilde{h}}{\partial\mathbf{p}} \quad , \quad \frac{d\mathbf{p}}{dt} = -\frac{\partial\tilde{h}}{\partial\mathbf{r}}, \tag{5.37}$$

hence the time integral of $-\partial\tilde{h}/\partial\mathbf{r}$ is simply the change in momentum, $\Delta\mathbf{p}$, that takes place during the collision. We therefore regain Eq. 5.6, and all the results which follow, including Eq. 5.17. (Note that, since we are not assuming a kinetic +

potential Hamiltonian, the canonical momentum $\mathbf{p}$ is not necessarily the ordinary relativistic momentum $\gamma m\mathbf{v}$, *during the interaction.* However, since we take $H = (p^2 + m^2)^{1/2}$ outside the scatterers, the net change in $\mathbf{p}$ during a collision does in fact equal the change in $\gamma m\mathbf{v}$, as before.)

Next, we allow each scatterer to rotate freely about its center of mass. The angular velocities ω are assumed to be small, and distributed isotropically. Continuing with a statistical treatment, we assume that the assignment of ω's to scatterers is random: they are uncorrelated with other quantities.

To evaluate the change in energy that a particle suffers during a collision with some scatterer, define a *scatterer rest frame*, which moves and rotates along with the scatterer, and whose origin coincides with the center of mass of the scatterer; we will use primes to denote vectors as viewed from this frame. We write the local Hamiltonian as

$$\tilde{H}(\mathbf{z}, t) = \tilde{h}(\mathbf{r}', \mathbf{p}'), \tag{5.38}$$

hence

$$\frac{\partial H}{\partial t} = (-\mathbf{W}' - \omega' \times \mathbf{r}') \cdot \frac{\partial \tilde{h}}{\partial \mathbf{r}'} + (-\omega' \times \mathbf{p}') \cdot \frac{\partial \tilde{h}}{\partial \mathbf{p}'}. \tag{5.39}$$

As before, we treat the scatterer as immobile for purposes of integrating $\partial H/\partial t$ along the trajectory followed during a collision. Invoking Hamilton's equations gives

$$\begin{aligned} \Delta H &= \int_{t_1}^{t_2} dt \left[(\mathbf{W}' + \omega' \times \mathbf{r}') \cdot \frac{d\mathbf{p}'}{dt} - (\omega' \times \mathbf{p}') \cdot \frac{d\mathbf{r}'}{dt} \right] \\ &= \mathbf{W}' \cdot \Delta\mathbf{p}' + \omega' \cdot \Delta\mathbf{L}' \\ &= \mathbf{W} \cdot \Delta\mathbf{p} + \omega \cdot \Delta\mathbf{L}, \end{aligned} \tag{5.40}$$

where $\Delta\mathbf{L}$ is the change in $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, the relativistic angular momentum of the particle. Squaring this and averaging over collisions, and proceeding under assumptions already discussed regarding the assignment of the $\mathbf{W}$'s and ω's to the

scatterers, we get

$$\begin{aligned}\langle(\Delta H)^2\rangle &= \frac{1}{3}\langle W^2\rangle\langle|\Delta\mathbf{p}|^2\rangle + \frac{1}{3}\langle\omega^2\rangle\langle|\Delta\mathbf{L}|^2\rangle \\ &= \frac{4}{3}p^2\langle W^2\rangle\langle\sin^2\frac{\alpha}{2}\rangle + \frac{1}{3}p^2\langle\omega^2\rangle\langle|\Delta\mathbf{a}|^2\rangle. \qquad (5.41)\end{aligned}$$

Here, we have introduced $\mathbf{a} = \mathbf{L}/p$ — a vector whose magnitude is on the order of the size of the scatterer — to extract the dominant energy dependence of $\langle|\Delta\mathbf{L}|^2\rangle$ from within the average.

We now continue as in Section 5.4, obtaining

$$\frac{\partial\eta}{\partial t} = \frac{2}{3L}\frac{\partial}{\partial E}\Big[\kappa p^4\frac{\partial}{\partial E}\Big(\frac{\eta}{pE}\Big)\Big], \qquad (5.42)$$

where

$$\kappa = \langle W^2\rangle\langle\sin^2\frac{\alpha}{2}\rangle + \frac{1}{4}\langle\omega^2\rangle\langle|\Delta\mathbf{a}|^2\rangle. \qquad (5.43)$$

This equation is very similar to Eq. 5.17, only the coefficient κ now reflects the effects of both translation and rotation of the scatterers.

As a final exercise, we will apply Eq. 5.43 to the case of hard-walled scatterers which are allowed rotational degrees of freedom. In this case, at a given collision,

$$\Delta\mathbf{a} = \mathbf{q}\times\Delta\mathbf{p}/p = 2\sin\theta\,\mathbf{q}\times\hat{\mathbf{n}}, \qquad (5.44)$$

where $\mathbf{q}$ is the location of the collision relative to the scatterer's center of mass, $\hat{\mathbf{n}}$ is a unit vector normal to the surface at the point of collision, and $\theta = 2\alpha$ is the angle of incidence. Thus,

$$\begin{aligned}\langle|\Delta\mathbf{a}|^2\rangle &= 4\langle\sin^2\theta\rangle\langle|\mathbf{q}\times\hat{\mathbf{n}}|^2\rangle \\ \kappa &= \Big[\langle W^2\rangle + \langle\omega^2\rangle\langle|\mathbf{q}\times\hat{\mathbf{n}}|^2\rangle\Big]\langle\sin^2\theta\rangle \\ &= \frac{1}{2}\Big[\langle W^2\rangle + \langle\omega^2\rangle\langle|\mathbf{q}\times\hat{\mathbf{n}}|^2\rangle\Big]. \qquad (5.45)\end{aligned}$$

This results in an equation for η identical to Eq. 5.22, only with $\langle W^2\rangle$ replaced by $\langle W^2\rangle + \langle\omega^2\rangle\langle|\mathbf{q}\times\hat{\mathbf{n}}|^2\rangle$. (The factor $\langle|\mathbf{q}\times\hat{\mathbf{n}}|^2\rangle$ is a geometrical quantity reflecting

the volume of space swept out by a rotating scatterer. The average is taken by over the combined surface area of all scatterers. Note that it vanishes identically if they are all uniform spheres.) It is simple to show that the same equation for η follows from Eq. 5.28, if the scatterers are allowed to translate and rotate, but may not change shape.

Chapter 6

Multiple-Time-Scale Approach to Ergodic Adiabatic Systems: Another Look

In Ref.[5], Ott used multiple-time-scale analysis both to demonstrate the adiabatic invariance of the quantity $\Omega(H,t)$, the *chaotic adiabatic invariant*, and also to pursue the question of the "goodness" of this quantity as an invariant. Unlike the results which have been presented so far in this Thesis — in which we have been interested only in the distribution of *energies* of an ensemble of trajectories evolving under a chaotic adiabatic Hamiltonian — Ott studied the evolution of the *phase space density* describing such an ensemble. Working to first order in the slowness parameter ϵ, he obtained an expression for this density, then applied this expression to solve for the growth of $M_1(t)$ and $M_2(t)$, the moments of energy of this distribution with respect to the adiabatic energy. In Chapter 2, taking a less formal approach, we have found disagreement with Ott's results concerning the goodness of the chaotic adiabatic invariant. In the present chapter we resolve this discrepancy. Re-examining the multiple-time-scale approach, we solve for the

evolution of the phase space density describing a chaotic adiabatic ensemble, and find a term which does not appear in Ref.[5]. With the addition of this term, the growth of the moments M_1 and M_2 is consistent with that predicted in Chapter 2. Finally, we apply our result to the problem of *adiabatic reaction forces*, within the framework considered by Berry and Robbins.[15] We find that the "extra term" in the phase space density leads to a first-order adiabatic reaction force which is distinct from the reaction forces originally derived in Ref.[15].

Our strategy is as follows. First, consider a chaotic adiabatic Hamiltonian $H(\mathbf{z}, \epsilon t)$, and a phase space density $F(\mathbf{z}, t)$ evolving under that Hamiltonian. We take the initial phase space density to be a function of energy shell alone: $F(\mathbf{z}, 0) = f_{00}(H(\mathbf{z}, 0))$, with f_{00} an arbitrary function of its argument. Using multiple-time-scale analysis and working to first order in ϵ, we obtain a solution for $F(\mathbf{z}, t)$ valid for times of $O(\epsilon^{-1})$. Applying our results to the specific case considered in Refs.[5–7], where the initial density is restricted to a single energy shell, we find expressions for dM_1/dt and dM_2/dt in agreement with those derived from the Fokker-Planck equation. Finally, we apply our result for F to the problem considered by Berry and Robbins.

To apply the multiple-time-scale method,[51] we follow Ott's expansion of F:

$$F(\mathbf{z}, t) = F_0(\mathbf{z}, \tau_2) + \epsilon F_1(\mathbf{z}, \tau_1, \tau_2) + \epsilon^2 F_2(\mathbf{z}, \tau_1, \tau_2) + \cdots, \tag{6.1}$$

where $\tau_1 = t$ and $\tau_2 = \epsilon t$ are the "fast" and "slow" times, respectively. (The independence of F_0 on τ_1 is an *ansatz*.) Since the Hamiltonian evolves on the slow scale, we introduce the notation $h(\mathbf{z}, \tau_2) = H(\mathbf{z}, \epsilon t)$. The initial conditions are: $F_0 = f_{00}(h)$, $F_1 = F_2 = \cdots = 0$, at $\tau_1 = \tau_2 = 0$. Plugging Eq. 6.1 into the Liouville equation $\partial F/\partial t + \{F, H\} = 0$, using $\partial/\partial t = \partial/\partial \tau_1 + \epsilon \partial/\partial \tau_2$, and ordering by powers of ϵ, we get, to $O(\epsilon^2)$:

$$\{F_0, h\} = 0 \tag{6.2}$$

$$\frac{\partial F_1}{\partial \tau_1} + \{F_1, h\} = -\frac{\partial F_0}{\partial \tau_2} \tag{6.3}$$

$$\frac{\partial F_2}{\partial \tau_1} + \{F_2, h\} = -\frac{\partial F_1}{\partial \tau_2}, \tag{6.4}$$

where $h = h(\mathbf{z}, \tau_2)$.

The solution of Eq. 6.2 is:

$$F_0(\mathbf{z}, \tau_2) = f_0(h, \tau_2), \tag{6.5}$$

where, aside from the initial condition $f_0(E, 0) = f_{00}(E)$, the function f_0 is so far arbitrary. This ambiguity is a feature of the multiple-time-scale method; we remove it by insisting that F_0 remain valid for times of $O(\epsilon^{-1})$, i.e. by removing terms at next order which grow secularly with time.

Following Ott, we multiply Eq. 6.3 by an arbitrary function $g(h)$ and integrate over phase space, obtaining

$$\frac{\partial}{\partial \tau_1} \int d\mathbf{z}\, g(h) F_1 = -\int d\mathbf{z}\, g(h) \frac{\partial F_0}{\partial \tau_2}. \tag{6.6}$$

Since the right side of this equation is independent of τ_1, $\int d\mathbf{z}\, g(h) F_1$ will grow secularly unless the term on the right is zero. We therefore set

$$0 = -\int d\mathbf{z}\, g(h) \Big[\frac{\partial f_0}{\partial E}(h, \tau_2) \frac{\partial h}{\partial \tau_2} + \frac{\partial f_0}{\partial \tau_2}(h, \tau_2) \Big], \tag{6.7}$$

where $\partial f_0/\partial E$ and $\partial f_0/\partial \tau_2$ refer to the derivatives of f_0 with respect to its first and second arguments, respectively. (In what follows, the arguments of h and $\partial h/\partial \tau_2$ are taken to be $(\mathbf{z}, \tau_2)$, if not specified otherwise; those of f_0, and of the functions Σ, u, f_1, and G_2 introduced below, are taken to be (E, τ_2), if not specified.)

Now define $\Sigma(E, \tau_2) \equiv \int d\mathbf{z}\, \delta(E - h) = (\partial/\partial E)\Omega(E, \tau_2)$. Letting $\langle \cdots \rangle_{E,\tau_2}$ denote the phase space average of $(\cdots)$ over the energy shell E of $h(\mathbf{z}, \tau_2)$, we have

$$\Big\langle \cdots \Big\rangle_{E,\tau_2} = (1/\Sigma) \int d\mathbf{z}\, \delta(E - h) \cdots, \tag{6.8}$$

from which

$$\int dz \cdots = \int dE\, \Sigma \left\langle \cdots \right\rangle_{E,\tau_2}. \tag{6.9}$$

With this result, Eq. 6.7, which holds for arbitrary g, yields

$$0 = \Sigma\Big(\frac{\partial f_0}{\partial E}u + \frac{\partial f_0}{\partial \tau_2}\Big) = \frac{\partial}{\partial \tau_2}(\Sigma f_0) + \frac{\partial}{\partial E}(u\Sigma f_0), \tag{6.10}$$

where $u(E,\tau_2) \equiv \langle \partial h/\partial \tau_2 \rangle_{E,\tau_2}$, and we have used the identity $\partial\Sigma/\partial\tau_2 + (\partial/\partial E)(\Sigma u) = 0$.

$F_0(\mathbf{z},\tau_2) = f_0(h,\tau_2)$ is now completely specified by the initial conditions, along with Eq. 6.10. Using Eqs. 6.5 and 6.10, we further obtain

$$\frac{\partial F_0}{\partial \tau_2}(\mathbf{z},\tau_2) = \frac{\partial f_0}{\partial E}(h,\tau_2)\Big[\frac{\partial h}{\partial \tau_2} - u(h,\tau_2)\Big], \tag{6.11}$$

which will be of use below.

We proceed to the evaluation of F_1. The solution of Eq. 6.3 contains both an inhomogeneous and a homogeneous term:

$$F_1(\mathbf{z},\tau_1,\tau_2) = F_{1i} + F_{1h} = -\int_0^{\tau_1} d\tau_1' \frac{\partial F_0}{\partial \tau_2}(\mathbf{Z},\tau_2) + f_1(h,\tau_2), \tag{6.12}$$

where $\mathbf{Z} = \mathbf{Z}(\mathbf{z},\tau_1,\tau_1',\tau_2)$ is the point in phase space reached by starting at $\mathbf{z}$ at time τ_1, then evolving a trajectory backward in time to τ_1', under the "frozen" (time-independent) Hamiltonian $h(\mathbf{z},\tau_2)$. So far, the homogeneous term f_1 is arbitrary apart from initial conditions ($f_1 = 0$ at $\tau_2 = 0$); to determine it completely, we remove secularities at $O(\epsilon^2)$. We proceed as before, multiplying both sides of Eq. 6.4 by arbitrary $g(h)$, and integrating:

$$\frac{\partial}{\partial \tau_1}\int dz\, g(h) F_2 = -\int dz\, g(h)\frac{\partial F_1}{\partial \tau_2} \tag{6.13}$$

$$= -\frac{\partial}{\partial \tau_2}\int dz\, g(h) F_1 + \int dz\, g'(h)\frac{\partial h}{\partial \tau_2}F_1. \tag{6.14}$$

(g' denotes the derivative of g with respect to its argument.) With manipulation, the right side becomes

$$-\int dE\, g(E)\Big[\frac{\partial}{\partial \tau_2}\big(\Sigma f_1\big) + \frac{\partial}{\partial E}\big(u\Sigma f_1\big) - \frac{\partial}{\partial E}\Big(\Sigma\frac{\partial f_0}{\partial E}\int_{-\tau_1}^{0} ds\, C(s)\Big)\Big]. \tag{6.15}$$

The quantity $C(s)$ (whose dependence on E and τ_2 has been suppressed) is an autocorrelation function,

$$C(s) = \Big\langle \Big(\frac{\partial h}{\partial \tau_2} - u\Big) \mathcal{O}_{\tau_2}(s) \Big(\frac{\partial h}{\partial \tau_2} - u\Big) \Big\rangle_{E,\tau_2}, \tag{6.16}$$

where $\mathcal{O}_{\tau_2}(s)$ is a time-evolution operator which acts to the right, evolving a point $\mathbf{z}$ for a time s under the frozen Hamiltonian h. Note that $C(s) = C(-s)$. For times τ_1 of $O(\epsilon^{-1})$, the integral $\int_{-\tau_1}^{0} ds\, C(s)$ becomes $(1/2)\int_{-\infty}^{+\infty} ds\, C(s) \equiv (1/2)G_2$. (We make the assumption that this integral converges.) The condition for removing secularities at $O(\epsilon^2)$ then becomes

$$\frac{\partial}{\partial \tau_2}\big(\Sigma f_1\big) + \frac{\partial}{\partial E}\big(u \Sigma f_1\big) - \frac{1}{2}\frac{\partial}{\partial E}\Big(\Sigma G_2 \frac{\partial f_0}{\partial E}\Big) = 0, \tag{6.17}$$

which, along with the initial conditions, specifies f_1.

We now have our central result, valid to $O(\epsilon^1)$ for times of $O(\epsilon^{-1})$:

$$F(\mathbf{z},t) = f_0(h,\tau_2) + \epsilon f_1(h,\tau_2) - \epsilon \frac{\partial f_0}{\partial E}(h,\tau_2) \int_0^{\tau_1} d\tau_1' \Big[\frac{\partial h}{\partial \tau_2}(\mathbf{Z},\tau_2) - u(h,\tau_2)\Big], \tag{6.18}$$

where f_0 and f_1 satisfy Eqs. 6.10 and 6.17, respectively. Ott's solution for F does not contain a term corresponding to our $F_{1h} = f_1$; we believe this to be the source of the above-mentioned conflict with the Fokker-Planck equation.

Let us now consider the case when the initial conditions are distributed over a single energy shell: $f_0(E,0) = \delta(E - E_0)/\Sigma(E,0)$. [The factor $1/\Sigma$ provides normalization: $\int dz\, F(\mathbf{z},0) = 1$.] The solution of Eq. 6.10 consistent with these initial conditions is

$$f_0(E,\tau_2) = \delta(E - \mathcal{E})/\Sigma(E,\tau_2), \tag{6.19}$$

where $\mathcal{E} = \mathcal{E}(\tau_2)$ is defined by $\Omega(\mathcal{E},\tau_2) = \Omega(E_0,0)$. [To demonstrate by inspection that Eq. 6.19 is a solution of Eq. 6.10, one needs the identity

$$d\mathcal{E}/dt = u(\mathcal{E},\tau_2), \tag{6.20}$$

which follows from the definitions of $\mathcal{E}$, u, Σ, and Ω.] Eq. 6.19 shows that, to lowest order, $F(\mathbf{z},t)$ remains distributed uniformly over the energy shell prescribed by the adiabatic invariance of Ω.

Continuing with these initial conditions, we now consider the moments $M_n(t) = \int d\mathbf{z}\, F(\mathbf{z},t)(h-\mathcal{E})^n$ which measure the error in the chaotic adiabatic invariant. Of the terms on the right side of Eq. 6.18, the first and third do not contribute to M_n (the latter because the average of $[\partial h/\partial\tau_2(\mathbf{Z},\tau_2) - u(h,\tau_2)]$ over any energy shell is zero), leaving

$$M_n(t) = \epsilon \int d\mathbf{z}\, f_1(h,\tau_2)(h-\mathcal{E})^n = \epsilon \int dE\, \Sigma f_1 (E-\mathcal{E})^n. \tag{6.21}$$

Differentiating with respect to time, one obtains (using Eqs. 6.17 and 6.20),

$$\frac{dM_1}{dt} = \epsilon^2 \int dE\, \Sigma f_1 [u - u(\mathcal{E},\tau_2)] + \epsilon^2 \Big[\frac{1}{2\Sigma}\frac{\partial}{\partial E}(\Sigma G_2)\Big]_{E=\mathcal{E}} \tag{6.22}$$

$$\frac{dM_2}{dt} = 2\epsilon^2 \int dE\, \Sigma f_1 (E-\mathcal{E})[u - u(\mathcal{E},\tau_2)] + \epsilon^2 G_2(\mathcal{E},\tau_2). \tag{6.23}$$

Expanding $u(E,\tau_2)$ in a Taylor series around $E = \mathcal{E}$, and disregarding moments higher than the second (since they may be shown to contribute terms of $O(\epsilon^3)$ or smaller) these equations become, to $O(\epsilon^2)$,

$$\frac{dM_1}{dt} = \epsilon \frac{\partial u}{\partial E}(\mathcal{E},\tau_2) M_1 + \frac{1}{2}\epsilon \frac{\partial^2 u}{\partial E^2}(\mathcal{E},\tau_2) M_2 + \epsilon^2 \Big[\frac{1}{2\Sigma}\frac{\partial}{\partial E}(\Sigma G_2)\Big]_{E=\mathcal{E}} \tag{6.24}$$

$$\frac{dM_2}{dt} = 2\epsilon \frac{\partial u}{\partial E}(\mathcal{E},\tau_2) M_2 + \epsilon^2 G_2(\mathcal{E},\tau_2). \tag{6.25}$$

(Since M_1, $M_2 \sim \epsilon$ for $t \sim \epsilon^{-1}$, all terms on the right scale like ϵ^2.) These expressions agree with those derived in Chapter 2, which resolves the discrepancy mentioned earlier.

Note that Eq. 6.18 directly leads to an evolution equation for the distribution of energies, $\eta(E,t)$, of an ensemble of systems evolving under a chaotic adiabatic Hamiltonian. We see this by writing $\eta(E,t) = \Sigma(E,\tau_2)\langle F(\mathbf{z},t)\rangle_{E,\tau_2} = \Sigma(f_0 + \epsilon f_1)$. Eqs. 6.10 and 6.17 then combine to give, to $O(\epsilon^2)$,

$$\frac{\partial \eta}{\partial t} = -\epsilon \frac{\partial}{\partial E}\big(u\eta\big) + \frac{1}{2}\epsilon^2 \frac{\partial}{\partial E}\Big[G_2 \Sigma \frac{\partial}{\partial E}\Big(\frac{\eta}{\Sigma}\Big)\Big], \tag{6.26}$$

which is exactly the Fokker-Planck equation of Chapter 2.

Finally, Eq. 6.18 has significance to the study of *adiabatic reaction forces* (see Chapter 1). Berry and Robbins[15] have introduced a model for investigating these forces. In this model, a heavy, slow particle is coupled to an *ensemble* of fast, chaotic trajectories. The position of the particle is denoted by $\mathbf{R}$, whereas the fast ensemble is represented by a phase space density $\rho(\mathbf{z}, t)$. This density evolves under a Hamiltonian h parametrized by the particle's position: $h = h(\mathbf{z}, \mathbf{R})$. (In this formulation, the slowly evolving variable $\mathbf{R}$ takes the place of the slow time τ_2.) The slow system is subject to a force

$$\mathbf{F}(t) = -\int d\mathbf{z}\, \rho \nabla h \qquad (6.27)$$

(where $\nabla \equiv \partial/\partial\mathbf{R}$) due to its coupling to the fast ensemble. To evaluate this force, we in turn need the response of ρ to the slow evolution of $\mathbf{R}$; this response is precisely the content of Eq. 6.18.

Following Ref.[15], we take the fast ensemble to be initially distributed over a single energy shell E_0 of $h(\mathbf{z}, \mathbf{R}(0))$. Then the leading contribution to $\mathbf{F}(t)$ is obtained by averaging $-\nabla h$ over the energy shell $\mathcal{E}(\mathbf{R}(t))$ determined by the chaotic adiabatic invariant. This term is dubbed the "adiabatic" force in Ref.[15]. This leading-order force is conservative: it is a simple exercise to show that one can obtain it by treating the adiabatic energy $\mathcal{E}(\mathbf{R})$ as a time-independent potential energy surface. Following an evaluation of ρ similar to Ott's, Berry and Robbins find, at next order in the rate of change of $\mathbf{R}$, two velocity-dependent contributions to $\mathbf{F}$ which they label "deterministic friction" (previously discussed by Wilkinson[8]) and "geometric magnetism"; both follow from a term in ρ corresponding to the term F_{1i} in Eq. 6.12 above.

Now, we have argued in this chapter that Ott's expression for the first-order phase space density missed a term. Might not this term lead to another first-order adiabatic reaction force? To see that this is indeed the case, replace ρ in Eq. 6.27

above with the "missing" term ϵF_{1h}; the result is an additional first-order reaction force given by

$$-\epsilon \int dE\, \Sigma f_1 \left\langle \nabla h \right\rangle_E. \tag{6.28}$$

This additional force can be understood as a correction to the adiabatic force, as follows. The latter was determined by assuming that, as the slow system evolves in time, the fast ensemble clings to the energy shell prescribed by the chaotic adiabatic invariant. This is true only at leading order. At next order, we find ρ distributed over a narrow range of energy shells near $\mathcal{E}(\mathbf{R})$. The true adiabatic force at time t is then a weighted sum of contributions $-\langle \nabla h \rangle$ from each of the shells to which the fast ensemble has diffused. The correction that this represents to the zeroth-order adiabatic force is given by Eq. 6.28.

The additional force given by Eq. 6.28 represents a velocity-*independent* contribution to $\mathbf{F}$ on the same order as geometric magnetism and deterministic friction.

Chapter 7

Conclusion

The unifying theme of this Thesis has been *chaotic adiabatic dynamics*, the evolution of systems evolving chaotically under a slowly time-dependent Hamiltonian. We conclude by briefly commenting on several issues related to the topics covered in Chapters 2 to 6.

We begin with our assumption of global chaos: the frozen Hamiltonian H_α is chaotic and ergodic for all values of α. Such systems represent an extreme end of possible Hamiltonians, the other extreme being integrable systems, in which all trajectories evolve regularly. The generic situation (in two or more degrees of freedom) is that phase space contains both regions of regular motion, and regions of chaotic motion. Any truly comprehensive study of adiabatic Hamiltonian dynamics must include an investigation of this generic case where integrability and chaos coexist in the frozen dynamics. (For such problems, phase space *separatrices* will play an important role. This has been studied in the adiabatic context by Tennyson *et al.*[52])

Not only is the property of global chaos non-generic, but it has proven difficult to find systems for which it can rigorously be established. In fact, a reason behind the prominence of billiard systems in the study of dynamical systems in general, is that

they provide some of the few examples for which global chaos may be shown to hold, analytically. We now discuss two other systems to which the approach presented in this Thesis may apply. These might be used in numerical investigations of our analytical results.

The first involves the classical hydrogenic atom in a strong magnetic field. When the field is held fixed in time, the dynamics, while not globally chaotic, is dominated by chaotic trajectories, at energies near ionization.[53] Thus, if we let the field change slowly with time, then after reduction to an effective Hamiltonian in two degrees of freedom (to get rid of the rotational symmetry about the axis of the magnetic field), we have a good approximation of a chaotic adiabatic system. Furthermore, there are scaling laws associated with this Hamiltonian which may be exploited in calculating the coefficients g_1 and g_2.

A smooth Hamiltonian system believed to be globally chaotic is the anisotropic Kepler problem.[54] By endowing the degree of anisotropy with a slow time dependence, and — as with the previous example — reducing to an effective two-degree-of-freedom Hamiltonian, we have another example of a chaotic adiabatic system.

Ott *et al.*[5–7] have discussed examples of chaotic adiabatic dynamics that arise in plasma physics.

Next, we briefly recall the result of Chapter 4 regarding the asymptotic distribution of particle speeds in a three-dimensional chaotic adiabatic billiard gas. The exponential distribution which was derived stands in contrast to the universal gaussian Maxwell-Boltzmann distribution which arises when the particles are allowed to interact. This raises the interesting question of how general the exponential distribution might, in fact, turn out to be. Can we somehow generalize it to the case of independent particles in a smooth time-dependent potential well?

Next, we discuss the use of the multiple-time-scale method in Chapter 6. This method has two major advantages over the Fokker-Planck approach of the other

chapters. First, it ultimately provides us with more knowledge regarding the evolution of a chaotic adiabatic ensemble: the phase space density F contains more information than the distribution of energies η. This may not seem to be of much importance, since throughout the Thesis we have been primarily interested in η anyway. However, on one count at least the distribution of energies is not enough: it is not possible to derive geometric magnetism from η. (For details, see Ref.[15]. Also, to see how deterministic friction, by contrast, *can* be obtained from η, see Ref.[8].) Thus, for a systematic derivation of all adiabatic reaction forces (up to first order, at least), one really needs to know the phase space density.

A second advantage of the multiple-time-scale method is that it provides a more rigorous derivation of the energy diffusion equation. One need not postulate a Fokker-Planck equation, it simply appears (see Eq. 6.26). (A drawback, however, is that the multiple-time-scale method does not provide a clear understanding of *why* η evolves diffusively.) It might make an interesting problem in mathematics to apply this approach to more general systems of equations — not necessarily Hamiltonian — which are slowly time-dependent, and which give rise to chaotic evolution. (In standard textbook discussions of the multiple-time-scale method,[51] the fast motion, while not necessarily representing Hamiltonian evolution, is regular, not chaotic.)

Finally, a few words about the quantal aspects of this problem, by which is meant the study of the quantal behavior of systems whose classical analogues exhibit chaotic adiabatic dynamics. Brown *et al.*[7] have commented that the quantal version of the adiabatic invariance of Ω is simply the statement that, at infinitely slow rate of change of the Hamiltonian, a system that begins in the nth quantal energy level will always remain in that level. For generic systems, this fact follows from the theory of avoided crossings: the probability for finding a degeneracy of energy levels by varying a single parameter in the Hamiltonian is zero. (On the other hand, systems with symmetries are allowed level crossings, hence the quan-

tum adiabatic theorem as stated above does not hold for such systems: we might start at the nth level, and end up at the n'th, where $n \neq n'$.) The correspondence between the quantal adiabatic theorem and the adiabatic invariance of Ω is established semi-classically: for large quantum number, the number of the energy level is proportional to the volume of phase space enclosed by the classical energy shell.

The classical-quantal correspondence becomes more complicated when one is interested in slow but finite rate of change of H. Consider a quantal system that begins in a single energy level, say the nth, and let H evolve at a rate proportional to ϵ. Then, on the basis of a correspondence with the classical results discussed in this Thesis, one might expect that after a time over which H has changed by order unity, the wave function will have diffused into a superposition of energy levels near the nth. Furthermore, the size of this spreading (measured by the variance in level number) ought to scale like ϵ. Wilkinson and Austin[55] have indeed shown that in the limit $\hbar \to 0$ the quantal system displays precisely this sort of diffusion; numerical results done on time-dependent billiard systems also support this line of argument.[56]

On the other hand, Berry and Robbins[15] have shown that, for a given quantal system, to first order in ϵ, the wave function remains tied to the nth energy level, thus there is no first-order energy diffusion. This discrepancy between these results, as discussed in Ref.[15], lies in the competition between two limits: the adiabatic and the semi-classical. Letting ϵ approach zero while holding $\hbar$ fixed, we find no energy diffusion at $O(\epsilon)$; however, letting $\hbar$ approach zero while holding ϵ fixed, the behavior of the quantal system approaches the classical behavior studied in this Thesis.

Finally, it is fair to state that our understanding of both classical and quantal chaotic adiabatic dynamics would benefit substantially from systematic numerical studies.

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