THE ORIGIN OF THERMODYNAMIC BEHAVIOUR

BY

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VERSION OF 1 SEPTEMBER, 1995

to Fraser
20 February, 1968—7 November, 1992
who loved to discuss all these questions

"It is not very difficult to show that the combination of the reversible laws of mechanics with Gibbsian statistics does not lead to irreversibility but that the notion of irreversibility must be added as a special ingredient...

...the explanation of irreversibility in nature is to my mind still open."

Bergmann (1967)

PROLOGUE

In 1935, Eddington wrote "The law that entropy always increases–the second law of thermodynamics-holds, I think, the supreme position among the laws of Nature.". Much has changed in science in the intervening half century, but I believe that Eddington's pronouncement still carries a great deal of truth.

The central question this book addresses is the dynamic origin of the Second Law of thermodynamics. Specifically, the goal is to define the *dynamical* foundation of the evolution of entropy to maximal states. This is accomplished through an application of recent results in ergodic theory to so-called "chaotic" dynamical systems (Lasota and Mackey, 1985, 1994; M.C. Mackey, 1989).

The Second Law of thermodynamics comes in so many forms that it is often confusing to understand precisely what a given author understands by the use of this term. This is unfortunate since the first statement of the Second Law was so clear. It was first enunciated by Clausius (1879), in his remarkable work building on the considerations of Carnot, when he wrote "Die Energie der Welt ist Konstant. Die Entropie der Welt strebt einem Maximum zu." (The energy of the world is constant. The entropy of the world tends to a maximum.) Though this simple declaration has been rephrased so many times that it is often unrecognizable, I find that Clausius' formulation is the most transparent. However, I will explicitly distinguish two variations on the original theme.

Let $S_{TD}(t)$ denote the thermodynamic entropy at time t.

Weak Form of the Second Law.

$$-\infty < S_{TD}(t_0) \leq S_{TD}(t) \leq 0 \qquad \textit{for all times } t_0 < t$$

and there exists a set (finite or not) of equilibrium entropies $\{S_{TD}^*(f)\}$ dependent on the initial preparation f of the system such that

$$\lim_{t \to +\infty} S_{TD}(t) = S_{TD}^*(f) \leq \max_f S_{TD}^*(f).$$

Thus the entropy difference $\Delta S(t) = S_{TD}(t) - \max_f S_{TD}^*(f)$ satisfies $\Delta S(t) \leq 0$ and

$$\lim_{t \to +\infty} \Delta S(t) \leq 0.$$

In this case system entropy converges to a steady state value S_{TD}^* which may not be unique. If it is not unique it characterizes a metastable state.

The second form of the Second Law of thermodynamics is more interesting.

Strong Form of the Second Law.

$$-\infty < S_{TD}(t_0) \leq S_{TD}(t) \leq 0 \qquad \textit{for all times } t_0 < t$$

and there is a unique limit S_{TD}^* (i.e. independent of the initial system preparation f) such that

$$\lim_{t \to +\infty} S_{TD} = S_{TD}^*$$

for all initial system preparations f. Under these circumstances,

$$\lim_{t \to +\infty} \Delta S(t) = 0.$$

In this case the system entropy evolves to a unique maximum irrespective of the way in which the system was prepared.

In my investigations of the connection between dynamics and entropy evolution, I have been heavily influenced by the work of Khinchin (1949), Dugas (1959), Kurth (1960), Truesdell (1960), Farquhar (1964), O. Penrose (1970, 1979), Lebowitz (1973), Lebowitz and Penrose (1973), G.W. Mackey (1974), Wehrl (1978), and Prigogine (1980). Because of the approach taken here and the nature of the material presented, a brief outline of the main points may be helpful.

Chapter 1 defines a thermodynamic system in terms of measure spaces, draws a one to one correspondence between a density and a thermodynamic state, and introduces the Boltzmann-Gibbs entropy of a density.

In Chapter 2, using a Maximal Entropy Postulate, it is a simple demonstration that the entropy of a density will assume a maximal value if and only if this density is (in the terminology of Gibbs) either the density of the

microcanonical or a generalized canonical ensemble. Then it is shown that the Boltzmann-Gibbs entropy of a density can be plausibly argued to coincide with the thermodynamic entropy S_{TD} of a system characterized by that density.

Chapter 3 introduces Markov operators. These are linear integral operators that describe the evolution of densities by dynamical or semi- dynamical systems. Fixed points of Markov operators, known as stationary densities, define states of relative or absolute thermodynamic equilibrium depending on whether there are multiple or unique stationary densities. Thus, a central question that must be answered in any treatment of thermodynamics is under what circumstance will the entropy change from its original value (determined by the way in which the system was prepared) to a final state corresponding to one of these states of relative or absolute equilibrium. Following this the conditional entropy, a generalization of the Boltzmann- Gibbs entropy, is introduced and identified with ΔS. Under particular conditions, the conditional entropy is shown to have its maximal value of zero if the stationary density of the state of thermodynamic equilibrium is that of the canonical ensemble. Then the distinction between invertible and noninvertible systems is made. This is used to provide the not too surprising proof that entropy is constant for invertible systems. It is only in noninvertible systems that the entropy *may* increase. Thus, irreversibility is necessary but not sufficient for the entropy to increase. Following this, a variety of sufficient conditions are derived for the existence of at least one state of thermodynamic equilibrium based on convergence properties of the system state density average.

Chapter 4 introduces a special type of Markov operator, the Frobenius- Perron operator. Following illustrative material demonstrating its utility in studying the evolution of densities by a variety of dynamical and semi- dynamical systems, we turn to a consideration of the conditions that guarantee the existence of a *unique* state of thermodynamic equilibrium. The necessary and sufficient condition for this existence is the property of ergodicity, which may be shared by both invertible and noninvertible systems.

Chapter 5 presents the concept of mixing, introduced in a qualitative sense by Gibbs, which is a stronger property than ergodicity though it still may be shared by noninvertible and invertible systems. However, it is not sufficient to permit the entropy of a system to change from its initial value.

Chapter 6 introduces a particular form of dynamical behaviour, called asymptotic periodicity, that is sufficient for the evolution of the entropy to a metastable state of relative equilibrium (weak form of the Second Law).

Chapter 7 is, in a sense, the core of this work. There it is shown that for there to be a global evolution of the entropy to its maximal value of zero (strong form of the Second Law) it is *necessary and sufficient* that the system have a property known as exactness.

In a very real way, the results of Chapter 7 raise as many questions as they answer. Though providing totally clear criteria for the global evolution of system entropy, at the same time these criteria suggest that all currently formulated physical laws may not be at the foundation of the thermodynamic behaviour we observe every day of our lives. This is simply because these laws are formulated as (invertible) dynamical systems, and exactness is a property that only noninvertible systems may display

One possibility is that the current invertible, dynamical system statements of physical laws are incorrect and that more appropriate formulations in terms of noninvertible semidynamical systems await discovery. Alternately, other phenomena may mask the operation of these invertible systems so they appear to be noninvertible to the observer. Chapters 8 through 11 explore this latter possibility.

In Chapter 8, we examine the effects of *coarse graining* of phase space, due either to measurement error or to an inherent graininess of phase space that is imposed by Nature. It is easy to show that if we observe a system with mixing dynamics, but operating in a coarse grained phase space, then the entropy of the coarse grained density will evolve to a maximum as time goes either forward ($t \to +\infty$) or backward ($t \to -\infty$). Thus, though coarse graining induces entropy increase to a maximum of zero it fails to single out any unique direction of time for this to occur. This illustrates that the origin of noninvertible behaviour is not a consequence of invertible dynamics operating in a coarse grained phase space.

Chapter 9 explores the consequence of taking a *trace* in which we observe only some of the important dynamical variables of a dynamics operating in a higher dimensional space (hidden variables). In this case the complete dynamics may be invertible and, consequently, have a constant entropy while the entropy of the trace system may smoothly evolve to a maximum (weak or strong form of the Second Law).

Chapters 10 and 11 respectively examine the effects of external perturbations on discrete and continuous time dynamics. This situation is usually called interaction with a heat bath. Interactions with a heat bath, depending on how they occur, can be shown to lead to either local (metastable) or global states of thermodynamic equilibrium.

In Chapter 10 we show that under very mild assumptions concerning the nature of the perturbation, discrete time

systems with the most uninteresting dynamics in the unperturbed situation will become either asymptotically periodic or exact in the presence of perturbations. Thus they will display evolution of entropy toward states of thermodynamic equilibrium (either form of the Second Law).

Chapter 11 continues this theme by examining the effects of white noise perturbations of continuous time systems whose dynamics are described by systems of ordinary differential equations. Again these perturbations induce exactness and the consequent increase of the conditional entropy to its maximum value of zero (strong form of the Second Law).

Lest there be any misapprehension on the part of the reader, let me state at the outset that it is my firm conviction that the answer to the question of the origin of the "arrow of time" does not lie in Chapters 8 through 11. Rather, I feel that the answer lies in yet undiscovered modifications of the laws of physics that render them noninvertible.

As should be evident from this survey of the contents, it is not my intent to develop statistical mechanics as a subject. This is done rather nicely from several points of view in a variety of texts. Kestin and Dorfman (1971), Reichl (1980), Ma (1985), Pathria (1985), and Grandy (1988) are representative of some of the more thought provoking of these.

Throughout, I have tried to include as much material as necessary so this book can be read as a unit. Proofs of almost all of the theorems are given, though they need not be read to grasp the thread of the argument. Examples are offered to try to illustrate the physical significance of the results discussed. To more clearly delineate material, the end of proofs are marked with a " $\square$ " and the end of examples by a " $\bullet$ ".

This work was started at the Universities of Oxford and Bremen, 1986-7 and continued in the same locations 1993-4. I thank Profs. J.D. Murray and Andrew Fowler (Oxford) and H. Schwegler (Bremen) for their hospitality during these periods. Several colleagues have helped me clarify various points, and I hope that they will not be offended by my lack of explicit acknowledgment of their interest. They know who they are. I am especially indebted to Helmut Schwegler for his continued interest and support in reading and commenting on almost every aspect of this work. He has given of his time and energy as only a true friend can.

My wife, Nancy, and my children–Fraser, David, Alastair, Linda, and Christopher–have all contributed a great deal through their love, interest, and encouragement.

Fraser (who died on 7 November, 1992 after a three year struggle against Ewing's sarcoma), and to whom I dedicate this book, always asked "Hi Mike, how's it going?". It is my personal sadness that he could not be present in body to ask the same question during the preparation of this second edition. But, as is always the case with Fraser, he is here in spirit.

Montreal, 15 May, 1994

PART I.
BACK TO BASICS

CHAPTER 1.
STARTERS

In this chapter we introduce some elementary concepts from measure theory as a start in our examination of the dynamical origin of increasing entropy. Section A draws a connection between thermodynamic systems and measure spaces. Section B briefly considers dynamics and phase spaces, while Section C introduces the notion of a density and postulates that the state of a thermodynamic system is characterized by a density. In Section D we introduce the Boltzmann Gibbs entropy, and prove that it is the unique (up to a multiplicative constant) entropy definition that satisfies the physical requirement (additivity) that entropy be an extensive quantity.

A. THERMODYNAMIC SYSTEMS.

In defining a thermodynamic system we need some terms and concepts come from measure theory.

We first start with a set X. Measure theorists often like to keep X pretty abstract, but for us X is going to be the **phase space** (more about this in the next section) on which all of our dynamics operates. Sometimes X will be a closed finite interval like $[0, 1]$, sometimes it may be infinite in extent like R^+, R^6, or even R^d, and sometimes X is a function space. In any event, whatever X is we are going to assume that it does not have any pathological properties.

Given a phase space X we turn to a definition of what measure theorists call a σ-algebra. Namely, we let $\mathcal{A}$ be a collection of subsets (subspaces) of X, and say that $\mathcal{A}$ is a σ-**algebra** if:

(1) $A \in \mathcal{A}$ implies that $X \setminus A \in \mathcal{A}$;
(2) Given a sequence (infinite or not) $\{A_k\}$ of subsets of X, $A_k \in \mathcal{A}$, then $\cup A_k \in \mathcal{A}$; and
(3) $X \in \mathcal{A}$.

(Note that properties 1 and 3 imply that the empty set $\emptyset$ is a member of $\mathcal{A}$ since $\emptyset = X \setminus X$).

The final notion we need for the definition of a thermodynamic system is that of measure. Any real valued function μ defined on a σ-algebra $\mathcal{A}$ is a **measure** if:

(1) $\mu(\emptyset) = 0$;
(2) $\mu(A) \geq 0$ for all $A \in \mathcal{A}$; and
(3) $\mu(\cup_k A_k) = \sum_k \mu(A_k)$ whenever $\{A_k\}$ is a sequence (infinite or not) of pairwise disjoint subsets of $\mathcal{A}$, *i.e.* $A_i \cap A_j = \emptyset$ for $i \neq j$.

With the three concepts of a set X, a σ-algebra $\mathcal{A}$, and a measure μ we call the triple $(X, \mathcal{A}, \mu)$ a **measure space**. If, in addition, we can find a sequence $\{A_k\}$ of subsets of the σ-algebra $\mathcal{A}$ such that

$$X = \bigcup_{k=1}^{\infty} A_k \qquad \text{and} \qquad \mu(A_k) < \infty$$

then we say that the measure space $(X, \mathcal{A}, \mu)$ is σ-**finite**. All of the measure spaces we consider will be σ-finite.

Example 1.1. If we were considering a phase space like $X = [0, 1]$ or $X = R$, then a reasonable σ algebra would be the smallest collection of closed intervals of the form $[a, b]$. These intervals have Lebesgue measure $\mu_L([a, b]) = b - a$.
●

Throughout, we will associate a thermodynamic system with a measure space through the following postulate.

POSTULATE A. A thermodynamic system is equivalent to a measure space.
Thus, every time we use the term thermodynamic system we are referring to the triple consisting of a phase space X, a σ-algebra $\mathcal{A}$, and a measure μ.

B. DYNAMICS.

We next consider a thermodynamic system operating in a phase space X. On this phase space the temporal evolution of our system is described by a **dynamical law** S_t that maps points in the phase space X into new points, *i.e.*, $S_t : X \to X$, as time t changes. In general X may be a d-dimensional phase space, either finite or not, and therefore x is a d-dimensional vector. Time t may be either continuous ($t \in R$) as, for example, it would be for a system whose dynamics were governed by a set of differential equations, or discrete (integer valued, $t \in Z$) if the dynamics are determined by discrete time maps.

We only consider autonomous processes in which the dynamics S_t are not an explicit function of the time t so it is always the case that $S_t(S_{t'}(x)) = S_{t+t'}(x)$. Thus, the dynamics governing the evolution of the system are the same

on the intervals $[0, t']$ and $[t, t + t']$. This is not a serious restriction since any nonautonomous system can always be reformulated as an autonomous one by the definition of new dependent variables.

Two types of dynamics will be important in our considerations, and some preliminary discussion will be helpful. Consider a phase space X and a dynamics $S_t : X \rightarrow X$. For every initial point x^0, the sequence of successive points $S_t(x^0)$, considered as a function of time t, is called a **trajectory**. In the phase space X, if the trajectory $S_t(x^0)$ is nonintersecting with itself, or intersecting but periodic, then at any given final time t_f such that $x^f = S_{t_f}(x^0)$ we could change the sign of time by replacing t by $-t$, and run the trajectory backward using x^f as a new initial point in X. Then our new trajectory $S_{-t}(x^f)$ would arrive precisely back at x^0 after a time t_f had elapsed: $x^0 = S_{-t_f}(x^f)$. Thus in this case we have a dynamics that may be reversed in time *completely unambiguously*. Dynamics with this character are known variously as **time reversal invariant** (Sachs, 1987) or **reversible** (Reichenbach, 1957) in the physics literature, and as **invertible** in the mathematics literature.

We formalize this by introducing the concept of a **dynamical system** $\{S_t\}_{t \in R}$ (or, alternately, $t \in Z$ for discrete time systems) on a phase space X, which is simply any group of transformations $S_t : X \rightarrow X$ having the two properties:

(1) $S_0(x) = x$; and
(2) $S_t(S_{t'}(x)) = S_{t+t'}(x)$ for $t, t' \in R$ or Z.

Since, from the definition, for any $t \in R$, we have

$$S_t(S_{-t}(x)) = x = S_{-t}(S_t(x)),$$

it is clear that dynamical systems are **invertible** in the sense discussed above since they may be run either forward or backward in time. Systems of ordinary differential equations are examples of dynamical systems as are invertible maps. All of the equations of classical and quantum physics are invertible.

To illustrate the second type of dynamics, consider a trajectory that intersects itself but is not periodic. Now starting from an initial point x^0 we find that the trajectory $\{S_t(x^0)\}$ eventually has one or more transversal crossings $x^\perp$ of itself. If we let $t_\perp$ be the time at which the first one of these crossings occurs, and choose our final time $t_f > t_\perp$, then picking $x^f = S_{t_f}(x^0)$ and reversing the sign of time to run the trajectory backward from x^f poses a dilemma once the reversed trajectory reaches $x^\perp$ because *the dynamics give us no clue* about which way to go! Situations like this are called **irreversible** in the physics literature, while mathematicians call them **noninvertible**.

Therefore, the second type of dynamics that is important to distinguish are those of **semidynamical systems** $\{S_t\}_{t>0}$, which is any semigroup of transformations $S_t : X \rightarrow X$, *i.e.*

(1) $S_0(x) = x$; and
(2) $S_t(S_{t'}(x)) = S_{t+t'}(x)$ for $t, t' \in R^+$ (or N).

The difference between the definition of dynamical and semidynamical systems lies solely in the restriction of t and t' to values drawn from the positive real numbers, or the positive integers, for the semidynamical systems. Thus, in sharp contrast to dynamical systems, semidynamical systems are **noninvertible** and may not be run backward in time in an unambigious fashion. Examples of semidynamical systems are given by noninvertible maps, delay differential equations, and some partial differential equations.

Often there is a certain confusion in the literature when the terms reversible and irreversible are used, and to avoid this **we will always use the adjectives invertible and noninvertible**. In spite of the enormous significance of distinguishing between dynamical and semidynamical systems later, at this point no assumption is made concerning the invertibility or noninvertibility of the system dynamics.

C. THERMODYNAMIC STATES.

The usual way of examining the dynamics of systems is by studying the properties of individual trajectories, but in keeping with the ergodic theory approach adopted here we opt instead to study the way in which the system dynamics operate on an infinite number of initial points.

More specifically, we will examine the way in which the dynamics alter densities. What do we mean by a density? If f is an L^1 function in the space X, *i.e.*, if

$$\int_X |f(x)| \, dx < \infty,$$

then f is a **density** if $f(x) \geq 0$ and $\| f \| = 1$. As usual, $\| f \|$ denotes the L^1 norm of the function f,

$$\| f \| = \int_X |f(x)| \, dx.$$

The examination of the evolution of densities by system dynamics is equivalent to examining the behaviour of an infinite number of trajectories. This apparently simple assumption concerning the way in which systems operate on densities is so fundamental and important to the understanding of the foundations of thermodynamics that it is given a special status.

POSTULATE B. A thermodynamic system has, at any given time, a state characterized by a density f(x), not necessarily independent of time.

Given a density f then the **f-measure** $\mu_{\mathbf{f}}(\mathbf{A})$ of the set A in the phase space X is defined by

$$\mu_f(A) = \int_A f(x)\, dx,$$

and f is called the **density** of the measure μ_f. The usual Lebesgue measure of a set A is denoted by $\mu_L(A)$, and the density of the Lebesgue measure is the uniform density, $f(x) = 1/\mu_L(X)$ for all points x in the phase space X. We always write $\mu_L(dx) = dx$.

The Lebesgue measure of the entire phase space, denoted by $\mu_L(X)$, may either be finite or infinite. If it is finite, we often take it to be normalized so $\mu_L(X) = 1$. It is important to realize that the measure of a set can be quite different depending on the density f. Thus for example, the Lebesgue measure of the positive real line R^+ is infinite, whereas the measure of R^+ with respect to the density $f(x) = ke^{-kx}$ is just

$$\mu_f(R^+) = \int_0^\infty ke^{-kx}\, dx = 1.$$

It is instructive to compare the approach used here with that of Boltzmann and Gibbs in their treatments of statistical mechanics. Both started from the assumption that they were dealing with systems of dimension $d = 2s$ whose dynamics were described by s position variables x_i and s momentum variables p_i. Boltzmann considered the phase space to be a $2s$ dimensional space which is usually called μ **space**. He then considered the evolution of a large number N of identical particles, each with the same dynamics, in μ space. N is large and typically on the order of Avagadro's number, 6×10^{23}. The limiting case of $N \to \infty$ is the **thermodynamic limit** in which case the Boltzmann approach is equivalent to studying the evolution of a density in μ space. Gibbs also considered N identical particles operating with these $2s$ dimensional dynamics in a phase space (commonly called the Γ **space**) of dimension $2sN$. He then considered an infinite number of copies of this original system, and gave this construct the name **ensemble**. Thus Gibbs studies the evolution of the ensemble density, and Γ space has proved to be the most useful in statistical mechanics.

This book is devoted to the study of systems by the evolution of densities, how system properties (dynamics) determine the character of the density evolution, and how this is translated into entropy behaviour. Later, it will become clear what types of systems may be described by the evolution of densities. However, if for now we accept Postulate B that such systems exist, then it will be easy to examine the consequences of this postulate.

D. BOLTZMANN-GIBBS ENTROPY.

Having postulated that a thermodynamic system has a state characterized by a density f, we are now in a position to develop the physically useful concept of entropy as both Boltzmann and Gibbs introduced the term.

First we define an **observable** $\mathcal{O}$ to be a real number characterizing some aspect of a thermodynamic system, for example the energy, pressure, or temperature. As such, an observable corresponds to a map $\mathcal{O}: X \to R$ from the phase space X that yields this number. The expected, or average, value of the observable $\mathcal{O}$ is just given by weighting $\mathcal{O}(x)$ with the system state density $f(x)$ and integrating over the entire phase space:

$$E(\mathcal{O}) = <\mathcal{O}> = \int_X \mathcal{O}(x)f(x)\, dx.$$

In his celebrated work Gibbs, assuming the existence of a system state density f on the phase space X, introduced the concept of the **index of probability** given by $\log f(x)$ where "log" denotes the natural logarithm. Though Gibbs identified $-\log f$ with entropy, now it is customary to introduce a quantity $H(f)$ which is the negative of the phase space average of the index of probability weighted by the density f, *i.e.*

$$H(f) = -\int_X f(x) \log f(x)\, dx.$$

This is now known as the **Boltzmann-Gibbs entropy** of a density f since precisely the same expression appears in Boltzmann's work (with the opposite sign) but the phase space is different for Boltzmann (μ space) and for Gibbs (Γ space). Clearly, the Boltzmann Gibbs entropy is just the expectation of the observable defined by the negative of the index of probability.

As it stands, the definition of the Boltzmann-Gibbs entropy may seem a bit obscure, and some motivation illustrates why it is the only reasonable candidate for a mathematical analog of the empirical thermodynamic entropy. It is easily shown that the only observable which is a function of a thermodynamic state that gives the requisite additive property to make the entropy an extensive quantity is the logarithmic function, and that it is unique up to a multiplicative constant (Khinchin, 1949; Skagerstam, 1974).

To be more specific, consider two systems A and B operating in the phase spaces X_A and X_B respectively, and each having the densities of states f_A and f_B. We now combine the two systems to form a new system C operating in the product space $X_C = X_A \times X_B$, so system C will have a density of states $f_C(x, y) = f_A(x)f_B(y)$ if A and B do not interact. Experimentally we expect that when the two systems are combined into a larger system C, then the entropy of system C should equal the sum of the individual entropies of A and B, since entropy is generally held to be an extensive system property. We wish to show that the Gibbs choice for the index of probability is the only choice (up to a multiplicative constant) that will ensure this.

To demonstrate this, assume that the index of probability is left as an unspecified observable $\mathcal{O}$. If the observable $\mathcal{O}$ is such that it transforms products to sums, $\mathcal{O}(f_C) = \mathcal{O}(f_A f_B) = \mathcal{O}(f_A) + \mathcal{O}(f_B)$, then the relation $H(f_A) + H(f_B) = H(f_C)$ holds. It is certainly clear that picking $\mathcal{O}(w) = d \log w$, where d is any arbitrary nonzero constant, will work but are there any other functions $\mathcal{O}$ with the requisite property?

Assume there exists a second continuous observable $\tilde{\mathcal{O}}$ such that

$$\tilde{\mathcal{O}}(f_A f_B) = \tilde{\mathcal{O}}(f_A) + \tilde{\mathcal{O}}(f_B).$$

Define two new functions $v_A(a)$ and $v_B(b)$ through

$$f_A(a) = e^{v_A(a)} \qquad \text{and} \qquad f_B(b) = e^{v_B(b)}.$$

Then we have

$$\tilde{\mathcal{O}}(e^{v_A + v_B}) = \tilde{\mathcal{O}}(e^{v_A}) + \tilde{\mathcal{O}}(e^{v_B}),$$

or with $h(w) \equiv \tilde{\mathcal{O}}(e^w)$ this becomes

$$h(v_A + v_B) = h(v_A) + h(v_B).$$

This, however, is just the famous Cauchy functional equation that has the unique solution

$$h(w) = \delta w \qquad \text{with } \delta \text{ an arbitrary constant}$$

(Kuczma, 1985). This in turn implies that $\tilde{\mathcal{O}}(e^w) = \delta w$ so

$$\tilde{\mathcal{O}}(w) = \delta \log w.$$

Thus the only observable that gives the requisite additive property for the Boltzmann-Gibbs entropy is the logarithmic function and it is unique up to a multiplicative constant.

We formalize the entropy definition by saying that the **Boltzmann Gibbs entropy** of the density f is defined by

$$H(f) = \int_X \eta(f(x)) \, dx \tag{1.1}$$

where the function $\eta(w)$ is given by

$$\eta(w) = \begin{cases} -w \log w & w > 0, \\ 0 & w = 0. \end{cases} \tag{1.2}$$

The function $\eta(w)$ has properties that are important for demonstrating properties of the entropy H (see Figure 1.1). First, note that $\eta(w)$ is continuous for $w \geq 0$ since $\eta(0) = 0$ by definition. Further, $\eta''(w) = -w^{-1}$ so $\eta(w)$ is strictly concave since $\eta''(w) < 0$ for all $w > 0$. From this it is an immediate consequence (see Figure 1.1) that

$$\eta(w) \leq (w - v)\eta'(v) + \eta(v) \tag{1.3}$$

for all $w, v > 0$. Combining equation (1.2) defining η with inequality (1.3) gives the **Gibbs inequality**

$$w - w \log w \le v - w \log v \qquad \text{for } w, v > 0. \tag{1.4}$$

Integrating (1.4) gives another useful inequality. If f and g are two densities, and $\eta(f(x))$ and $\eta(g(x))$ are both integrable, then we have directly from (1.4) that

$$- \int_X f(x) \log f(x) \, dx \le - \int_X f(x) \log g(x) \, dx, \tag{1.5}$$

which we call the **integrated Gibbs inequality**. Only when $f = g$ does the equality hold.

E. SUMMARY. This chapter has introduced some key concepts and postulates necessary in our examination of the foundation of evolution of entropy. We have identified thermodynamic systems with measure spaces and states of thermodynamic systems with densities. We have also defined the Boltzmann Gibbs entropy and proved it is the unique (up to a multiplicative constant) definition of entropy that is consistent with the physically motivated requirement of entropy additivity. In the next chapter we turn our attention to maximal entropy principles and their consequences.

Figure 1.1. The graph of $\eta(x)$ as a function of x. The solid line tangent to the curve at $x = v$ has slope $\eta'(v)$, while the dashed line connecting the points v and w has slope $[\eta(w) - \eta(v)]/(w - v)$. This illustrates the origin of inequality (1.3).

CHAPTER 2.
MAXIMAL ENTROPY PRINCIPLES.

In this chapter we examine the surprising consequences of maximizing the Boltzmann Gibbs entropy subject to various constraints. In Section A we show that for a system operating in a phase space of finite measure with no other constraints, the entropy will assume a maximal value if and only if the density (in the terminology of Gibbs) is the density of the microcanonical ensemble. Further, in Section B for a general phase space it is demonstrated that given the expectation value of a particular observable, the Boltzmann-Gibbs entropy of a density will attain its maximum if and only if the density is a generalization of the density of the canonical ensemble.

In Section C we show that the mathematical definition of the Boltzmann-Gibbs entropy of a density can be plausibly argued to coincide with the thermodynamic entropy of a system characterized by that density, and that all of equilibrium thermodynamics follows.

Section D shows how other constraints, coupled with the maximal entropy principle, yield the densities of the Maxwell Boltzmann or other distributions. Section E shows how the use of a maximal entropy principle can be used to derive the Planck blackbody radiation law. Section F briefly considers how the maximal entropy principle can be extended to situations in which there are known expectation values of several observables.

A. MICROCANONICAL ENSEMBLES.

Armed only with the integrated version of the Gibbs inequality (1.5) we may immediately understand the origin of the classical Gibbs microcanonical ensemble as reflecting a manifestation of extremal properties of the entropy. Consider a given space X with finite Lebesgue measure, $\mu_L(X) < \infty$ (forgo the normalization $\mu_L(X) = 1$ temporarily), and all possible densities f. Then the only density that maximizes the entropy is the (uniform) density of the Lebesgue measure of X. More precisely,

Theorem 2.1. *When $\mu_L(X) < \infty$, the density that maximizes the Boltzmann-Gibbs entropy is the uniform density*

$$f_*(x) = \frac{1}{\mu_L(X)}. \tag{2.1}$$

For any other density $f \neq f_*$, $H(f) < H(f_*)$.

Proof. Pick an arbitrary density f so, by definition, the entropy of f is

$$H(f) = -\int_X f(x) \log(f(x)) \, dx.$$

With $g(x) = 1/\mu_L(X)$ the integrated Gibbs inequality (1.5) gives

$$H(f) \leq -\int_X f(x) \log g(x) \, dx = -\log\left[\frac{1}{\mu_L(X)}\right] \int_X f(x) \, dx,$$

or $H(f) \leq -\log\left[\frac{1}{\mu_L(X)}\right]$ since f is a density. The equality holds if and only if $f = f_*$. The entropy of f_* is easily calculated to be

$$H(f_*) = -\int_X \frac{1}{\mu_L(X)} \log\left[\frac{1}{\mu_L(X)}\right] \, dx = -\log\left[\frac{1}{\mu_L(X)}\right],$$

so $H(f) \leq H(f_*)$ for any density f, or $H(f) < H(f_*)$ for $f \neq f_*$. Clearly, if X is normalized so $\mu_L(X) = 1$, then $H(f) \leq 0$. $\square$

Example 2.1. The uniform density f_* defined by (2.1) is a generalization of the density of the microcanonical ensemble introduced by Gibbs in his work on the foundations of thermodynamics.

Specifically, Gibbs considered the special case of a conservative mechanical system, *i.e.* one in which the forces are such that the work $W(x_1, x_2)$ required to move a particle between two points x_1 and x_2 in the phase space X is independent of the path connecting x_1 and x_2. For conservative systems the energy U is a constant of the motion, which simply means U is constant along any given trajectory. Furthermore, any density f which is a function of the energy U alone, $f(U)$, will also be a constant of the motion. (This invariance of the density along trajectories is what

Gibbs referred to as *conservation of extension in phase.*) Inasmuch as it is necessary to have an ensemble with an (ultimately) time independent density to describe the behaviour of a system in thermal equilibrium, Gibbs reasoned that a natural first choice would be to pick an ensemble characterized by the density

$$f(U) = \begin{cases} \text{Constant} & U = U_0 \\ 0 & \text{otherwise}, \end{cases} \tag{2.2}$$

where the energy U_0 is to be specified.

The density in equation (2.2) is the density of what Gibbs called the **microcanonical ensemble**, and it is clearly a special case of the uniform density (2.1) which maximized the entropy of a finite space. In the microcanonical ensemble the phase space X is taken to be the space X^* of conjugate position and momenta (q, p) restricted by the requirement that $U(p, q) = U_0$. The constant appearing in the density (2.2) is simply related to the measure of the restricted space X^* by Constant $= 1/\mu_L(X^*)$. •

Notice that in the derivation of the density (2.1) maximizing the entropy on a finite space, there was no reference to the nature of the dynamics of the system generating the density. This is in sharp contrast to the usual approach in thermodynamics in which the dynamics are quite specifically used to argue for the plausibility of the microcanonical density (2.1). The fact that a generalization of this density appears in such a natural way merely illustrates the generality of both the density and the method used to obtain it, and that the existence of the density of the microcanonical ensemble is independent of the system dynamics.

B. CANONICAL ENSEMBLES.

Even more fascinating consequences can emerge from the extremal properties of entropy that offer insight into the basic foundation of thermodynamics of both classical and quantum systems. In this section we state and prove a theorem that is used to deduce all of conventional equilibrium thermodynamics in the next section.

Theorem 2.2. *Assume that an (observable) nonnegative measurable function $\mathcal{O}(x)$ is given as well as the average $< \mathcal{O} >$ of that function over the entire space X, weighted by the density f:*

$$< \mathcal{O} >= \int_X \mathcal{O}(x) f(x) \, dx. \tag{2.3}$$

(Note that $< \mathcal{O} >$ is nonnegative and may be time dependent.) Then the maximum of the entropy $H(f)$, subject to the constraint (2.3), occurs for the density

$$f_*(x) = Z^{-1} e^{-\nu \mathcal{O}(x)} \tag{2.4}$$

where Z is defined by

$$Z = \int_X e^{-\nu \mathcal{O}(x)} \, dx, \tag{2.5}$$

and ν is implicitly determined from

$$< \mathcal{O} >= Z^{-1} \int_X \mathcal{O}(x) e^{-\nu \mathcal{O}(x)} \, dx. \tag{2.6}$$

Proof. The proof again uses the integrated Gibbs inequality. From (1.5), for densities f and f_*,

$$\begin{aligned} H(f) &\leq - \int_X f(x) \log f_*(x) \, dx \\ &= - \int_X f(x)[- \log Z - \nu \mathcal{O}(x)] \, dx \\ &= \log Z + \nu \int_X f(x) \mathcal{O}(x) \, dx \\ &= \log Z + \nu < \mathcal{O} > . \end{aligned}$$

However it is easy to show that

$$H(f_*) = \log Z + \nu < \mathcal{O} > \tag{2.7}$$

and therefore $H(f) \leq H(f_*)$, with the equality holding if and only if $f = f_*$.   □

The choice of notation in (2.4) and (2.5) was intentional to draw the connection with the density of the Gibbs canonical ensemble.

Example 2.2. If X^* is the conjugate position-momentum (q, p) space, $\mathcal{O}(x)$ is the system energy functional, and $< \mathcal{O} >$ the average (over the phase space) energy of the system, then Z as given by (2.5) can be identified directly with the **partition function** and the density f_* given in (2.4) that maximizes the entropy is to be identified with the density of the **Gibbs canonical ensemble**.

In deriving the density of the Gibbs canonical ensemble, it is implicit in the writing of the average $< \mathcal{O} >$, given by equation (2.3), over the entire phase space that if the density (2.4) is to describe a state of thermodynamic equilibrium then the quantity $\mathcal{O}(x)$ must eventually be independent of time at long times. An even more restrictive requirement would be that $\mathcal{O}(x)$ is a constant of the motion. If $\mathcal{O}(x)$ is identified with the system energy U, then we are dealing with a system in which the energy is conserved. •

Example 2.3. As another illustration of the application of Theorem 2.2, consider the family of densities f with a given variance, *i.e.*

$$\sigma^2 = \int_{-\infty}^{\infty} x^2 f(x) \, dx.$$

Under this constraint, the maximal Boltzmann Gibbs entropy is attained when the density is Gaussian,

$$f_*(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}.$$

This is quite easy to show, since for an arbitrary density f,

$$
\begin{aligned}
H(f) &\leq -\int_{-\infty}^{\infty} f(x) \log \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2} \right\} dx \\
&= \log \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \right\} + \frac{1}{2\sigma^2} \int_{-\infty}^{\infty} x^2 f(x) \, dx \\
&= \frac{1}{2} - \log \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \right\} = H(f_*). \quad •
\end{aligned}
$$

C. THE THERMODYNAMIC CONNECTION.

All of conventional equilibrium thermodynamics can be deduced from the density (2.4). Let us see how.

It is a fundamental assumption of thermodynamics that

POSTULATE C. There exists a one to one correspondence between states of thermodynamic equilibrium and states of maximum entropy.
We add to this the following.

POSTULATE D. Given an observable $\mathcal{O}(x)$ and its average $< \mathcal{O} >$, the density given by (2.4)-(2.6) maximizing the entropy with respect to $\mathcal{O}$ corresponds to the density of the state of thermodynamic equilibrium attained physically.

If there is but one state of thermodynamic equilibrium that is attained regardless of the way in which the system is prepared then this is called a **globally stable equilibrium** and is associated with a globally stable state of maximal entropy (strong form of the Second Law). If, however, there are multiple states of thermodynamic equilibrium, each corresponding to a state of locally maximal entropy and dependent on the initial preparation of the system, then we say that these are **local** or **metastable states of equilibrium** (weak form of the Second Law).

Given these observations, it is natural to examine the consequences of associating the equilibrium thermodynamic entropy S_{TD}^* with the maximal Boltzmann Gibbs entropy H given by (2.7):

$$H(f_*) \leftrightarrow S_{TD}^*.$$

Since we have not specified units for H, a multiplicative constant c^{-1} may be necessary, *viz.*

$$H(f_*) = S_{TD}^*/c,$$

which implies from (2.7) that the equilibrium thermodynamic entropy is given by

$$S_{TD}^* = c \log Z + c\nu < \mathcal{O} >$$

If, as before, we make the association of $< \mathcal{O} >$ with the internal thermodynamic energy U,

$$< \mathcal{O} >= U,$$

we wish to then associate the parameter ν with some function of the temperature T. At this point, it should be noted that

$$< \mathcal{O} >= -\frac{1}{Z}\frac{dZ}{d\nu}.$$

Taking the derivative of $< \mathcal{O} >$ with respect to the parameter ν in this equation we have

$$\frac{d < \mathcal{O} >}{d\nu} = \frac{1}{Z^2}\left[\frac{dZ}{d\nu}\right]^2 - \frac{1}{Z}\left[\frac{d^2 Z}{d\nu^2}\right]$$
$$=< \mathcal{O} >^2 - < \mathcal{O}^2 > .$$

Remembering that the variance $D^2(\mathcal{O}|f_*)$ of a function $\mathcal{O}$ with respect to a density f_* is simply given by

$$D^2(\mathcal{O}|f_*) =< \mathcal{O}^2 > - < \mathcal{O} >^2$$
$$=< (\mathcal{O}- < \mathcal{O} >)^2 >$$

and that the variance is by necessity non-negative, $D^2 \geq 0$, we immediately have that

$$\frac{d < \mathcal{O} >}{d\nu} = -D^2(\mathcal{O}|f_*) \leq 0.$$

Therefore, if there is any connection between variations in the parameter ν and the average energy $< \mathcal{O} >= U$, it must be an inverse one. Since our experience tells us that that temperature T and energy U are directly proportional to one another, this leads us to conclude that if the parameter ν and the temperature T are related to one another then it must be an inverse relationship.

Next in our investigation of the potential physical meaning of the parameter ν, consider two systems:

(1) System A, operating in a phase space X_A, characterized by an energy functional $\mathcal{O}_A(x_a)$, average energy $< \mathcal{O}_A >$, parameter ν_A; and

(2) System B, operating in a phase space X_B, characterized by an energy functional $\mathcal{O}_B(x_b)$, average energy $< \mathcal{O}_B >$, and parameter ν_B.

By Theorem 2.2, the densities maximizing the entropy for systems A and B are, respectively,

$$f_{*A}(x_a) = \frac{1}{Z_A}e^{-\nu_A \mathcal{O}_A(x_a)} \qquad \text{with} \qquad Z_A = \int_{X_A} e^{-\nu_A \mathcal{O}_A(x_a)}\, dx_a, \tag{2.8}$$

and

$$f_{*B}(x_b) = \frac{1}{Z_B}e^{-\nu_B \mathcal{O}_B(x_b)} \qquad \text{with} \qquad Z_B = \int_{X_B} e^{-\nu_B \mathcal{O}_B(x_b)}\, dx_b. \tag{2.9}$$

We combine systems A and B into a third system C, operating on the product space $X_A \times X_B$, so the new system C has an energy functional $\mathcal{O}_C(x_a, x_b)$ and average energy $< \mathcal{O}_C >$, and is characterized by a parameter ν_C. Again by Theorem 2.2 the density maximizing the entropy of the combined system C will be given by

$$f_{*C}(x_a, x_b) = \frac{1}{Z_C}e^{-\nu_C \mathcal{O}_C(x_a, x_b)} \tag{2.10}$$

with

$$Z_C = \int_{X_A \times X_B} e^{-\nu_C \mathcal{O}_C(x_a, x_b)}\, dx_a\, dx_b.$$

If systems A and B do not interact, then the density of the combined system C will be the product of the individual densities of systems A and B:

$$f_C(x_a, x_b) = f_A(x_a)f_B(x_b). \tag{2.11}$$

Furthermore, the energy of the combined system, $\mathcal{O}_C$, will be the sum of the separate energies of system A and system B:

$$\mathcal{O}_C(x_a, x_b) = \mathcal{O}_A(x_a) + \mathcal{O}_B(x_b) \qquad \text{and} \qquad <\mathcal{O}_C> = <\mathcal{O}_A> + <\mathcal{O}_B>. \tag{2.12}$$

Remember from Theorem 2.2 that the $<\mathcal{O}>$'s are nonegative. Inserting equations (2.8) and (2.9) into the right hand side of (2.11), and (2.10) into the left hand side along with the relations (2.12) gives

$$\frac{1}{Z_C} e^{-\nu_C[\mathcal{O}_A(x_a) + \mathcal{O}_B(x_b)]} = \frac{1}{Z_A Z_B} e^{-\nu_A \mathcal{O}_A(x_a) - \nu_B \mathcal{O}_B(x_b)} \tag{2.13}$$

Now consider two possibilities. First, assume that the two systems A and B are characterized by the same parameter $\nu = \nu_A = \nu_B$. Then it is clear from (2.13) that $\nu_C = \nu$. If the parameter ν is a monotone function of temperature then this argument implies that combining two systems of the same temperature ($\nu_A = \nu_B$) results in a system of the same temperature.

Next, assume that $\nu_A < \nu_B$. Then, how can equation (2.13) be satisfied? Clearly, if the combined system C has a parameter ν_C such that

$$\nu_C \mathcal{O}_C(x_a, x_b) = \nu_A \mathcal{O}_A(x_a) + \nu_B \mathcal{O}_B(x_b),$$

then (2.13) will be satisfied. What is the value of the parameter ν_C? It is easily obtained by multiplying the last relationship by $f_C = f_A f_B$ and integrating over the product space $X_C = X_A \times X_B$ to obtain

$$\nu_C <\mathcal{O}_C> = \nu_A <\mathcal{O}_A> + \nu_B <\mathcal{O}_B>. \tag{2.14}$$

Furthermore, by writing (2.14) in the form

$$\nu_C = \nu_A r + \nu_B(1 - r),$$

where $0 < r = \frac{<\mathcal{O}_A>}{<\mathcal{O}_A> + <\mathcal{O}_B>} < 1$, it is clear that $\nu_C < \nu_B$. Alternately, equation (2.14) can be rewritten in the form

$$\nu_C = \nu_A(1 - s) + \nu_B s,$$

where $0 < s = \frac{<\mathcal{O}_B>}{<\mathcal{O}_A> + <\mathcal{O}_B>} < 1$, so $\nu_A < \nu_C$. Thus we have proved that when $\nu_A < \nu_B$ the parameter ν_C of the combined system is limited by

$$\nu_A < \nu_C < \nu_B.$$

If ν is interpreted as a monotone function of temperature this last result is in accord with our experience, since combining two systems of two different temperatures T_A and T_B will result in a combined system with a temperature T_C intermediate between T_A and T_B.

Thus, we conclude from these arguments that ν is a monotone function of the inverse temperature. If we take ν to be

$$\nu = \frac{1}{kT}$$

where k is Boltzmann's constant, then the entropy expression in (2.7) becomes

$$S_{TD}^* = c \log Z + cU/kT,$$

or

$$TS_{TD}^* = cT \log Z + (c/k)U. \tag{2.15}$$

If the constant c is taken to be identical with Boltzmann's constant, $c \equiv k$, then (2.15) immediately gives the **Gibb's function**

$$F = U - TS_{TD}^*, \tag{2.16}$$

the fundamental equation of equilibrium thermodynamics relating the **Helmholtz free energy**

$$F = -kT \log Z$$

to the internal energy U, temperature T, and equilibrium entropy S_{TD}^*.

Thus, by the use of Postulates A through D in conjunction with the identification of certain parameters and functions with corresponding quantities of thermodynamic interest, the result is the fundamental relationship on which all of equilibrium thermodynamics is based.

D. BOLTZMANN AND OTHER STATISTICS.

In addition to the relative ease with which the fundamental relationships of equilibrium thermodynamics can be deduced by a suitable identification of quantities in the density of the canonical ensemble, other results can be obtained by considering situations in which the energy functional is specified.

Continuous Energy Spectrum. First, consider the situation in which we have a system for which the energy functional is continuous and given by

$$\mathcal{O}(p) = \epsilon_0 + \frac{p^2}{2m},$$

where ϵ_0 is a zero point energy and p is the momentum, taken to be continuous. This might, for example, describe the situation in a one dimensional classical gas. The partition function is

$$Z = \sqrt{\frac{2\pi m}{\nu}} e^{-\nu \epsilon_0},$$

while the density maximizing the entropy is just

$$f_*(p) = \sqrt{\frac{\nu}{2\pi m}} e^{-\frac{\nu p^2}{2m}}, \tag{2.17}$$

and the parameter ν and the average energy $< \mathcal{O} >$ are connected by the relation

$$\nu^{-1} = < \mathcal{O} > -\epsilon_0$$

as before. Taking $\nu^{-1} = kT$ as we have argued for in the previous section, (2.17) takes the form

$$f_*(p) = \sqrt{\frac{1}{2\pi m kT}} e^{-\frac{p^2}{2m kT}},$$

which is the continuous **Maxwell-Boltzmann distribution** for particle momenta in one dimension, and $kT = < \mathcal{O} > -\epsilon_0$.

This picture changes quite radically if the assumption concerning the continuity of the energy spectrum $\mathcal{O}$ of the system is replaced by the assumption that it is discrete.

Discrete Two-level Energy Spectrum. As an example consider the situation in which the energy functional has only two values

$$\mathcal{O}(0) = \epsilon_0 \qquad \text{or} \qquad \mathcal{O}(1) = \epsilon_0 + \delta\epsilon,$$

where ϵ_0 and $\delta\epsilon$ are both constants with the dimensions of energy. ϵ_0 is to be thought of as some "ground state energy" $\mathcal{O}(0)$, while $\delta\epsilon$ is the value by which the energy can increment to its second level $\mathcal{O}(1)$. Now in searching for a density which maximizes the entropy we must interpret the integrals in equations (1.1), (2.3), and (2.6) as Stieltjes integrals from which we easily calculate that the partition function Z is given by

$$Z = e^{-\nu \epsilon_0}(1 + e^{-\nu \delta\epsilon}),$$

and thus the density maximizing the entropy is simply

$$f_*(0) = \frac{1}{1 + e^{-\nu \delta\epsilon}} \qquad \text{and} \qquad f_*(1) = \frac{e^{-\nu \delta\epsilon}}{1 + e^{-\nu \delta\epsilon}}.$$

Discrete Equally Spaced Multi-level Spectrum. Alternately, consider the situation in which the energy function can take on a number of discrete values of the form

$$\mathcal{O}(n) = \epsilon_0 + n\delta\epsilon \qquad n = 0, 1, \cdots, \tag{2.18}$$

where ϵ_0 and $\delta\epsilon$ are interpreted as before.

In this case the partition function Z is given by

$$Z = \frac{e^{-\nu \epsilon_0}}{1 - e^{-\nu \delta\epsilon}}, \tag{2.19}$$

and the density maximizing the entropy is

$$f_*(n) = [1 - e^{-\nu \delta\epsilon}] e^{-\nu n \delta\epsilon} \qquad n = 0, 1, \cdots. \tag{2.20}$$

General Discrete Multi-level Spectrum. Finally, we look at the situation in which the system energy may take any one of $(m+1)$ discrete values,

$$\mathcal{O}(n) = \epsilon_0 + \epsilon_n, \qquad n = 0, \cdots, m$$

where m may be finite or not. Now the partition function is easily calculated to be

$$Z = e^{-\nu \epsilon_0} \sum_{i=0}^{m} e^{-\nu \epsilon_i},$$

and the density maximizing the Boltzmann Gibbs entropy is

$$f_*(n) = \frac{e^{-\nu \epsilon_n}}{\sum_{i=0}^{m} e^{-\nu \epsilon_i}}, \qquad n = 0, \cdots, m,$$

which is just the density of the **discrete Maxwell Boltzmann distribution**.

E. BLACKBODY RADIATION.

In the previous section when we considered the case where the energy had a discrete and equally spaced multi-level spectrum, had we allowed all values of $n \in R^+$ and not restricted ourselves to integer values of n in equation (2.18), the corresponding result would have been

$$f_*(n) = \nu \delta \epsilon \, e^{-\nu n \delta \epsilon},$$

which does not seem too different from (2.20). However, the differences become immediately apparent when the average energy $< \mathcal{O} >$ is calculated in the discrete (integral n) case:

$$< \mathcal{O} > = \sum_{n=0}^{\infty} [\epsilon_0 + n\delta\epsilon] f_*(n)$$

$$= \epsilon_0 + \frac{\delta\epsilon \, e^{-\nu\delta\epsilon}}{1 - e^{-\nu\delta\epsilon}}. \tag{2.21}$$

If it is assumed that the energy functional in (2.18) is that of a system in which there is a strict relationship between the frequency of oscillation and the incremental energy $\delta\epsilon$ of the form

$$\delta\epsilon = \hbar\omega,$$

and that $\nu = 1/kT$ as we have argued for in Section C, then (2.21) takes the form

$$< \mathcal{O}(\omega, T) > -\epsilon_0 = \hbar\omega \frac{e^{-\frac{\hbar\omega}{kT}}}{1 - e^{-\frac{\hbar\omega}{kT}}}. \tag{2.22}$$

This will be immediately recognized as the Planck formula for the average energy of a system of oscillators (relative to the ground state energy ϵ_0) at a temperature T and frequency ω. From this it is quite straightforward to derive the Planck formula for the spectrum of black body radiation $\epsilon(\omega, T)$ from the general relation

$$\epsilon(\omega, T) = [< \mathcal{O}(\omega, T) > -\epsilon_0] \frac{\omega^2}{\pi^2 c^3}, \tag{2.23}$$

where c is the velocity of light. Substituting (2.22) into (2.23) immediately gives the **Planck blackbody radiation formula**

$$\epsilon(\omega, T) = \frac{\hbar}{\pi^2 c^3} \frac{\omega^3}{e^{\frac{\hbar\omega}{kT}} - 1}. \tag{2.24}$$

Note that had we used the result for the average energy of an ensemble with a continuous dependence on n in (2.18), then the result would have been

$$\epsilon(\omega, T) = \frac{kT}{\pi^2 c^3} \omega^2, \tag{2.25}$$

the **Rayliegh-Jeans radiation law** with its "ultraviolet catastrophe". The same expression results from (2.24) in the high temperature limit with $\hbar\omega \ll kT$, while the low temperature limit with $\hbar\omega \gg kT$ gives the **Wien radiation law**

$$\epsilon(\omega, T) = \frac{\hbar}{\pi^2 c^3} \omega^3 e^{-\frac{\hbar\omega}{kT}}.$$

F. GENERAL ENTROPY MAXIMA.

It is quite easy to state and prove an obvious generalization of Theorem 2.2 applicable to systems in which there are multiple known averages $< \mathcal{O}_i >$. This generalization is contained in:

Theorem 2.3. *Assume that a sequence of m non-negative measurable functions $\mathcal{O}_i(x)$, $i = 1, \ldots, m$, and their averages $< \mathcal{O}_i >$ over the entire space X are given. Then the maximum of the entropy $H(f)$ for all densities f, subject to the conditions*

$$< \mathcal{O}_i >= \int_X \mathcal{O}_i(x) f(x) \, dx \tag{2.26}$$

occurs for the density

$$f_*(x) = \frac{1}{Z} \prod_{i=1}^m e^{-\nu_i \mathcal{O}_i(x)} \tag{2.27}$$

where

$$Z = \int_X \prod_{i=1}^m e^{-\nu_i \mathcal{O}_i(x)} \, dx, \tag{2.28}$$

and the ν_i's are implicitly determined from

$$< \mathcal{O}_i >= \frac{1}{Z} \int_X \mathcal{O}_i(x) e^{-\nu_i \mathcal{O}_i(x)} \, dx. \tag{2.29}$$

Proof. The demonstration is an extension of the proof of Theorem 2.2. □

The density (2.27) maximizing the entropy is a generalization of the density of the grand canonical ensemble. If we know that a given system has a number of independent averages (2.26) of functions $\mathcal{O}_i(x)$, then the content of Theorem 2.3 can be used to construct the density that maximizes the entropy. This density can, in turn, be used to construct a generalized thermodynamics for that system. Grad (1952) and Jaynes (1957) have followed this procedure.

G. MAXIMAL ENTROPY PRINCIPLES.

As attempts to justify Postulate D on dynamical grounds increasingly met with failure, more and more authors tried to enshrine this hypothesis as a basic principle, often known as the **Maximal Entropy Principle**. Tolman (1938) seems to have been one of the first to espouse this point of view. He argued that since the techniques being used in thermodynamics were statistical in nature, one had to have some principle that would guide the selection of the proper density out of the unlimited number of possibilities. The Maxmimal Entropy Principle certainly offers one such guide. Jaynes (1957), Scalapino (1961), and Katz (1967) have written extensively on the use of the maximal entropy principle in reformulating classical and quantum statistical mechanics, and Lewis (1967) has tried to justify it on dynamical grounds.

It may appear that the use of the maximal entropy principle gives a great deal (equilibrium thermodynamics) for very little. Such is surely not the case. In actuality the hardest aspect of the understanding of thermodynamics is determining which systems, described by densities, will evolve toward equilibrium in such a way that the entropy is maximized.

H. SUMMARY.

Based on the topics covered in this chapter it is clear that the central questions of what systems can be reasonably described by densities that approach a limit that maximizes the entropy rank as the most important ones that must be answered if we are to have any clear and comprehensive understanding of the foundations of thermodynamics since (Postulate D) we assume that the density maximizing the entropy characterizes the physically attained state of thermodynamic equilibrium. The treatment of these problems constitutes the remainder of this book.

PART II.
DYNAMICS AND THERMODYNAMICS

CHAPTER 3.
INVERTIBLE AND NONINVERTIBLE SYSTEMS.

From the perspective of the previous chapter, the central problem in thermodynamics is "How may one guarantee that the entropy of a system will increase to its maximum value regardless of the manner in which it was prepared?" In this chapter we start our investigation of this question.

We first introduce in Section A the concept of a Markov operator, which describes the evolution of densities in a variety of important physical situations. Frobenius-Perron operators, special types of Markov operators, are touched on only briefly as they are introduced formally in Chapter 4.

In Section B we turn to a consideration of the behaviour of the entropy of a sequence of densities evolving under the action of a Markov operator. We first define the conditional entropy, a generalization of the Boltzmann-Gibbs entropy, argue that it is a reasonable analog of the entropy difference ΔS, and then show that this entropy is either stationary (constant) or increasing. Following this it is demonstrated that for an invertible Markov operator the entropy is always constant, while for noninvertible Markov operators the entropy *may* increase. This establishes the not too surprising result that noninvertibility is necessary (though not necessarily sufficient) for the entropy of any system to increase.

Fixed points of the Markov and Frobenius-Perron operators, known as stationary densities, correspond to states of (relative or absolute) thermodynamic equilibrium, and several sufficient conditions for the existence of these equilibrium states are given in Section C.

A. MARKOV OPERATORS.

In every situation considered by theoretical physics, as developed to this point in time, the evolution of densities may be studied by the use of the linear Markov, Frobenius-Perron, or Koopman operators. This is in spite of the fact that the underlying system dynamics responsible for the evolution of the density may be highly nonlinear.

The Frobenius-Perron and Koopman operators, introduced formally in the next chapter, are the two most useful types of operators to describe the evolution of densities in systems for which the dynamics are totally deterministic, *i.e.* the dynamics evolve according to a very specific law that in principle permits the accurate specification of a system trajectory at any point in time.

Example 3.1. As an example in which the evolution of the density is described by the Frobenius-Perron operator, consider a set of ordinary differential equations operating in R^d:

$$\frac{dx_i}{dt} = F_i(x) \qquad i = 1, \ldots, d. \tag{3.1}$$

As shown in Chapter 4, starting from an initial density $f(x)$, the evolution of the time dependent density $f(t,x) \equiv P^t f(x)$ (here P is a Frobenius-Perron operator) is described by the **generalized Liouville equation**

$$\frac{\partial f}{\partial t} = -\sum_i \frac{\partial (fF_i)}{\partial x_i}. \qquad \bullet \tag{3.2}$$

The Frobenius-Perron and Koopman operators are special cases of the more general Markov operator which may be used in the description of both deterministic and stochastic systems. Since the first results on invertibility and noninvertibility that are of importance for an understanding of thermodynamics can be stated for Markov operators, we start with them and defer the formal introduction of the Frobenius-Perron and Koopman operators to the next chapter.

Any linear operator $P : L^1 \to L^1$ that satisfies

(1) $P^t f \geq 0$; and
(2) $\| P^t f \| = \| f \|$

for all $t \in R$ and $f \geq 0$, $f \in L^1$ is called a **Markov operator**. *If we restrict ourselves to only considering densities f, then any operator P which when acting on a density again yields a density is a Markov operator.* It is important to remember that although we usually state results concerning the dynamical behavior of Markov operators in terms of their action on densities, these results also usually hold for all L^1 functions.

Example 3.2. As an example of a system in which the evolution of the density is governed by the operation of a Markov operator, consider the system of stochastic differential equations

$$\frac{dx_i}{dt} = F_i(x) + \sigma(x)\xi_i, \qquad i = 1, \ldots, d \tag{3.3}$$

obtained when the system of ordinary differential equations (3.1) is perturbed by white noise ξ_i of amplitude $\sigma(x)$. Then, as we consider in Chapter 11, starting from an initial density $f(x)$ the evolution of the time dependent density $f(t,x) \equiv P^t f(x)$ (now P is a Markov operator) satisfies

$$\frac{\partial f}{\partial t} = -\sum_i \frac{\partial(fF_i)}{\partial x_i} + \frac{1}{2}\sum_{i,j} \frac{\partial^2(\sigma^2 f)}{\partial x_i \partial x_j}, \tag{3.4}$$

a modified form of the generalized Liouville equation (3.2) known as the **Fokker-Planck equation**. •

Markov operators have a number of useful properties. Since they are easy to demonstrate, we only state them here and leave their proof as an exercise. In stating these properties, as well as later, we will find it useful to introduce the notation

$$f^+(x) = \max(0, f(x)) \quad \text{and} \quad f^-(x) = \max(0, -f(x)).$$

There are four properties that hold for every $f \in L^1$ (note that we are not restricting ourselves to densities, or even to nonnegative f):

(1) $(P^t f(x))^+ \le P^t f^+(x)$
(2) $(P^t f(x))^- \le P^t f^-(x)$
(3) $|P^t f(x)| \le P^t |f(x)|$
(4) $\| P^t f \| \le \| f \|$.

The last is the most important, and it states the *contractive property* of P. This contractivity implies that during the iteration of two functions f_1 and f_2 by a Markov operator P, the distance between the two functions, $f = f_1 - f_2$, can only decrease or stay constant and will never increase.

With the concept of the Markov operator, we can introduce the important notions of fixed points and stationary densities. If an L^1 function f_* satisfies $P^t f_* = f_*$ for all t, then f_* is called a **fixed point** of the Markov operator.[1] If, further, f_* is a density, then f_* is known as a **stationary density**. The importance of stationary densities comes from the fact that *the existence of a stationary density may be associated with a state of thermodynamic equilibrium* using the material at the end of the next section.

Example 3.3. For the system of ordinary differential equations (3.1), the stationary densities f_* are given by the solutions of

$$-\sum_i \frac{\partial(f_*F_i)}{\partial x_i} = 0,$$

while for the stochastic differential equations (3.3) the f_* are the solutions of

$$-\sum_i \frac{\partial(f_*F_i)}{\partial x_i} + \frac{1}{2}\sum_{i,j} \frac{\partial^2(\sigma^2 f_*)}{\partial x_i \partial x_j} = 0. \bullet$$

In precise analogy with the definitions of dynamical and semidynamical systems in Chapter 1, we may discuss invertible and noninvertible Markov operators. Given a Markov operator P^t, then P^t is an **invertible Markov operator** if:

(1) $P^0 f = f$ and
(2) $P^t(P^{t'} f) = P^{t+t'} f \qquad$ for all $t, t' \in R$ (or Z).

Clearly, allowing $t, t' \in R$ or Z is the origin of the invertibility.

---

[1] There is a result concerning the fixed points of a Markov operator P^t that will be used a number of times. That is, if $P^t f_* = f_*$ for all t, then $P^t f_*^+ = f_*^+$ and $P^t f_*^- = f_*^-$. The demonstration is quite easy, since if f_* is a fixed point of P^t, then $f_*^+ = (P^t f_*)^+ \le P^t f_*^+$ and $f_*^- = (P^t f_*)^- \le P^t f_*^-$. Thus $\int_X [P^t f_*^+(x) - f_*^+(x)]\,dx + \int_X [P^t f_*^-(x) - f_*^-(x)]\,dx = \int_X P^t |f_*(x)|\,dx - \int_X |f_*(x)|\,dx = \| P^t |f_*| \| - \| |f_*| \| \le 0$ since P^t is contractive. Since $P^t f_*^+ - f_*^+ \ge 0$ and $P^t f_*^- - f_*^- \ge 0$, then we must have $P^t f_*^+ = f_*^+$ and $P^t f_*^- = f_*^-$.

Example 3.4. As an example of an invertible Markov operator, again consider the evolution of the density f described by the Liouville equation (3.2) for dynamics determined by the system of ordinary differential equations (3.1). Replacing t by $-t$ in (3.1) gives dynamics described by $dx/dt = -F_i(x)$, and the corresponding generalized Liouville equation (3.2) becomes

$$\frac{\partial f}{\partial t} = \sum_i \frac{\partial (f F_i)}{\partial x_i},$$

so the equation for the evolution of the density $f(t, x)$ is simply related to (3.2) by a change of sign corresponding to the transformation $t \to -t$ or, equivalently, to a reversal of the dynamics $F_i \to -F_i$.•

If the definition of an invertible Markov operator is replaced by

(1) $P^0 f = f$ and

(2) $P^t(P^{t'} f) = P^{t+t'} f$ for all $t, t' \in R^+$ (or N),

then P is a **noninvertible Markov operator**.

Example 3.5. The stochastic differential equation (3.3) with its associated Fokker-Planck equation (3.4) is an example of an equation governing the evolution of a noninvertible Markov operator. Going through the same exercise of replacing t by $-t$ in the stochastic differential equation yields a corresponding Fokker-Planck equation

$$\frac{\partial f}{\partial t} = \sum_i \frac{\partial (f F_i)}{\partial x_i} + \frac{1}{2} \sum_{i,j} \frac{\partial^2 (\sigma^2 f)}{\partial x_i \partial x_j}$$

that is different from the original equation (3.4) since the sign of the second term on the right hand side, arising from the noise, is reversed. As a consequence the equation for the evolution of the density $f(t, x)$ does not correspond to a reversal of the dynamics $F_i \to -F_i$.•

Example 3.6. To illustrate some of the concepts of this section, choose the discrete time transformation

$$S(x) = \begin{cases} 2x & 0 \le x < \frac{1}{2} \\ 2(1-x) & \frac{1}{2} \le x \le 1, \end{cases} \tag{3.5}$$

so $x_{t+1} = S(x_t)$, $t \ge 0$. This noninvertible transformation is commonly known as the **hat** or **tent map** after the appearance of its graph shown in Figure 3.1.

To investigate how the tent map (3.5) transforms densities, we first derive an expression for the operator P corresponding to this transformation. (This operator is actually a Frobenius Perron operator.) To do this, suppose first of all that we start with some initial density f which is transformed by one application of the map S into a new density Pf. Then the fraction of the density Pf contained in some interval $[0, x]$ is given by

$$\int_0^x Pf(s)\, ds.$$

After one application of the map S the points in $[0, x]$, which have contributed to Pf, had their origin in the counterimage of the interval $[0, x]$ under the action of S. This is denoted by $S^{-1}([0, x])$ and defined by $S^{-1}([0, x]) = \{y : S(y) \in [0, x]\}$. With these comments, it must be the case that the fraction of the density Pf in the interval $[0, x]$ is equal to the fraction of the original density f in the set $S^{-1}([0, x])$, or that

$$\int_0^x Pf(s)\, ds = \int_{S^{-1}([0,x])} f(s)\, ds.$$

For the tent map it is a straightforward calculation to show that the counterimage of an interval $[0, x]$ is given explicitly by the union of two intervals:

$$S^{-1}([0, x]) = [0, \tfrac{1}{2}x] \cup [1 - \tfrac{1}{2}x, 1].$$

Substituting this into the previous integral expression between f and P gives the result

$$\int_0^x Pf(s)\, ds = \int_0^{\frac{x}{2}} f(s)\, ds + \int_{1-\frac{x}{2}}^1 f(s)\, ds.$$

Finally, differentiating both sides of this expression with respect to x gives an explicit form for Pf in terms of f:

$$Pf(x) = \tfrac{1}{2}[f(\tfrac{1}{2}x) + f(1 - \tfrac{1}{2}x)]. \tag{3.6}$$

This expression for the Frobenius-Perron operator P corresponding to the tent map (3.5) is a noninvertible Markov operator. It is a straightforward exercise to show that the uniform density $f_* = 1$ is a stationary density for the operator P defined by (3.6) since it satisfies $Pf_* = f_*$. $\bullet$

In closing this section, it is appropriate to point out a useful consequence of the Radon-Nikodym theorem. We consider two measures μ_* and ν_* on a phase space X, and assume that $\mu_*(A) = 0$ for all sets $A \subset X$ such that $\nu_*(A) = 0$, and *vice versa*. Then it follows from the Radon-Nikodym theorem that there are unique non-negative integrable functions g and h such that

$$\nu_*(A) = \int_A g(x)\, \mu_*(dx),$$

and

$$\mu_*(A) = \int_A h(x)\, \nu_*(dx).$$

Now assume that f is a density with respect to the measure μ_*. This then implies from the above that

$$\int_X f(x)\, \mu_*(dx) \equiv 1 \equiv \int_X f(x)h(x)\, \nu_*(dx),$$

or that when f is a density with respect to the measure μ_*, then (fh) is a density with respect to the measure ν_*. Conversely, if f is a density with respect to the measure ν_* then (fg) is a density with respect to μ_*.

In the special case that one of the measures is the Lebesgue measure, $\nu_* = \mu_L$ for example, then it is an immediate consequence of these observations that if f_* is the density of the measure μ_* we can identify $h = f_*$ and $g = 1/f_*$.

Now consider a Markov operator P with a stationary density f_*. By definition, $\| Pf \| = \| f \|$ if f is a density, which can be rewritten as

$$\int_X \frac{Pf(x)}{f_*(x)}\, \mu_*(dx) = \int_X \frac{f(x)}{f_*(x)}\, \mu_*(dx) = 1.$$

Since (f/f_*) is a density with respect to μ_* we can define a new Markov operator R by

$$Rh = \frac{P(hf_*)}{Pf_*},$$

where h is a density with respect to μ_* and (hf_*) is a density with respect to the Lebesgue measure μ_L.

Markov operators, whether invertible or noninvertible, are quite general. In many situations it is possible to talk about the evolution of densities in physical systems by studying the properties of special types of Markov operators like the Frobenius-Perron and Koopman operators. On some occasions we may be able to state results that are only true in a discrete time system. If this is the case, then a note to this effect will be made. Otherwise, it is to be implicitly understood that all results hold for both continuous and discrete time systems.

B. CONDITIONAL ENTROPY.

Before starting an examination of the behaviour of the entropy of a density under the action of a Markov operator, we introduce a generalization of the Boltzmann-Gibbs entropy, the **conditional entropy**. We start with a motivating example.

Example 3.7. We examine the behaviour of the Boltzmann Gibbs entropy when the system dynamics are governed by the quadratic map

$$S(x) = rx(1 - x) \tag{3.7}$$

operating on the phase space $[0, 1]$ when $r = 4$. (It is precisely for this value of r, and no other, that the map is onto, see Figure 3.2.) This transformation, like the tent map, is not invertible, and indeed can be obtained from the tent map (3.5) from $S_Q = h^{-1} \circ S_T \circ h$, where S_Q and S_T denote, respectively, the quadratic and tent maps and the conjugating function h is given by

$$h(x) = \frac{1}{2} - \frac{1}{\pi}\sin^{-1}(1 - 2x)$$

so
$$h^{-1}(x) = \frac{1}{2} - \frac{1}{2}\cos(\pi x).$$

[Two functions S_T and S_Q are said to be **conjugate** if there exists a transformation h such that $S_Q = h^{-1} \circ S_T \circ h$, where "$\circ$" denotes composition.]

To construct the Frobenius-Perron operator P governing the evolution of densities by the quadratic transformation (3.7), proceed as for the tent map. Given a set $[0, x]$ it is straightforward to show that the counterimage of this set consists of the union of two disjoint intervals:

$$S^{-1}([0,x]) = [0, \tfrac{1}{2}(1 - \sqrt{(1-x)}] \cup [\tfrac{1}{2}(1 + \sqrt{(1-x)}, 1].$$

Thus, the operator P corresponding to the quadratic map (3.7) with $r = 4$ is

$$Pf(x) = \frac{1}{4\sqrt{(1-x)}}\{f(\tfrac{1}{2} - \tfrac{1}{2}\sqrt{(1-x)}) + f(\tfrac{1}{2} + \tfrac{1}{2}\sqrt{(1-x)})\} \tag{3.8}$$

It is easy to verify that the nonuniform density

$$f_*(x) = \frac{1}{\pi\sqrt{x(1-x)}} \tag{3.9}$$

is a stationary density of P defined by (3.8).

Now consider the Boltzmann-Gibbs entropy of a density evolving under the action of the operator P defined by equation (3.8). Pick as an initial density $f = 1$, so $H(f) = 0$. Further, with this choice of initial density, from (3.8)

$$Pf(x) = \frac{1}{2\sqrt{1-x}},$$

and the Boltzmann-Gibbs entropy of Pf is given by

$$H(Pf) = -\int_0^1 \frac{1}{2\sqrt{1-x}}\log\left[\frac{1}{2\sqrt{1-x}}\right]\, dx = \log 2 - 1.$$

Obviously, $H(Pf) < H(f) = 0$, and the Boltzmann-Gibbs entropy has decreased! $\bullet$

In Chapter 2 we associated the equilibrium thermodynamic entropy S_{TD}^* with the maximum Boltzmann Gibbs entropy $H(f_*)$, and showed how this and other assumptions led to the fundamental relation (2.16) of equilibrium thermodynamics. However, as the previous example clearly shows, the time dependent Boltzmann Gibbs entropy may in fact decrease. This behaviour is unacceptable if we are to be able to draw a connection between the behaviour of the Boltzmann-Gibbs entropy and the temporal behaviour of thermodynamic entropy. The way out of this difficulty involves the definition of a generalization of the Boltzmann-Gibbs entropy called the conditional entropy.

If f and g are two densities such that supp $f \subset$ supp g [supp f denotes the **support** of f], then the **conditional entropy** of the density f with respect to the density g is

$$\begin{aligned}
H_c(f|g) &= \int_X g(x)\eta\left(\frac{f(x)}{g(x)}\right)\, dx \\
&= -\int_X f(x)\log\left[\frac{f(x)}{g(x)}\right]\, dx \tag{3.10}
\end{aligned}$$

Note that the conditional entropy is always defined, *i.e.* H_c is finite or equal to $-\infty$, since g is a density and η is a bounded function. As is evident from the defining equation (3.10), $H_c(f|g)$ measures the deviation between the two densities f and g.

There are two important properties of $H_c(f|g)$:

(1) Since f and g are both densities, the integrated Gibbs inequality (1.5) implies that $H_c(f|g) \leq 0$. It is only when $f = g$ that the equality holds.

(2) If g is the constant density of the microcanonical ensemble, *i.e.* $g = 1/\mu_L(X)$ throughout the phase space X, then $H_c(f|g) = H(f) - \log\mu_L(X)$. If the space X is normalized, then $g = 1$ and $H_c(f|1) = H(f)$. This illustrates how the conditional entropy is a generalization of the Boltzmann-Gibbs entropy.

From the definition of $H_c(f|g)$ it follows that

$$H_c(f|g) = H(f) + \int_X f(x) \log g(x)\, dx$$
$$= H(f) - H(g) + \int_X [f(x) - g(x)] \log g(x)\, dx.$$

Replace f by $P^t f$ and identify $g = f_*$ where f_* is a stationary density of P. Then we have

$$H_c(P^t f|f_*) = H(P^t f) - H(f_*) + \int_X [P^t f(x) - f_*] \log f_*(x)\, dx.$$

Under the conditions of Theorem 2.2, the Boltzmann-Gibbs entropy $H(f)$ is maximized by the density f_* given by equation (2.4) and

$$H(f_*) = \log Z + \nu <\alpha> . \tag{3.11}$$

Thus, within the context of Theorem 2.2 we conclude that the conditional entropy will be zero whenever the Boltzmann-Gibbs entropy is at its maximum value of $H(f_*)$ if, in addition, $\lim_{t\to\infty} P^t f = f_*$.

These observations, in conjunction with our formulations of the weak and strong forms of the Second Law, immediately suggest that the conditional entropy H_c be interpreted as the difference between the thermodynamic entropy and the equilibrium entropy. With only the few tools developed so far, the behaviour of the entropy of a sequence of densities $\{P^t f\}$ evolving under the action of a Markov operator may be examined in light of our identification of H_c with ΔS.

The first result along these lines validating this association is a result stating that the conditional entropy is never decreasing. More precisely,

Theorem 3.1. *(Voigt, 1981). Let P be a Markov operator. Then*

$$H_c(P^t f|P^t g) \geq H_c(f|g)$$

for $f \geq 0$, and all densities g.

Proof. Though Voigt (1981) has given the full proof, we only consider the situation in which $g > 0$ so f/g is bounded, and $P^t g > 0$, as this is quite easy.

Remembering our comments at the end of the previous section, we define a new operator $R : L^\infty \to L^\infty$ (remember that L^∞ just consists of bounded measurable functions) by

$$R^t h = \frac{P^t(hg)}{P^t g}.$$

This new operator has the properties that $R^t h \geq 0$ when $h \geq 0$, $R^t 1 = 1$, and if g is a stationary density of the operator P^t then $g R^t h = P^t(hg)$.

For any function $\eta(u)$, $u \geq 0$, with a concave graph (*i.e.* $\eta'' \leq 0$), and a linear operator $P^t : L^p \to L^p$, $1 \leq p \leq \infty$ that satisfies $P^t 1 = 1$ and $P^t f \geq 0$, the **Jensen inequality**

$$\eta(P^t f) \geq P^t \eta(f) \tag{3.12}$$

holds for all nonnegative L^p functions f whenever $P^t \eta(f)$ exists (Kuczma, 1985). [Insight into the origin of the Jensen inequality (3.12) can be obtained by considering Figure 1.1. Pick a point $u \in [0, v]$ so we can write $u = \alpha v$ with $\alpha \in [0, 1]$. It is a simple matter of geometry to show that $\eta(u) \equiv \eta(\alpha v) \geq \alpha \eta(v)$.]

It is easy to show that the operator R^t satisfies the Jensen inequality so

$$\eta(R^t h) \geq R^t \eta(h). \tag{3.13}$$

If we take h to be f/g and $\eta(u) = -u \log u$, then the left hand side of this inequality becomes

$$\eta(R^t h) = -\frac{P^t f}{P^t g} \log \left[\frac{P^t f}{P^t g} \right]$$

while the right hand side is

$$R^t \eta(h) = \frac{P^t((\eta \circ h)g)}{P^t g} = -\frac{P^t \left(f \log \left[\frac{f}{g} \right] \right)}{P^t g}.$$

Thus (3.13) is equivalent to

$$-P^t f \log \left[\frac{P^t f}{P^t g} \right] \geq -P^t \left[f \log \left(\frac{f}{g} \right) \right].$$

Integration of this expression over the entire phase space gives

$$
\begin{aligned}
H_c(P^t f | P^t g) &\geq - \int_X P^t \left\{ f(x) \log \left[\frac{f(x)}{g(x)} \right] \right\} dx \\
&= - \int_X f(x) \log \left[\frac{f(x)}{g(x)} \right] dx \\
&= H_c(f|g),
\end{aligned}
$$

which completes the proof. $\square$

Notice in this theorem that if $g = f_*$ is a stationary density of P^t so $P^t f_* = f_*$, then

$$H_c(P^t f | f_*) \geq H_c(f | f_*).$$

Thus the conditional entropy with respect to a stationary density is always a nondecreasing function bounded above by $H_{max} = H_c(f_* | f_*) = 0$. In examining the behaviour of $H_c(P^t f | f_*)$ we therefore know that it has a limit as $t \to \infty$, though more information about P^t is required to define the limiting value.

In the special case that the system is operating on a finite space and the Markov operator P^t has the density of the microcanonical ensemble as a stationary density, i.e. $P^t 1 = 1$, then this theorem implies that

$$H(P^t f) \geq H(f)$$

for all nonnegative f. Coupling this with the observation from Chapter 2 that on a finite space the maximum entropy is $H_{max} = -\log \left[\frac{1}{\mu_L(X)} \right]$, we have

$$H_{max} = -\log \left[\frac{1}{\mu_L(X)} \right] \geq H(P^t f) \geq H(f)$$

for all t so, once again, $H(P^t f)$ has a limit as $t \to \infty$.

The conclusions of Theorem 3.1 seem to be precisely the same as those reached by Boltzmann (1909) in his pioneering work on the mechanical foundations of thermodynamics. However, things are not quite as transparent as this since to this point nothing has been said about the invertibility or noninvertibility of the Markov operator P with respect to the behaviour of the entropy. This distinction is crucial for the limiting value of $H_c(P^t f | f_*)$ since the entropy for an invertible Markov operator is constant and determined by the way in which the system is prepared. More precisely, for invertible Markov operators we can state the following theorem.

Theorem 3.2. *If P is an invertible Markov operator, then the conditional entropy is constant for all times t, and equal to the value determined by the choice of the initial densities f and g. That is,*

$$H_c(P^t f | P^t g) = H_c(f|g)$$

for all t.

Proof. Since P is invertible, by Theorem 3.1 it follows that

$$H_c(P^{t+t'} f | P^{t+t'} g) = H_c(P^{t'} P^t f | P^{t'} P^t g) \geq H_c(P^t f | P^t g) \geq H_c(f|g)$$

for all times t and t'. Pick $t' = -t$ so for all times t

$$H_c(f|g) \geq H_c(P^t f|P^t g) \geq H_c(f|g)$$

and therefore

$$H_c(P^t f|P^t g) = H_c(f|g)$$

for all t. $\square$

From this theorem, in any system whose evolution of densities is described by an invertible Markov operator the entropy is forever fixed at a value determined by the initial state. Or, put another way, the entropy is uniquely determined by the method of preparation of the system. A specialized form of the proof of Theorem 3.2 was used by Loschmidt (1876) in his *Umkehreinwand* (objection based on time reversal) argument against the Boltzmann approach to statistical mechanics.

Example 3.8. In particular, for the system of ordinary differential equations (3.1) whose density evolves according to the Liouville equation (3.2) we can assert that the entropy of the density $P^t f$ will be constant for all time and will have the value determined by the initial density f with which the system is prepared. This result can also be proved directly by noting that from the definition of the entropy we may write

$$H_c(f|f_*) = - \int_{R^d} f(x) \left[\log\left(\frac{f}{f_*}\right) + \frac{f_*}{f} - 1 \right] dx$$

when the stationary density is f_*. Differentiating with respect to time gives

$$\frac{dH_c}{dt} = - \int_{R^d} \frac{df}{dt} \log\left[\frac{f}{f_*}\right] dx \tag{3.14}$$

or, after substituting from (3.2) for $(\partial f/\partial t)$, and integrating by parts under the assumption that f has compact support,

$$\frac{dH_c}{dt} = \int_{R^d} \frac{f}{f_*} \sum_i \frac{\partial(f_* F_i)}{\partial x_i} dx.$$

Since f_* is a stationary density of P^t, it is clear from (3.2) that

$$\frac{dH_c}{dt} = 0,$$

and we conclude that the conditional entropy $H_c(P^t f|f_*)$ does not change from its initial value when the dynamics evolve in this manner. •

Thus, not too surprisingly, we conclude that *noninvertibility in system dynamics*, as reflected in an evolution of densities via a noninvertible Markov operator, *is necessary for the entropy to increase* as the system evolves. We cannot, however, assert that noninvertibility is sufficient to guarantee this, and indeed it is not the case.

Based on much more specific assumptions, this result concerning the necessity of noninvertibility was well known to Clausius (1879) and Boltzmann (1909), two of the founders of modern thermodynamic theory. How, then, did Boltzmann arrive at his conclusion that the entropy would increase to a maximum in a collection of particles moving under the action of (invertible) Hamiltonian dynamics? Both he and Clausius tried to circumvent this clear problem [the use of invertible (Hamiltonian) dynamics] by the addition of their *Stosszahlansatz* (molecular chaos) *postulate*. This reduces, quite simply, to a *postulate of noninvertibility*.

Spohn (1978) has put forward a slightly different interpretation of the conditional entropy defined in (3.10) when g is taken to be a unique stationary density f_*. This is done by starting from a (local phenomenological) balance equation for the entropy density $\mathcal{S}$

$$\frac{d\mathcal{S}}{dt} = -J_{\mathcal{S}} + \sigma,$$

where $J_{\mathcal{S}}$ is interpreted as an energy flow and $\sigma (\geq 0)$ is an entropy production. In the special case of a system coupled to a reservoir at a single temperature he identifies $\mathcal{S}$ with the Boltzmann-Gibbs entropy $H(f)$, the entropy production σ with

$$\sigma = \frac{dH_c(f|f_*)}{dt},$$

and the energy flow $J_{\mathcal{S}}$ with

$$J_{\mathcal{S}} = \frac{d}{dt} \int_X f(x) \log f_*(x)\, dx.$$

These relations follow immediately as a special case of the definition of the conditional entropy if one takes $g = f_*$, writes the definition (3.10) of the conditional entropy in the form

$$H(f) = - \int_X f(x) \log f_*(x)\, dx + H_c(f|f_*),$$

and takes the time derivative. In this interpretation the conditional entropy $H_c(f|f_*)$ is to be viewed as the entropy production integrated over time. It is a consequence of Theorem 3.1 that $\sigma \geq 0$ and that system noninvertibility is necessary (though not sufficient) for $\sigma > 0$.

C. EXISTENCE OF EQUILIBRIA.

As we have observed in the early part of this chapter, a stationary density f_* of a Markov operator P satisfies $P^t f_* = f_*$ for all times t. As a consequence, the existence of a stationary density f_* may be put into a one to one correspondence with a state of thermodynamic equilibrium. Thus, *in our attempts to ultimately examine the various ways in which systems approach equilibrium states*, and whether or not these routes to equilibrium correspond to situations in which the entropy increases to a maximum, *it is important to first have some concept of the conditions sufficient to ensure the existence of at least one state of thermodynamic equilibrium.* That is the goal of this section.

Throughout, use will be made of properties of the **system state density average**, defined by either

$$A_t f = \frac{1}{t} \sum_{k=0}^{t-1} P^k f \tag{3.15a}$$

in the discrete time case, or by

$$A_t f = \frac{1}{t} \int_0^t P^k f\, dk \tag{3.15b}$$

in the continuous time case, where P is a Markov operator.

First, note that from the definition of $A_t f$ in the discrete time case we can write the difference of two system state density averages as

$$A_t f - A_t P f = \frac{1}{t}(f - P^t f)$$

so

$$\| A_t f - A_t P f \| \leq \frac{1}{t} \left[\| f \| + \| P^t f \| \right] \leq \frac{2}{t} \| f \|$$

by the triangle inequality ($\| f + g \| \leq \| f \| + \| g \|$) and the contractive property of Markov operators. Similarly, in the continuous time case for any $\epsilon > 0$ we obtain

$$\| A_t f - A_t P^\epsilon f \| \leq \frac{2\epsilon}{t} \| f \|.$$

Taking the limit as $t \to \infty$ in both cases shows that

$$\lim_{t \to \infty} \| A_t f - A_t P^\epsilon f \| = 0$$

where $\epsilon = 1$ in the discrete time case.

As usual, on a measure space $(X, \mathcal{A}, \mu_*)$ the **scalar product** of an L^1 function f with a bounded measurable function $g \in L^\infty$, denoted by $< f, g >_*$, is defined by

$$< f, g >_* = \int_X f(x) g(x)\, \mu_*(dx).$$

Note that if $\mu_*(dx)$ is absolutely continuous with respect to the Lebesgue measure $\mu_L(dx) = dx$, then

$$< f, g >_* = \int_X f(x)g(x)f_*(x)\, dx = < ff_*, g >,$$

where the omission of a subscript "L" on the right hand term simply means that it is the scalar product with respect to the Lebesgue measure. Furthermore, a sequence $\{f_t\}$ of L^1 functions f_t is said to be **weakly convergent** to an L^1 function f if

$$\lim_{t \to \infty} < f_t, g > = < f, g > \qquad \text{for all} \quad g \in L^\infty.$$

Then we have the first sufficient condition for the existence of a state of thermodynamic equilibrium with a corresponding stationary density f_* of the Markov operator describing the evolution of system states.

Sufficient Equilibrium Condition (SEC) 3.3. *Given an initial system density f evolving under the action of a Markov operator P and a system state density average $A_t f$, if there is a subsequence $\{A_{\alpha_t} f\}$ of the sequence $\{A_t f\}$ that is weakly convergent to a density f_*, then $P^t f_* = f_*$ for all times t and a state of thermodynamic equilibrium exists.*

The proof follows immediately from the observation that since P is a linear operator, $P^t A_{\alpha_t} f = A_{\alpha_t} P^t f$ and thus $\{A_{\alpha_t} P^t f\}$ is weakly convergent to $P^t f_*$. However, $\{A_{\alpha_t} f\}$ and $\{A_{\alpha_t} P^t f\}$ have the same limit so $P^t f_* = f_*$.

Let $\mathcal{F}$ be a sequence of L^p functions. $\mathcal{F}$ is called **weakly precompact** if every sequence $\{f_t\}$ of functions $f_t \in \mathcal{F}$ contains a weakly convergent subsequence $\{f_{\alpha_t}\}$ converging to an L^p function f. Furthermore, the sequence $\{f_t\}$ is called **strongly convergent** to an L^p function f if

$$\lim_{t \to \infty} \| f_t - f \| = 0.$$

The concept of weak precompactness and strong convergence allow us to establish a second sufficient condition for the existence of a state of thermodynamic equilibrium. It is a special case of a result of Kakutani and Yoshida known as the **Abstract Ergodic Theorem**.

Sufficient Equilibrium Condition (SEC) 3.4. *If, for all initial system densities f evolving under the action of a Markov operator P, the sequence of system state density averages $\{A_t f\}$ is weakly precompact, then $\{A_t f\}$ is strongly convergent to a stationary density f_* and a state of thermodynamic equilibrium exists.*[2]

How does one test for the existence of this state of thermodynamic equilibrium using the weak precompactness condition of SEC 3.4? One test for weak precompactness is (Dunford and Schwartz, 1957):

Weak Precompactness Condition (WPC) 1. *Any set $\mathcal{F}$ of L^1 functions f satisfying $|f(x)| \le g(x)$, where $g(x) \ge 0$ is also an L^1 function, is weakly precompact.*

Thus, if f is a density then identifying an upper bound L^1 state function g ensures that $\mathcal{F}$ is weakly precompact.

This upper bound criterion for weak precompactness immediately leads to a third sufficient condition for the existence of a state of thermodynamic equilibrium. To see this, first assume that for a system in which densities f evolve under the action of a Markov operator P we have $P^t f \le g$ for all times t. As a consequence, $0 \le A_t f \le g$ so $|A_t f| \le g$ and thus the sequence $\{A_t f\}$ is weakly precompact. An application of SEC 3.4 then completes the proof of

Sufficient Equilibrium Condition (SEC) 3.5. *If, for an initial density f evolving under the action of a Markov operator P there is an upper bound state function g such that $P^t f \le g$ for all times t, then P has a stationary density f_* and a state of thermodynamic equilibrium is guaranteed.*

To this point there was no restriction on the phase space X in which our system is operating. If, however, the phase space X has finite measure then there is a second criterion for weak precompactness:

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[2] To prove this, first note that since $\{A_t f\}$ is assumed to be weakly precompact, there must exist a subsequence $\{A_{\alpha_t} f\}$ that is weakly convergent to a function f_* that satisfies $P^t f_* = f_*$ by SEC 3.3. Write $f = (f - f_*) + f_*$. For $\epsilon \ge 0$ it is a consequence of the Hahn-Banach theorem that there is an L^1 function g such that $f - f_*$ can be written as $f - f_* = P^t g - g + r$, wherein $\| r \| \le \epsilon$. Then we have $A_t f = A_t(P^t g - g) + A_t r + A_t f_*$. Since $P^t f_* = f_*$, it follows that $A_t f_* = f_*$ and thus $\| A_t f - f_* \| = \| A_t(f - f_*) \| \le \| A_t(P^t g - g) \| + \| A_t f \|$. By our initial observations after the definition of the system state density average, $\| A_t(P^t g - g) \|$ is strongly convergent to zero as $t \to \infty$, and $\| A_t f \| \le \| r \| < \epsilon$ by assumption. Thus for sufficiently large times t we have $\| A_t f - f_* \| \le \epsilon$ and $\{A_t f\}$ is strongly convergent to f_* since ϵ is arbitrary. To show that f_* is a density, note that if f is a density we have $P^t f \ge 0$ and $\| P^t f \| = \| f \|$ for all times t. Consequently, $A_t f \ge 0$ and $\| A_t f \| = 1$ and since $\{A_t f\}$ is strongly convergent to f_* it follows that f_* is a density.

Weak Precompactness Condition (WPC) 2. *If $\mu(X) < \infty$ and $M > 0$, then the set of all L^1 functions f whose L^p norm for some $p > 1$ satisfies $\| f \|_{L^p} \leq M$ is weakly precompact.*

Now assume that $\| P^t f \| < M$ for all times t so that $\| A_t f \| \leq M$ by the triangle inequality. This observation in conjunction with the Abstract Ergodic Theorem (SEC 3.4) and the second criterion for weak precompactness, WPC2, demonstrates

Sufficient Equilibrium Condition (SEC) 3.6. *If there is some initial density f evolving in a finite phase space X under the action of a Markov operator P, and a positive constant M and $p > 1$ such that $\| P^t f \|_{L^p} \leq M$ for all times t, then P has a stationary density f_* and a state of thermodynamic equilibrium exists.*

A third condition for weak precompactness which we will use later is given by

Weak Precompactness Condition (WPC) 3. *A set of L^1 functions $\mathcal{F}$ on a finite phase space X is weakly precompact if and only if: (a) $\| f \| \leq M < \infty$ for all $f \subset \mathcal{F}$; and (b) For every positive ϵ there is a $\delta > 0$ such that*

$$\int_A |f(x)| \, \mu(dx) < \epsilon \qquad if \quad \mu(A) < \delta \quad and \quad f \in \mathcal{F}.$$

None of these four sufficient conditions for the existence of a state of thermodynamic equilibrium offer any insight into the uniqueness of that state. If it is known that the state is unique and thus that the stationary density is likewise unique, then the following theorem tells us that the stationary density f_* is the long time limit of the system state density average for all initial system preparations.

Theorem 3.7. *For a system in which densities evolve under the action of a Markov operator P with a unique positive stationary density $f_* > 0$ over the entire phase space X,*

$$\lim_{t \to \infty} A_t f = f_*$$

for all initial system preparations characterized by an initial density f.[3]

D. SUMMARY.

The results of this chapter are essential for our investigation of the foundation of the dynamics responsible for the operation of various forms of the Second Law of Thermodynamics.

We have first introduced Markov operators, which control the evolution of densities under the action of system dynamics. This is important because densities characterize thermodynamic states, and in particular stationary densities of Markov operators define states of relative or absolute thermodynamic equilibrium.

Next, we have introduced the concept of conditional entropy, which is a generalization of the Boltzmann–Gibbs entropy. Though Theorem 3.1 demonstrates that entropy is always a nondecreasing function, we have also shown that it is only when densities evolve under the action of a noninvertible Markov operator that the entropy may increase (Theorem 3.2). Thus, *noninvertibility is necessary* (though not necessarily sufficient) *for system entropy to increase.*

Finally, four sufficient conditions for the existence of a state of thermodynamic equilibrium have been given (SEC 3.3 through 3.6) based on various convergence properties of the system state density average. These sufficient conditions provide no insight into the possible uniqueness of this state of equilibrium. However, if it is known that the equilibrium state is unique and characterized by a strictly positive stationary density, then Theorem 3.7 tells us that this unique density will be the long time limit of the system state density average for all initial system preparations.

In the next chapter, we turn to a consideration of the necessary and sufficient conditions for the existence of a unique state of thermodynamic equilibrium characterized by a unique stationary density f_* of the Markov operator.

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[3] In the case when the system is prepared in such a way that f/f_* is bounded the proof is almost trivial since, with $c = \sup(f/f_*)$, we have $P^t f_* \leq P^t(c f_*) = c P^t f_* = c f_*$ so $A_t f \leq c A_t f_* = c f_*$ and $\{A_t f\}$ is weakly precompact and convergent to a stationary density by the Abstract Ergodic Theorem (SEC 3.4). Since f_* is unique by assumption, the proof is complete. When the initial system preparation is such that f/f_* is not bounded the proof is technically more complicated and may be found in Lasota and Mackey (1985, pages 85-6).

Figure 3.1. The graph of the tent map (3.5).

Figure 3.2. The graph of the quadratic map (3.7) when $r = 4$.

CHAPTER 4.
ERGODICITY AND UNIQUE EQUILIBRIA.

In the last chapter we proved the necessity of irreversibility for increases in entropy to take place. Then conditions sufficient to guarantee the existence of relative states of thermodynamic equilibrium were given. The two interrelated questions of the existence of a unique state of thermodynamic equilibrium, and the global approach of the entropy to an absolute maximum, were not addressed.

This chapter provides a complete answer to the first of these questions by giving a necessary and sufficient criterion for the existence of a unique state of thermodynamic equilibrium as characterized by a unique stationary density f_*.

We start with a formal development of the Frobenius-Perron and Koopman operators in Sections A and B, having given an informal introduction to the Frobenius-Perron operator when discussing the tent map in Chapter 3. These operators are specific types of Markov operators appropriate for describing the evolution of densities by nonsingular dynamical or semidynamical systems. Section C briefly considers the subject of Poincaré recurrence.

We then define the property of ergodicity for a system, which is both necessary and sufficient to guarantee the existence of a unique state of thermodynamic equilibrium. We close with a proof that ergodicity, and hence the uniqueness of a state of thermodynamic equilibrium, is necessary and sufficient for the weak (Cesàro) convergence of the sequence $\{P^t f\}$ to a unique stationary density f_* for all initial densities f. In spite of this convergence property, ergodicity is insufficient to guarantee that the entropy will increase to its unique maximum value.

A. THE FROBENIUS PERRON OPERATOR.

To formalize the development of the Frobenius-Perron operator introduced in the previous chapter, a few new concepts are needed. A transformation S_t is said to be **measurable** if $S_t^{-1}(A) \subset X$ for all $A \subset X$. Furthermore, given a density f_* and associated measure μ_*, a measurable transformation S_t is **nonsingular** if $\mu_*(S_t^{-1}(A)) = 0$ for all sets A such that $\mu_*(A) = 0$.

If S_t is a nonsingular transformation, then the unique operator $P^t : L^1 \to L^1$ defined by

$$\int_A P^t f(x)\, dx = \int_{S_t^{-1}(A)} f(x)\, dx \tag{4.1}$$

is called the **Frobenius-Perron operator** corresponding to S.

From our comments in Chapter 3 and the formal definition, if f is a density, then equation (4.1) defining the Frobenius-Perron operator has an intuitive interpretation. Start with an initial density f and integrate this over a set B that will evolve into the set A under the action of the transformation S_t. However, the set B is $S_t^{-1}(A)$. This integrated quantity must be equal, since S_t is nonsingular, to the integral over the set A of the density obtained after one application of S_t to f. This final density is $P^t f$.

The fact that the Frobenius-Perron operator is unique is a straightforward consequence of the Radon-Nikodym theorem. It is clear from the definition that the Frobenius-Perron operator is a Markov operator, and so P^t is a linear contracting operator. Also, if $f \geq 0$ then $P^t f \geq 0$ and $\| P^t f \| = \| f \|$. Finally it is easy to show that if $S_{nt} = S_t \circ \cdots \circ S_t$, and P^{nt} and P^t are, respectively, the Frobenius-Perron operator corresponding to S_{nt} and S_t, then $P^{nt} = P^t \circ \cdots \circ P^t = (P^t)^n$.

An important property of the Frobenius-Perron operator which we will have occasion to use is contained in:

Property 4.1. *If P^t is the Frobenius-Perron operator associated with a nonsingular transformation S_t, then for all nonnegative functions f*

$$supp\ f \subset S_t^{-1}(supp\ P^t f)$$

(supp denotes support). More generally for every set A, $P^t f(x) = 0$ for all elements $x \in A$ if and only if $f(x) = 0$ for all $x \in S_t^{-1}(A)$.

Proof. By definition

$$\int_A P^t f(x)\, dx = \int_{S_t^{-1}(A)} f(x)\, dx$$

so

$$\int_X 1_A(x) P^t f(x)\, dx = \int_X 1_{S_t^{-1}(A)}(x) f(x)\, dx.$$

Thus if $P^t f(x) = 0$ on A then $f(x) = 0$ on $S_t^{-1}(A)$ and conversely. Take $A = X \setminus \text{supp}\,(P^t f)$ so $P^t f(x) = 0$ for all $x \in A$ and thus $f(x) = 0$ for all $x \in S_t^{-1}(A)$. This in turn implies that $\text{supp}\,f \subset X \setminus S_t^{-1}(A)$. Since $S_t^{-1}(A) = X \setminus S_t^{-1}(\text{supp}\,P^t f)$ the proof is complete. $\square$

Sometimes (as for the tent and quadratic maps of Examples 3.6 and 3.7) the implicit defining equation (4.1) for the Frobenius- Perron operator allows one to obtain an explicit formula for P^t. For example if $A = [a, x]$ then (4.1) becomes

$$\int_a^x P^t f(s)\, ds = \int_{S_t^{-1}([a,x])} f(s)\, ds \tag{4.2}$$

which, after differentiating, becomes

$$P^t f(x) = \frac{d}{dx} \int_{S_t^{-1}([a,x])} f(s)\, ds. \tag{4.3}$$

This process may be carried even further if the transformation is invertible so $S_t^{-1} = S_{-t}$ and S_{-t} has a continuous derivative with respect to x. Then,

$$S_t^{-1}([a, x]) = [S_{-t}(a), S_{-t}(x)],$$

and (4.3) becomes

$$P^t f(x) = f(S_{-t}(x)) \left| \frac{dS_{-t}(x)}{dx} \right|. \tag{4.4}$$

An extension of (4.4), valid for higher dimensional spaces $X = R^d$ when S_t is invertible, may also be derived. We first of all require a change of variables formula for integrals. If S_t is a nonsingular transformation and f a bounded integrable function, then for every set A we have

$$\int_{S_t^{-1}(A)} f(S_t(x))\, dx = \int_A f(x)\, \mu_{S_t^{-1}}(dx) = \int_A f(x) J^{-1}(x)\, dx,$$

wherein the measure $\mu_{S_t^{-1}}$ is

$$\mu_{S_t^{-1}}(B) = \mu_L(S_t^{-1}(B)).$$

and the density of the measure $\mu_{S_t^{-1}}$ with respect to the Lebesgue measure μ_L is J^{-1}, *i.e.*

$$\mu_L(S_t^{-1}(B)) = \int_B J^{-1}(x)\, dx.$$

From this it is relatively straightforward to obtain a generalization of equation (4.4) valid for any invertible transformation S_t operating in R^d. First consider the defining equation for the Frobenius-Perron operator corresponding to an invertible S_t:

$$\int_A P^t f(x)\, dx = \int_{S_{-t}(A)} f(x)\, dx,$$

and change the variables on the right hand side by using $y = S_t(x)$ so

$$\int_{S_{-t}(A)} f(x)\, dx = \int_A f(S_{-t}(y)) J^{-t}(y)\, dy.$$

Thus we have

$$\int_A P^t f(x)\, dx = \int_A f(S_{-t}(x)) J^{-t}(x)\, dx$$

so

$$P^t f(x) = f(S_{-t}(x)) J^{-t}(x). \tag{4.5}$$

Given a density f and associated measure μ_f, then a measurable transformation S_t is said to be **f measure preserving** if

$$\mu_f(S_t^{-1}(A)) = \mu_f(A)$$

for all sets A. Measure preserving transformations are necessarily nonsingular. Since the concept of measure preservation is not only dependent on the transformation but also on the measure, we alternately say that the measure μ_f is **invariant** with respect to the transformation S_t if S_t is f measure preserving.

Example 4.1. We can either say that the tent map (3.5) preserves the Lebesgue measure or that the Lebesgue measure is invariant with respect to the tent map. In an entirely analogous fashion, we say that the quadratic map (3.7) with $r = 4$ preserves the measure defined by

$$\mu_*(x) = \int_0^x f_*(s)ds$$

where the density f_* is the stationary density (3.9) of the Frobenius- Perron operator P, given by (3.8), corresponding to the quadratic map. If $A = [0, x]$, this takes the more explicit form

$$\mu_*(x) = \int_0^x \frac{1}{\pi\sqrt{s(1-s)}}ds = \frac{1}{2} - \frac{1}{\pi}\sin^{-1}(1 - 2x).$$

We also express this by saying that the measure μ_* is invariant with respect to the quadratic map. Note that the quadratic map does not preserve the Lebesgue measure, and that μ_* is just the conjugating function h of Example 3.7 used in transforming between the quadratic and tent maps, $S_Q = \mu_*^{-1} \circ S_T \circ \mu_*.\bullet$

It is possible to draw a connection between states of thermodynamic equilibrium, invariant measures and stationary densities of the Frobenius-Perron operator through the following theorem.

Theorem 4.2. *Let S_t be a nonsingular transformation and P^t the Frobenius-Perron operator associated with S_t. Then there exists a state of thermodynamic equilibrium whose density f_* is a stationary density of P^t if and only if the measure μ_**

$$\mu_*(A) = \int_A f_*(x)dx$$

is invariant with respect to S_t.

Proof. If μ_* is an invariant measure, then by definition $\mu_*(A) = \mu_*(S_t^{-1}(A))$ or

$$\int_A f_*(x)\,dx = \int_{S_t^{-1}(A)} f_*(x)\,dx = \int_A P^t f_*(x)\,dx,$$

which follows from the definition of the Frobenius-Perron operator. Thus $P^t f_* = f_*$ and f_* is a stationary density. The converse is equally easy to prove. Note in particular that the Lebesgue measure is invariant if and only if $P^t 1 = 1$. $\square$

This theorem is important because of the three way connection it draws between the existence of a state of thermodynamic equilibrium and the attendant stationary density f_*, the invariance of the associated measure μ_*, and the f_* measure preserving nature of S_t. In particular the density $f_* = 1$ of the microcanonical ensemble corresponds to a state of thermodynamic equilibrium if and only if the system dynamics preserve the Lebesgue measure. That is, systems preserving the Lebesgue measure may be appropriately described by the microcanonical ensemble. Of course it is important to realize that this theorem says nothing about either the uniqueness of this state of thermodynamic equilibrium or of the invariant measure corresponding to it.

B. THE KOOPMAN OPERATOR.

Next, we turn to a definition of the Koopman (1931) operator, which bears an important relationship to the Frobenius-Perron operator. If S_t is a nonsingular transformation and f is a bounded measurable function, *i.e.*, $f \in L^\infty$, then the operator $U^t : L^\infty \to L^\infty$ defined by

$$U^t f(x) = f(S_t(x))$$

is called the **Koopman operator** with respect to S_t.

As with the Markov and Frobenius-Perron operators, the Koopman operator has several easily demonstrated properties. The first is that U^t is a linear operator, while the second is that $||U^t f||_{L^\infty} \leq ||f||_{L^\infty}$ so U^t is a contracting operator. The most important and useful, however, is that the operator U^t is adjoint to the Frobenius-Perron operator, *i.e.*

$$< P^t f, g > = < f, U^t g > . \tag{4.6}$$

(To demonstrate that U^t and P^t are adjoint, check the property first with $g(x) = 1_A(x)$. This gives the defining relationship for the Frobenius-Perron operator. Since it is true for characteristic functions it is true for simple functions and thus for all g.)

Having introduced the Koopman operator we can now state, without proof, a famous theorem due to Birkhoff (1931) that gives information about the behaviour of trajectories of measurable transformations with an invariant measure. We introduce this theorem not because it is central to our investigation of the foundations of statistical thermodynamics, but rather because of the historical interest of a consequence of this result, given in Theorem 4.6 after our definition of ergodicity. Hence we have the following.

Theorem 4.3. *(Birkhoff Individual Ergodic Theorem.) Let S_t be a measurable transformation operating in a phase space X, and g be an integrable function. If there is an invariant measure μ, then there exists a second integrable function g^* such that*

$$g^*(x) = \lim_{t \to \infty} \frac{1}{t} \sum_{k=0}^{t-1} g(S_k(x)), \tag{4.7}$$

i.e. the time average of g along a trajectory converges to a definite value g^*.

The limiting value g^* of the time average is in fact a fixed point of the Koopman operator. This is easily seen by replacing x by $S_t(\mathrm{x})$ in equation (4.7) to immediately give the relation $g^*(x) = g^*(S_t(x)) = U^t g^*(x)$, thus finishing the demonstration.

Rewriting equation (4.6) in the integral form

$$\int_X g(x) P^t f(x)\, dx = \int_X f(x) g(S_t(x))\, dx$$

gives some insight into the relation between the Frobenius- Perron and Koopman operators. If for some set A in the phase space X we pick

$$f(x) = 0 \qquad \text{for all} \qquad x \notin A \qquad \text{and} \qquad g(x) = 1_{X \setminus S_t(A)}(x),$$

then the integral form of (4.6) may be written as

$$\int_X 1_{X \setminus S_t(A)}(x) P^t f(x)\, dx = \int_X f(x) 1_{X \setminus S_t(A)}(S_t(x))\, dx$$
$$= \int_A f(x) 1_{X \setminus S_t(A)}(S_t(x))\, dx.$$

Since $S_t(x) \notin X \setminus S_t(A)$ for $x \in A$, the right hand integral is clearly zero. Also, the left hand integral is simply the L_1 norm so $\|1_{X \setminus S_t(A)} P^t f\| = 0$, implying that $1_{X \setminus S_t(A)}(x) P^t f(x) = 0$ or

$$P^t f(x) = 0 \qquad \text{for} \qquad x \notin S_t(A).$$

Thus the Frobenius-Perron operator P^t transports the function f, supported on the set A, forward in time to a function supported on some subset of $S_t(A)$ [see Property 4.1.]. Consequently densities are transformed by P^t in a way analogous to the way points are transformed by S_t.

Next consider the Koopman operator $U^t f(x) = f(S_t(x))$ with the same f so

$$f(S_t(x)) = 0 \qquad \text{if} \qquad S_t(x) \notin A,$$

implying that

$$U^t f(x) = 0 \qquad \text{for} \qquad x \notin S_t^{-1}(A) \tag{4.8}$$

Therefore U^t can be thought of as transporting the density f supported on A backwards in time to a density supported on a subset of $S_t^{-1}(A)$.

If the system S_t is invertible and nonsingular, then these observations are even more transparent since $S_t^{-1}(x) = S_{-t}(x)$ and (4.5) becomes

$$P^t f(x) = U^{-t} f(x) J^{-t}(x) \tag{4.9}$$

which makes our comments connecting the actions of the Frobenius- Perron and Koopman operators more explicit. Note that if the transformation S_t is Lebesgue measure preserving then $J^{-t}(x) = 1$ and (4.9) becomes

$$P^t f(x) = U^{-t} f(x). \tag{4.10}$$

C. RECURRENCE.

For transformations S_t with an invariant measure operating in a phase space X, a point x in a subset A of the phase space X is called a **recurrent point** if there is some time $t > 0$ such that $S_t(x)$ is also in A. An important result, which deals with recurrent points, has become known as the Poincaré recurrence theorem.

Poincaré Recurrence Theorem. *Let S_t be a transformation with an invariant measure μ_* operating in a finite phase space X, $\mu_*(X) < \infty$, and let A be a subset of X with positive f_* measure. Then there exists a point x in A that is recurrent.*

Proof. (Adapted from Petersen [1983]). Assume the contrary, *i.e.* that there are no recurrent points in A. This then implies that $S_t^{-1}(A) \cap A = \emptyset$ for all times $t > 0$, and thus $S_t^{-1}(A) \cap S_{t'}^{-1}(A) = \emptyset$ for all positive times $t \neq t'$. Since S_t is measure preserving this implies that $\mu_*(S_t^{-1}(A)) = \mu_*(S_{t'}^{-1}(A))$ and this, coupled with the pairwise disjoint nature of the sets $S_t^{-1}(A)$ and $S_{t'}^{-1}(A)$, leads to

$$\sum_{t=0}^{\infty} \mu_*(A) = \sum_{t=0}^{\infty} \mu_*(S_t^{-1}(A)) = \mu_* \left(\bigcup_{t=0}^{\infty} S_t^{-1}(A) \right) \leq \mu_*(X) \leq \infty.$$

The only way in which this inequality can be satisfied is for $\mu_*(A)$ to be zero, which is a contradiction. Thus we conclude that A contains recurrent points. $\square$

The proof of the Poincaré recurrence theorem also demonstrates that the set of nonrecurrent points has measure zero, so almost every point is recurrent! Furthermore, repeated application of the theorem tells us that a recurrent point of A will return to A infinitely often.

Following Loschmidt's 1876 objections to Boltzmann's attempt to justify thermodynamics using (invertible) classical mechanics, this recurrence result was used by Zermelo (1896) as the basis for an attack on Boltzmann's celebrated "H theorem" concerning the behaviour of the entropy. In what has become known as the *Wiederkehreinwand* (objection based on recurrence). Zermelo argued that, because of recurrence, almost all points would constantly revisit the same areas of phase space and thus it would be impossible for the entropy to ever monotonically increase to its maximum.

Zermelo was right in his assertion that the entropy of a system whose dynamics are governed by Hamiltons equations, or any set of ordinary differential equations for that matter, cannot change as we have proved in Example 3.8. He was wrong, however, to base his argument on the result of the Poincaré recurrence theorem. The fallacy in the argument is to be found in his implicit assumption that densities (on which the behaviour of the entropy depends) will behave like points and also be recurrent as, perhaps, in the Spectral Decomposition Theorem 6.1. Just because points are recurrent, densities need not be, and indeed in Chapter 7 we give a necessary and sufficient condition for the entropy of a system to increase to its maximum that is completely compatible with the Poincaré recurrence theorem.

D. DENSITIES AND FLOWS.

Given a set of ordinary differential equations

$$\frac{dx_i}{dt} = F_i(x), \qquad i = 1, \dots, d \tag{4.11}$$

operating in a bounded region of R^d, it is possible to derive an evolution equation for $P^t f(x)$ by using the invertibility of (4.11) in conjunction with (4.5). However, it is much easier to derive an evolution equation for $U^t f(x)$, and then to use the adjointness property (4.6) to obtain an analogous result for $P^t f(x)$.

Thus, start with the definition of the Koopman operator written in the slightly more explicit form

$$U^t f(x^0) = f(S_t(x^0)),$$

where x^0 is the d-dimensional vector of initial conditions. From this we have

$$\frac{U^t f(x^0) - f(x^0)}{t} = \frac{f(S_t(x^0)) - f(x^0)}{t} = \frac{f(x(t)) - f(x^0)}{t},$$

where $x(t) = S_t(x^0)$. By the mean value theorem, there must be a constant θ satisfying $0 < \theta < 1$ such that

$$\frac{U^t f(x^0) - f(x^0)}{t} = \sum_i f_{x_i}(x(\theta t)) x_i'(\theta t)$$

$$= \sum_i f_{x_i}(x(\theta t)) F_i(x(\theta t))$$

$$= \sum_i f_{x_i}(S_{\theta t}(x^0)) F_i(S_{\theta t}(x^0)).$$

[Here we have used the convention $f_x = (\partial f / \partial x)$]. Taking the limit as $t \to 0$ and noting that $f(x) = f(S_t(x^0)) = U^t f(x^0)$ we have

$$\frac{\partial f}{\partial t} = \sum_i F_i(x) \frac{\partial f}{\partial x_i} \tag{4.12}$$

which is the desired evolution equation for $f(x) = U^t f(x^0)$.

Now, to obtain the analogous evolution equation for $P^t f(x)$ use the adjointness relation (4.6) with a function g that has compact support. Then it is straightforward to show that

$$\left\langle \frac{P^t f - f}{t}, g \right\rangle = \left\langle f, \frac{U^t g - g}{t} \right\rangle. \tag{4.13}$$

Taking the limit as $t \to 0$ in (4.13) in conjunction with (4.12) gives

$$\lim_{t \to 0} \left\langle f, \frac{U^t g - g}{t} \right\rangle = \left\langle f, \sum_i F_i(x) \frac{\partial g}{\partial x_i} \right\rangle$$

$$= \int_{R^d} f(x) \sum_i F_i(x) \frac{\partial g}{\partial x_i} \, dx$$

$$= \sum_i \int_{R^d} \left[\frac{\partial (fgF_i)}{\partial x_i} - g \frac{\partial (fF_i)}{\partial x_i} \right] \, dx$$

$$= - \sum_i \int_{R^d} g \frac{\partial (fF_i)}{\partial x_i} \, dx.$$

[In going from the third to the fourth line we have used the fact that g has compact support.] The last line is simply

$$- \left\langle \sum_i \frac{\partial (fF_i)}{\partial x_i}, g \right\rangle,$$

and thus, with

$$\lim_{t \to 0} \frac{P^t f(x) - f(x)}{t} = \frac{\partial f(x(t))}{\partial t}$$

we have the following evolution equation for $f(t, x) = P^t f(x)$:

$$\frac{\partial f}{\partial t} = - \sum_i \frac{\partial (fF_i)}{\partial x_i}. \tag{4.14}$$

As noted in Chapter 3, we call this the **generalized Liouville equation**.

The partial differential equation (4.14), describing the temporal evolution of the density f by the Frobenius Perron operator P^t, is quite familiar from mechanics. In fact, from Theorem 4.2 we can obtain a necessary and sufficient condition for a measure μ_* to be an invariant measure with respect to the system of ordinary differential equations (4.11). Since μ_* will be invariant if and only if f_* is a stationary density of P^t, from (4.14) this reduces to

$$0 = \sum_i \frac{\partial (f_* F_i)}{\partial x_i}, \tag{4.15}$$

which is immediately recognized as **Liouville's theorem**.

More specifically, if we wish to know when the Lebesgue measure

$$\mu_L(A) = \int_A dx_1 \cdots dx_d = \int_A dx,$$

with its associated density $f_* = 1$, is invariant, simply replace f_* in (4.15) by 1 to give

$$\sum_i \frac{\partial F_i}{\partial x_i} = 0,$$

which is sometimes called **Liouville's equation**.

Example 4.2. If the system of ordinary differential equations (4.11) is a Hamiltonian system,

$$\frac{dq_i}{dt} = \frac{\partial \mathcal{H}}{\partial p_i}, \qquad \frac{dp_i}{dt} = -\frac{\partial \mathcal{H}}{\partial q_i}, \qquad i = 1, \ldots, s,$$

where $s = 2d$, and p and q are the momenta and position variables and $\mathcal{H}(p, q)$ is the system Hamiltonian, then (4.14) takes the form

$$\frac{\partial f}{\partial t} = -\sum_{i=1}^{s} \left[\frac{\partial f}{\partial q_i} \frac{\partial \mathcal{H}}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial \mathcal{H}}{\partial q_i} \right].$$

From this it is clear that Hamiltonian systems always preserve the Lebesgue measure. However, this is not the only invariant measure as may be easily shown by taking an arbitrary function G of the system Hamiltonian $\mathcal{H}$ satisfying $G(\mathcal{H}) \geq 0$ and $\int_{R^s} G(\mathcal{H}) \, d\mathcal{H} = 1$ so G is a density. Then it is once again possible to show that Hamiltonian systems preserve the measure $\mu_{G(\mathcal{H})}$. •

E. ERGODICITY.

We are ready to begin consideration of the characteristics the dynamics S_t must have to guarantee the existence of a unique state of thermodynamic equilibrium that maximizes the entropy. The density maximizing the entropy should also be an equilibrium density, so our search is really one for the properties of S_t necessary to guarantee that a density f_* is a stationary density of the Frobenius-Perron operator corresponding to S_t, i.e. $P^t f_* = f_*$, and that f_* is unique.

We start by defining a few new terms. First, any set A such that $S_t^{-1}(A) = A$ is called an **invariant set**. Given a density f_* on a space X, any invariant set A such that $\mu_*(A) = 0$ or $\mu_*(X \setminus A) = 0$ is called **trivial**.

A nonsingular transformation S_t is said to be f_* **ergodic** if every invariant set A is a trivial subset of the phase space X, i.e. either $\mu_*(A) = 0$ or $\mu_*(X \setminus A) = 0$. If the phase space is finite and f_* is the uniform density of the microcanonical ensemble, then we say that S_t is **uniformly ergodic** instead of f_* ergodic. In the older physics and mathematics literature, ergodic systems were often called **metrically transitive** or **metrically indecomposable**.

Example 4.3. Probably the simplest example of a physical system that is ergodic is a one dimensional harmonic oscillator[4] (O. Penrose, 1979), but to illustrate the property of ergodicity, we consider a dynamical system in which momentum (p) and position (q) evolve according to

$$\frac{dp}{dt} = \alpha, \quad \frac{dq}{dt} = \beta, \qquad \alpha \neq \beta \tag{4.16}$$

on a unit torus (doughnut). For concreteness, we could imagine that the dynamics (4.16) describe the behaviour of a single gas particle (atom or molecule). Imagine cutting the torus apart in both directions and laying it down in the

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[4] Although the one dimensional harmonic oscillator is ergodic, a system of $d > 1$ independent autonomous oscillators (p and q are, respectively, momentum and position):

$$\frac{dp_k}{dt} = -\omega_k^2 q_k, \qquad \frac{dq_k}{dt} = p_k, \qquad k = 1, \cdots, d$$

is ergodic if and only if the frequencies ω_k are linearly independent (Lasota and Mackey, 1994, Example 7.7.1 and Remark 7.7.1).

plane so we have a phase space $X = [0, 1) \times [0, 1)$. Then, starting from any initial point (q_0, p_0) in X, the trajectory of our particle, emanating from that initial position, is given by

$$p(t) = p_0 + \alpha t, \quad q(t) = q_0 + \beta t \pmod 1 \tag{4.17}$$

as depicted by the solid lines in Figure 4.1.

If either α or β is irrational, then (4.16) is an example of a uniformly ergodic transformation [Arnold and Avez, 1968]. If, instead of examining the trajectory behaviour of a single particle, we look at the motion of many individual particles with initial conditions located in some subset of the phase space X (as an approximation to the behaviour of a density), then we obtain the behaviour of Figure 4.2 in which is shown the first six iterations of 10^4 particles with initial conditions located in the subset $[0, \frac{1}{10}] \times [0, \frac{1}{10}]$ by the uniformly ergodic dynamics

$$S(p, q) = (\sqrt{2} + p, \sqrt{5} + q) \pmod 1,$$

obtained from (4.17) by restricting the time t to the set of nonnegative integers and picking $\alpha = \sqrt{2}$, $\beta = \sqrt{5}$. This clearly illustrates an important property that ergodic dynamics *may* display, namely particles with nearby initial conditions may remain close to one another in spite of the fact that in the limit as $t \to \infty$ the entire phase space has eventually been visited.

This example of an ergodic transformation (if α and/or β are irrational) can also be viewed as a Hamiltonian system

$$\frac{dp}{dt} = -\frac{\partial \mathcal{H}}{\partial q}, \quad \frac{dq}{dt} = \frac{\partial \mathcal{H}}{\partial p}$$

where the Hamiltonian $\mathcal{H}$ is given by $\mathcal{H} = -\alpha q + \beta p$. Note, however, that substitution of the explicit expressions for $p(t)$ and $q(t)$ from (4.17) into the Hamiltonian gives $\mathcal{H} = \beta p_0 - \alpha q_0$, and thus the "energy" of this system (ergodic or not) is forever determined by its initial values. •

By themselves, neither the definition of ergodicity nor its illustration are terribly instructive with respect to the question of how one might prove ergodicity and the relation of ergodicity to the existence of stationary densities and to states of thermodynamic equilibrium. The following two results help clarify the property of ergodicity and its connection with the uniqueness of a state of thermodynamic equilibrium. First we have:

Theorem 4.4. *Let S_t be a nonsingular transformation and U^t the associated Koopman operator. Then S_t is ergodic if and only if the fixed points of U^t are constant functions, i.e. if the only solutions of*

$$g(S_t(x)) = g(x) \tag{4.18}$$

are constants.

Proof. Assume that S_t is ergodic but that g is not constant. Then there is some constant r such that the sets

$$A = \{x : g(x) \leq r\} \qquad \text{and} \qquad B = \{x : g(x) > r\}$$

have positive measure. A is invariant since

$$S_t^{-1}(A) = \{x : S_t(x) \in A\} = \{x : g(S_t(x)) \leq r\}$$
$$= \{x : g(x) \leq r\} = A,$$

as is B. Since A and B are invariant, S cannot be ergodic which is a contradiction so g must be constant.

Now assume that S_t is not ergodic but that (4.18) is only satisfied by constant g. Then by definition there must be a nontrivial invariant set A. Set $g = 1_A$. Since A is nontrivial g is not constant. Further since A is invariant $A = S_t^{-1}(A)$ and

$$g(S_t(x)) = 1_A(S_t(x)) = 1_{S_t^{-1}(A)}(x) = g(x),$$

so (4.18) is satisfied by a nonconstant function which is a contradiction. Thus S_t must be ergodic.   □

This result can sometimes be used to prove the ergodicity of a given system, for example to show that the system (4.17) is ergodic if $\alpha \neq \beta$ and if α and/or β is irrational.[5]

The second result is even more important as it establishes a one to one correspondence between the uniqueness of a state of thermodynamic equilibrium and the ergodicity of the dynamics.

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[5] To do this we set

$$S(p, q) = (p + \alpha t, q + \beta t) \qquad \text{mod } 1$$

Theorem 4.5. *Let S_t be a nonsingular transformation and P^t the corresponding Frobenius Perron operator. There is a unique state of thermodynamic equilibrium with associated stationary density f_*, $P^t f_* = f_*$ if and only if S_t is ergodic.*

Proof. Assume that $f_* > 0$ is the unique stationary density of P^t, but that S_t is not ergodic. If S_t is not ergodic there must exist a nontrivial set A, which is invariant so that $S_t^{-1}(A) = A$. If we also set $B = X \setminus A$ then $S_t^{-1}(B) = B$. Since A and B are clearly disjoint we can write f_* in the form $f_* = 1_A f_* + 1_B f_*$. Furthermore since $P^t f_* = f_*$ we have

$$P^t(1_A f_*) + P^t(1_B f_*) = 1_A f_* + 1_B f_*.$$

Since $1_B f_*$ is equal to zero on the set $A = X \setminus B = S_t^{-1}(A)$, by Property 4.1, $P^t(1_B f_*)$ is also zero on A and we conclude that

$$P^t(1_A f_*) = 1_A f_* \qquad \text{and} \qquad P^t(1_B f_*) = 1_B f_*.$$

Since A and B are clearly disjoint this means that there are two stationary densities of P^t, $1_A f_*$ and $1_B f_*$, which is a contradiction. Thus S_t is f_* ergodic.

Next, assume that S_t is ergodic but that f_1 and f_2 are different stationary densities of P^t. Let $g = f_1 - f_2$ so it is clear that $P^t g = g$ and, by our observations in footnote 1 of Chapter 3, we have

$$P^t g^+ = g^+ \qquad \text{and} \qquad P^t g^- = g^- \tag{4.19}$$

Since f_1 and f_2 are different densities it is also the case that $g^+ \neq 0$ and $g^- \neq 0$. Define two sets A and B by $A = \text{supp } g^+ = \{x : g^+(x) > 0\}$ and $B = \text{supp } g^- = \{x : g^-(x) > 0\}$. A and B are obviously disjoint and have positive measure. From the relations (4.19) and an inductive extension of Property 4.1. it is also clear that

$$A \subset S_t^{-1}(A) \subset \cdots \subset S_t^{-n}(A),$$

and

$$B \subset S_t^{-1}(B) \subset \cdots \subset S_t^{-n}(B).$$

Since A and B are disjoint, $S_t^{-n}(A)$ and $S_t^{-n}(B)$ are also disjoint for $n > 0$ and, as a consequence, the sets

$$A^* = \bigcup_{n=0}^{\infty} S_t^{-n}(A) \qquad \text{and} \qquad B^* = \bigcup_{n=0}^{\infty} S_t^{-n}(B)$$

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and use the fact that the phase space $X = (p, q)$ is periodic in p and q with period 1 to expand the function g in (4.18) in a Fourier series:

$$g(p, q) = \sum_{k_p, k_q} a_{k_p k_q} e^{2\pi i (k_p p + k_q q)},$$

where the summation is taken over all possible integers k_p, k_q. Substituting this series representation for g into (4.18) we obtain

$$\sum_{k_p, k_q} a_{k_p k_q} e^{2\pi i (k_p p + k_q q)} = \sum_{k_p, k_q} a_{k_p k_q} e^{2\pi i (k_p p + k_q q)} e^{2\pi i t (k_p + k_q)}.$$

Thus, for all t and all k_p, k_q we must have

$$a_{k_p k_q} = a_{k_p k_q} e^{2\pi i t (k_p + k_q)}. \tag{*}$$

This last expression can be satisfied under two circumstances: Either when $a_{k_p k_q} = 0$, or when the integers k_p and k_q are such that

$$k_p \alpha + k_q \beta = 0. \tag{**}$$

If α and β are rational, then we can always find nonzero integers k_p and k_q such that (*) is satisfied. As a consequence, the nonconstant function

$$g(p, q) = \sum_{k_p, k_q} a_{k_p k_q} e^{2\pi i (k_p p + k_q q)},$$

satisfies $g(p, q) = U^t g(p, q) = g(S_t(p, q))$, and S_t is not ergodic by Theorem 4.4. Conversely, if α and/or β, $\alpha \neq \beta$, are irrational then the only integers k_p and k_q for which (**) is satisfied are the trivial values $k_p = k_q = 0$ which means that α and β are linearly independent. In this case the only Fourier coefficient that can be nonzero is $a_{0,0}$ so that the function $g(p, q) = a_{0,0}$ is a constant. Then, since there are only constant solutions g to the equation (4.18) we have proved the ergodicity of (4.17) when α and/or β are irrational.

are also disjoint. Furthermore, since

$$S_t^{-1}(A^*) = \bigcup_{n=1}^{\infty} S_t^{-n}(A) = \bigcup_{n=1}^{\infty} S_t^{-n}(A) = A^*,$$

and similarly for B^*, A^* and B^* are also invariant sets. Since A and B are both of positive measure, A^* and B^* must also be of positive measure and A^* and B^* are thus nontrivial invariant sets which contradicts the ergodicity of S_t. Thus we conclude that f_1 and f_2 cannot be different stationary densities. $\square$

What does this result, in conjunction with Theorem 4.2, tell us? First consider the microcanonical ensemble with its uniform density. Then a given dynamics S_t will be measure preserving with respect to the Lebesgue measure if and only if the uniform density of the microcanonical ensemble is a stationary density of the Frobenius-Perron operator corresponding to S_t. Furthermore, from Theorem 4.5 the uniform density of the microcanonical ensemble will be the unique stationary density of P^t if and only if the system S_t is uniformly ergodic. Hence, the existence of a unique state of thermodynamic equilibrium, characterized by the uniform density of the microcanonical ensemble which maximizes the Boltzmann-Gibbs entropy to zero, is totally dependent on the operation of a uniformly ergodic dynamics that preserves the Lebesgue measure.

In the more general case, the nonuniform density f_* of the canonical ensemble which maximizes the conditional entropy will be the unique density corresponding to a state of thermodynamic equilibrium if and only if it is the stationary density of the Frobenius-Perron operator corresponding to an f_* ergodic system S_t with respect to which the measure

$$\mu_*(A) = \int_A f_*(x)\, dx$$

is invariant.

Thus in complete generality *ergodicity is necessary and sufficient to guarantee the existence of a unique state of thermodynamic equilibrium at which entropy is maximal.* That this unique state exists is, of course, only half of the picture for we must also understand what kind of systems can evolve to that state.

For ergodic dynamics there is an important and simply proved consequence of the Birkhoff individual ergodic theorem, Theorem 4.3. That is:

Theorem 4.6. *S_t is f_* ergodic (with unique stationary density f_*) operating in a finite normalized phase space X if and only if for any integrable function g the time average of g along the trajectory of S_t is equal to the f_* weighted average of g over the entire phase space. That is,*

$$\lim_{t \to \infty} \frac{1}{t} \sum_{k=0}^{t-1} g(S_k) = \int_X g(x) f_*(x)\, dx = <g> \tag{4.20a}$$

in the discrete time case, or

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T g(S_t(x))\, dt = \int_X g(x) f_*(x)\, dx = <g> \tag{4.20b}$$

in the continuous time case.

Proof. The proof that ergodicity implies the equality of temporal and spatial averages follows first from the observation that multiplying by f_* in (4.7), integrating over X and noting that

$$\int_X g(x) f_*(x)\, dx = \int_X g(S_t(x)) f_*(x)\, dx = \int_X g(x) P^t f_*(x)\, dx$$

by the adjointness of U^t and P^t gives, after passing to the limit,

$$\int_X g^*(x) f_*(x)\, dx = \int_X g(x) f_*(x)\, dx.$$

The second essential point to note is that the limiting function g^* is a fixed point of the Koopman operator U^t. Thus, since S_t is f_* ergodic, by Theorem 4.4 we know that g^* must be constant with respect to x. We have directly that

$$\int_X g^*(x) f_*(x)\, dx = g^* \int_X f_*(x)\, dx = g^* = \int_X g(x) f_*(x)\, dx,$$

so it follows immediately that

$$g^* = \int_X g(x) f_*(x) \, dx,$$

and this, in conjunction with Theorem 4.3, completes the proof. The converse is equally easy to prove. $\square$

In the physics literature the statement of this theorem is usually used as the definition of ergodicity: namely that an ergodic system is one for which the spatial and temporal averages coincide.

Theorem 4.6 also offers a way to derive an extension of the Poincaré recurrence theorem that gives an explicit formula for the fraction of the iterates of an f_* measure preserving and ergodic transformation S_t that fall in a subset A of a finite phase space X. Using the characteristic function 1_A of the set A, the fraction of the points $\{S_t(x)\}$ that are in A is given simply by

$$\lim_{t \to \infty} \frac{1}{t} \sum_{k=0}^{t-1} 1_A(S_k(x)).$$

By equation (4.20), this is simply $\mu_*(A)$. Thus the sojourn time in a set A is directly proportional to the f_* measure of A.

To conclude this section we state one last theorem concerning necessary and sufficient convergence properties for the ergodicity of a transformation S_t and thus, by our comments following Theorem 4.5, for the existence of a unique state of thermodynamic equilibrium.

Theorem 4.7. *Let S_t be a nonsingular transformation and P^t the corresponding Frobenius Perron operator with stationary density f_* for all points in the phase space X. Then S_t is f_* ergodic if and only if $\{P^t f\}$ is Cesàro convergent to f_* for all densities f, i.e., if*

$$\lim_{t \to \infty} \frac{1}{t} \sum_{k=0}^{t-1} < P^k f, g > = < f_*, g > \tag{4.21a}$$

in the discrete time case, or if

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T < P^t f, g > \, dt = < f_*, g > \tag{4.21b}$$

in the continuous time case, for all bounded measurable functions g.

Proof. We only give the proof for the discrete time case, as the continuous time proof follows directly using continuity arguments. Assume S_t is f_* ergodic which, by Theorem 4.5, implies that f_* is the unique stationary density of P^t. Then by Theorem 3.7 we have

$$\lim_{t \to \infty} \frac{1}{t} \sum_{k=0}^{t-1} P^k f = f_*$$

immediately. Multiplication by a bounded measurable function g and integration over the entire phase space X gives

$$\lim_{t \to \infty} \frac{1}{t} \sum_{k=0}^{t-1} < P^k f, g > = < f_*, g >$$

and (4.21a) is recovered.

Conversely, assume that (4.21a) holds and pick $g(x) = 1_X(x)$ so we have

$$\lim_{t \to \infty} \frac{1}{t} \sum_{k=0}^{t-1} \int_X P^k f(x) \, dx = \int_X f_*(x) \, dx,$$

which implies that

$$\lim_{t \to \infty} \int_X \left\{ \frac{1}{t} \sum_{k=0}^{t-1} P^k f(x) - f_*(x) \right\} \, dx = 0$$

or that
$$\lim_{t \to \infty} ||A_t f - f_*|| = 0$$

for all densities f. Assume that the density f is a stationary density of P^t so $P^t f = f$ for all t and, as a consequence, $A_t f = f$ for all t. Then we have
$$||f - f_*|| = 0,$$

or $f = f_*$ is the unique stationary density of P^t. Since P^t has a unique stationary density f_*, by Theorem 4.5 S_t is f_* ergodic. $\square$

Since Frobenius-Perron operators are specialized Markov operators, there is a certain logic to extending the concept of ergodicity to Markov operators. Thus let P^t be a Markov operator with a stationary density f_*. We will say that P^t is $\mathbf{f_*}$ **ergodic** if $\{P^t f\}$ is Cesàro convergent to f_* for all initial densities f.

F. SUMMARY.

This chapter introduces the important notion of the Frobenius- Perron and Koopman operators, which describe the evolution of densities by nonsingular dynamical or semidynamical systems. This is by way of an introduction to the notion of f_* ergodicity in these systems, a type of mild irregular dynamical behaviour both necessary and sufficient for the existence of a unique stationary density f_* and thus a unique state of thermodynamic equilibrium (Theorem 4.5). However, ergodicity by itself cannot guarantee the approach of the entropy to the maximum value corresponding to this unique state, in spite of the fact that ergodicity is also necessary and sufficient for the weak Cesàro convergence of the sequence $\{P^t f\}$ to f_* for all initial densities f (Theorem 4.7). Our identification of states of thermodynamic equilibrium with densities, in conjunction with the contents of Theorems 4.5 and 4.7, shows that f_* ergodicity, Cesàro convergence of $\{P^t f\}$ to f_*, and the uniqueness of a state of thermodynamic equilibrium with density f_* are all equivalent. We have also discussed the concept of Poincarè recurrence, pointing out it was incorrectly utilized by Zermelo to criticize the work of Boltzmann.

In the next chapter we introduce the dynamic property of mixing.

Figure 4.1. A single trajectory of the ergodic system (4.16) in (p, q) phase space, starting from the initial point (p_0, q_0). $\alpha = \sqrt{2}$ and $\beta = \sqrt{5}$, thus ensuring uniform ergodicity. The numbers indicate successive portions of the trajectory and the arrows show the direction.

Figure 4.2. The iteration of 10^4 initial points concentrated on a small region of phase space by a discrete time version (4.17) of (4.16). α and β as in Figure 4.1.

CHAPTER 5.
MIXING.

In this chapter, we consider systems with irregular dynamical behaviors that are stronger than ergodic. Namely, we consider with dynamics described by measure preserving transformations that have the property of strong, or Hopf, mixing. Systems with mixing dynamics have entropies that are forever fixed by their mode of preparation. This is followed by a brief discussion of Kolmogorov systems in Section B. The final Section C discusses the behaviour of temporal correlation between dynamical variables, showing that mixing is necessary and sufficient for the decay of temporal correlations to zero.

The dynamical property of mixing, like ergodicity, will not account for the evolution of system entropy. However, it is important to discuss mixing for three reasons. First, there is a general, though not universal, misconception that mixing is, in fact, sufficient to allow the evolution of entropy to a maximum. This is most certainly not the case. Second, comparison of the temporal correlation and entropy behaviour of mixing and asymptotically periodic dynamics (Chapter 6) shows that there is no special connection to be drawn between the behavior of the correlation function and the emergence of thermodynamic behaviour. Finally, as we will show in Chapter 8, if there is a certain imprecision in our knowledge of the values of the state variables in a mixing system then this is sufficient to cause the system entropy to evolve to its maximal value.

A. MIXING.

Gibbs (1902) realized that ergodicity, while necessary and sufficient to guarantee the existence of a unique state of thermodynamic equilibrium characterized by a stationary density f_*, was inadequate to guarantee the approach of a system to that equilibrium. As a consequence he qualitatively discussed a property stronger than ergodicity which is now called **(strong) mixing**.[6] This was subsequently developed mathematically by Koopman (1931), von Neumann (1932), and Hopf (1932).

Let S_t be an f_* measure preserving transformation operating on a finite normalized $[\mu_*(X) = 1]$ space. Then S_t is called **f_* mixing** if

$$\lim_{t \to \infty} \mu_*(A \cap S_t^{-1}(B)) = \mu_*(A)\mu_*(B) \tag{5.1}$$

for all subsets A and B of X. If f_* is the uniform density of the microcanonical ensemble, then in analogy with our definition of ergodicity we say that S_t is **uniformly mixing**. Notice in particular that with $A = X$ the f_* measure of any subset B of the phase space does not change under the action of a mixing transformation.

Example 5.1. To see how mixing works, examine Figure 5.1 where the evolution of 10^4 points by the uniformly mixing transformation

$$S(x, y) = (x + y, x + 2y) \qquad (\text{mod } 1)$$

is shown in the phase space $[0, 1] \times [0, 1]$. As in Example 4.3, one could once again think of this as depicting the motion of a large number of imaginary atoms with different initial conditions in their two dimensional phase space. In contrast to the uniformly ergodic transformation of Figure 4.2, here the mixing dynamics act to very quickly spread the particles (or initial set of points) throughout phase space in thread like structures.[7] •

Example 5.2. As a second example of a uniformly mixing transformation we introduce the **baker transformation**, so called because of the similarity of its operation to the kneading and folding operations involved in the preparation of pastry dough. We take the phase space X to be the unit square $X = [0, 1] \times [0, 1]$ and define the baker transformation by

$$S(x, y) = \begin{cases} (2x, \frac{1}{2}y) & 0 \le x \le \frac{1}{2} \\ (2x - 1, \frac{1}{2} + \frac{1}{2}y) & \frac{1}{2} < x \le 1. \end{cases} \tag{5.2}$$

To see pictorially how the baker transformation works, consult Figure 5.2a where X is indicated as a dotted region. The first operation involved in the application of S, shown in Figure 5.2b, involves a compression of X in the y direction and a concomitant stretching in the x direction by a factor of 2. Finally, in Figure 5.2c, this deformed area is divided vertically at $x = 1$ and the right hand portion is placed on top of the left hand portion to give the final result of one application of S to the entire space X. Since it is clear from this geometric construction that the counterimage of any

---

[6] There is another type of mixing, weak mixing, but we will not find it of use in our investigations here (see Lasota and Mackey, 1994).

[7] The transformation of Example 5.1 is an example of an **Anosov (or C) diffeomorphism**. Consult Arnold and Avez (1968, Chapter 3) for an extensive discussion of these and their continuous time analogs, the **Anosov (or C) flows.**

rectangle A in X is again a rectangle or a pair of rectangles with the same total area as A, the baker transformation S is measurable and preserves the Lebesgue measure.

To further illustrate the operation of the baker transformation and to show that it is in fact uniformly mixing, consider Figure 5.3a where two sets A and B of the phase space X are indicated with $\mu_L(B) = \frac{1}{2}$. By taking repeated counterimages of B with the baker transformation we find that after t counterimages (3 are shown), $S_t^{-1}(B) = S_{-t}(B)$ consists of 2^{t-1} vertical rectangles of equal area whose total area is $\mu_L(B)$. Clearly the measure of the set $A \subset S_t^{-1}(B) = S^{-t}(B)$ approaches $\mu_L(A)\mu_L(B) = \mu_L(A)/2$ in the limit as t becomes large and the condition (5.1) defining mixing is satisfied. (A more mathematical proof with less insight is possible by analytically calculating the successive counterimages).

If, instead of running the baker transformation backward we run it forward in time (Figure 5.3b) the behaviour is remarkably similar to that found for counterimages. Namely after t applications of the baker transformation $S_t(B)$ consists of 2^t horizontal rectangles whose measure is still equal to $\mu_L(B)$. It is this characteristic of mixing transformations that gives rise to the thready behaviour seen in Figure 5.1. •

The behaviour of the uniformly mixing baker transformation as time runs either backward (Figure 5.3a) or forward (Figure 5.3b) simply reflects the fact that the defining relation (5.1) for mixing could equally well be written

$$\lim_{t \to \infty} \mu_*(A \cap S_t(B)) = \mu_*(A)\mu_*(B), \tag{5.3}$$

for all $t \in R$ whenever S_t is invertible. Again taking $A = X$ we see that the measure of any set B is unchanged by either forward or backward action of invertible mixing dynamics.

Example 5.3. A third example of a mixing transformation in a continuous time system is given by a model of an ideal gas in which the position of the ith particle is denoted by a position vector q_i and a momentum vector p_i, so (q_i, p_i) is a point in R^6. It is assumed that the particles in the gas are physically indistinguishable from one another, and that the gas is so dilute that for any bounded region of the phase space there are at most a finite number of particles present at any given time. Under the assumption that the particles move with constant speed and do not interact, the transformation describing the evolution of this system is given by

$$S_t(p, q) = (p, q + pt). \tag{5.4}$$

The surprising result is that this system of noninteracting particles is mixing (Lasota and Mackey, 1994). •

Example 5.4. There is a whole class of continuous time systems of importance in classical mechanics which are mixing. These systems, known as geodesic flows on manifolds with negative curvature, have been intensively studied by Anosov (1963, 1967), and discussed in Arnold and Avez (1968) and Abraham and Marsden (1978). Sinai (1963, 1970) has shown that the Boltzmann-Gibbs model of a dilute gas (spherical molecules with totally elastic collisions) is an example of this type of system and is thus mixing. •

It is a straightforward consequence of the definition that mixing implies ergodicity.[8] Furthermore, an f_* measure preserving transformation S_t, with associated Frobenius-Perron operator P^t and stationary density f_*, is mixing if and only if the sequence $\{P^t f\}$ is weakly convergent to the density f_* for all initial densities f. If $f_* = 1$, then S_t is uniformly mixing if and only if $\{P^t f\}$ is weakly convergent to the density of the microcanonical ensemble for all initial densities f.

This is expressed more formally in:

Theorem 5.1. *Let S_t be an ergodic transformation, with stationary density f_* of the associated Frobenius- Perron operator, operating in a phase space of finite f_* measure. Then S_t is f_* mixing if and only if $\{P^t f\}$ is weakly convergent to f_* for all densities f, i.e.,*

$$\lim_{t \to \infty} <P^t f, g> = <f_*, g>$$

---

[8] To see this assume that S_t is mixing and that the set B in (5.1) is an invariant set which means, by definition, that $S_t^{-1}(B) = B$. Since A in (5.1) is arbitrary, take $A = B$, which implies from the definition (5.1) of mixing that

$$\lim_{t \to \infty} \mu_*(A \cap S_t^{-1}(B)) = \mu_*(B \cap B) = \mu_*(B) = \mu_*^2(B).$$

This, in turn, implies that $\mu_*(B) = 0$ or 1 so B is a trivial subset of X and S_t is ergodic.

for every bounded measurable function g.

Proof. The proof that mixing implies the weak convergence of $\{P^t f\}$ to f_* is easily accomplished by first writing the definition of $\mu_*(A \cap S_t^{-1}(B))$ in a functional form so

$$
\begin{aligned}
\lim_{t \to \infty} \mu_*(A \cap S_t^{-1}(B)) &= \lim_{t \to \infty} \int_{A \cap S_t^{-1}(B)} f_*(x)\, dx \\
&= \lim_{t \to \infty} \int_X 1_{A \cap S_t^{-1}(B)}(x) f_*(x)\, dx \\
&= \lim_{t \to \infty} \int_X 1_A(x) 1_{S_t^{-1}(B)}(x) f_*(x)\, dx \\
&= \lim_{t \to \infty} \int_X 1_A(x) 1_B(S_t(x)) f_*(x)\, dx \\
&= \lim_{t \to \infty} < 1_A f_*, U^t 1_B > \\
&= \lim_{t \to \infty} < P^t 1_A f_*, 1_B > \\
&= \lim_{t \to \infty} < P^t f, g >,
\end{aligned}
$$

for functions $f = 1_A f_*$ and $g = 1_B$.

In a similar fashion, the right hand side of the defining relation (5.1) can be written as

$$
\begin{aligned}
\mu_*(A)\mu_*(B) &= \int_X 1_A(x) f_*(x)\, dx \int_X 1_B(x) f_*(x)\, dx \\
&= < 1_A f_*, 1 > < f_*, 1_B > \\
&= < f, 1 > < f_*, g > .
\end{aligned}
$$

Thus, combining these two results yields, for $f = 1_A f_*$ and $g = 1_B$,

$$
\lim_{t \to \infty} < P^t f, g > = < f, 1 > < f_*, g > .
$$

Since this result holds for characteristic functions, it must also be true for simple functions and thus all others since every L^1 function is the strong limit of a sequence of simple functions, and every bounded measurable (L^∞) function is the uniform limit of simple functions. Finally, taking f to be a density completes the proof. This argument is easily reversed to prove the converse. $\square$

In our subsequent discussion, we will call a Markov operator P^t with stationary density $\mathbf{f_*}$ **mixing** if $\{P^t f\}$ is weakly convergent to f_*.

Gibbs (1902), Krylov (1979), and many other authors have emphasized the importance of mixing for the understanding of thermodynamic behaviour. Indeed, at first one might think that the weak convergence of the sequence $\{P^t f\}$ to the density f_* of the canonical ensemble, or to the density $f_* = 1$ of the microcanonical ensemble, no matter what initial density f was chosen, would be exactly what is required to guarantee the approach of the entropy to its maximum. Such is not the case. It is most certainly true that mixing is necessary for this convergence of the entropy, but it is also not sufficient as we show in Chapter 7.

Example 5.5. As an illustration of this fact we again return to our example of the uniformly mixing baker transformation. The baker transformation (5.2) is clearly invertible, so

$$
S^{-1}(x, y) = \begin{cases} (\frac{1}{2}x, 2y) & 0 \le y \le \frac{1}{2} \\ (\frac{1}{2} + \frac{1}{2}x, 2y - 1) & \frac{1}{2} < y \le 1, \end{cases} \tag{5.5}
$$

and we may apply equation (4.5) directly to obtain an expression for the Frobenius-Perron operator corresponding to S. The only other fact that we must use is that S preserves the Lebesgue measure so $J^{-t} = 1$, which can be verified directly from (5.2). Thus

$$
P_S f(x, y) = \begin{cases} f(\frac{1}{2}x, 2y) & 0 \le y \le \frac{1}{2} \\ f(\frac{1}{2} + \frac{1}{2}x, 2y - 1) & \frac{1}{2} < y \le 1, \end{cases}
$$

so $P_S 1 = 1$ and the density of the microcanonical ensemble is a stationary density of P_S.

Since the stationary density of P_S is the uniform density (it is easily proved that $f_* = 1$ is the unique stationary density) we may calculate the entropy of $P_S f$ as

$$H(P_S f) = - \int_0^{\frac{1}{2}} \int_0^1 f(\tfrac{1}{2}x, 2y) \log f(\tfrac{1}{2}x, 2y) \, dx \, dy$$
$$- \int_{\frac{1}{2}}^1 \int_0^1 f(\tfrac{1}{2} + \tfrac{1}{2}x, 2y - 1) \log f(\tfrac{1}{2} + \tfrac{1}{2}x, 2y - 1) \, dx \, dy$$

A change of variables on the right hand side in the two integrals gives

$$H(P_S f) = H(f),$$

and we have proved that $H(P_S^t f) = H(f)$ for all positive times t and all densities f. This argument also extends to negative times when the baker transformation is being run backward. Thus the uniformly mixing baker transformation has an entropy that is constant for all of time and equal to the entropy of the initial density f with which the system was prepared.

This is illustrated in Figure 5.4. At $t = 0$ we prepare the phase space with an initial density

$$f(x, y) = \tfrac{3}{2} 1_{X_1}(x) + \tfrac{1}{2} 1_{X_2}(x) \tag{5.6}$$

where $X_1 = [0, \tfrac{1}{2})$ and $X_2 = [\tfrac{1}{2}, 1]$ (Figure 5.4b). Then the entropy of the initial state is

$$H(f) = -\tfrac{1}{4}\{\log \tfrac{1}{2} + 3 \log \tfrac{3}{2}\} \simeq -0.13.$$

After one application of the baker transformation (Figure 5.4c) we have

$$f_1(x, y) = \tfrac{1}{2} 1_{Y_1}(y) + \tfrac{3}{2} 1_{Y_2}(y)$$

where $Y_1 = [0, \tfrac{1}{2})$ and $Y_2 = [\tfrac{1}{2}, 1]$. It is an easy matter to show that $H(f_1) \equiv H(f)$. Further applications of the baker transformation yield $H(f_t) \equiv H(f)$ (Figure 5.4d for $t = 2$) which also holds for negative times (Figure 5.4a for $t = -1$) since the baker transformation is invertible. ●

This example illustrates the content of the following theorem which is a consequence of Theorem 3.2.

Theorem 5.2. *Let S_t be an invertible f_* mixing transformation. Then the system entropy is forever fixed at the value corresponding to the way in which the system was prepared:*

$$H_c(P^t f | f_*) \equiv H_c(f | f_*)$$

for all $t \in R$.

B. KOLMOGOROV SYSTEMS.

In this section, a concept that will be used in Chapter 9 is briefly introduced, namely that of Kolmogorov systems, or K systems.

We use the notation $S_t(\mathcal{A}) = \{S_t(A) : A \in \mathcal{A}\}$, $t \in R$ (or Z), where $\mathcal{A}$ is a sigma algebra. If S_t is an invertible transformation operating on a normalized space, and both S_t and S_{-t} are f_* measure preserving, then S_t is said to be a **K-system** if there is a sigma algebra $\mathcal{A}_0 \in \mathcal{A}$ such that:

(1) $S_{-t}(\mathcal{A}_0) \in \mathcal{A}_0$;

(2) The sigma algebra defined by

$$\bigcap_{t=0}^{\infty} S_{-t}(\mathcal{A}_0)$$

is trivial in the sense that it only contains sets of f_* measure 0 or 1; and

(3) The smallest sigma algebra containing

$$\bigcup_{t=0}^{\infty} S_t(\mathcal{A}_0)$$

is identical to $\mathcal{A}$.

Kolmogorov systems have behaviors stronger than mixing in that if a transformation is a K-system then this also implies that it is mixing (Walters, 1982). The other property of K-systems that is important for thermodynamic considerations is that since they are f_* measure preserving they have a unique stationary density f_*. However, since they are invertible, by Theorem 3.2 the entropy of a K-system is identically equal to the initial entropy determined by the initial density with which the system is prepared. In fact, our example of the baker transformation (5.2), which we used to illustrate uniform mixing, is an example of a Kolmogorov system (Lasota and Mackey, 1994).

C. THE DECAY OF CORRELATIONS.

To understand the connection between mixing and the decay of correlations requires the introduction of a few concepts. If we have a time series $x(t)$ [either discrete or continuous], and two bounded integrable functions $\sigma, \eta : X \to R$, then the **correlation** of σ with η is defined as

$$R_{\sigma,\eta}(\tau) = \lim_{T \to \infty} \frac{1}{T} \sum_{t=0}^{T-1} \sigma(x(t+\tau))\eta(x(t))$$

in the discrete time case, or

$$R_{\sigma,\eta}(\tau) = \lim_{T \to \infty} \frac{1}{T} \int_0^T \sigma(x(t+\tau))\eta(x(t)) \, dt$$

in the continuous case. The **average** of the function σ is just

$$< \sigma > = \lim_{T \to \infty} \frac{1}{T} \sum_{t=0}^{T-1} \sigma(x(t)),$$

or

$$< \sigma > = \lim_{T \to \infty} \frac{1}{T} \int_0^T \sigma(x(t)) \, dt,$$

so it is clear that

(1) $R_{\sigma,\eta}(0) = < \sigma\eta >$; and

(2) $R_{\sigma^2}(0)R_{\eta^2}(0) \geq R_{\sigma,\eta}(\tau)$. This follows directly by writing out the expression $< [\alpha\sigma(t) + \beta\eta(t+\tau)]^2 >$ for real and nonzero α and β, and noting that it must be nonnegative.

The **covariance** of σ with η, $C_{\sigma,\eta}(\tau)$, is defined by

$$C_{\sigma,\eta}(\tau) = R_{\sigma,\eta}(\tau) - < \sigma >< \eta >,$$

while the **normalized covariance** $\rho_{\sigma,\eta}(\tau)$ is

$$\rho_{\sigma,\eta}(\tau) = \frac{R_{\sigma,\eta}(\tau) - < \sigma >< \eta >}{< \sigma\eta > - < \sigma >< \eta >}.$$

Clearly, $\rho_{\sigma,\eta}(0) = 1$.

Now assume we have an ergodic transformation S_t with consequent unique stationary density f_*, operating in a finite normalized phase space X, and that S_t is generating the sequence of values $\{x(t)\}$. Then the correlation of σ with η can be written in both the discrete and continuous time case as

$$R_{\sigma,\eta}(\tau) = \int_X \sigma(S_\tau(x))\eta(x)f_*(x) \, dx \tag{5.7}$$

by use of the extension of the Birkhoff Ergodic Theorem 4.6. Using the definition of the Koopman operator, along with the adjointness of the Frobenius-Perron and Koopman operators, equation (5.7) can be rewritten in the form

$$R_{\sigma,\eta}(\tau) = < \eta f_*, U^\tau \sigma > = < P^\tau(\eta f_*), \sigma > . \tag{5.8}$$

Writing the defining relation for mixing transformations as in the proof of Theorem 5.1, it is clear that for general functions η and σ we have

$$\lim_{t \to \infty} < P^t(\eta f_*), \sigma > = < \eta f_*, 1 >< f_*, \sigma >,$$

so (5.8) yields

$$\lim_{\tau \to \infty} R_{\sigma,\eta}(\tau) = < \eta >< \sigma >$$

when S_t is mixing. Thus we have the following result connecting mixing with the limiting behaviour of the normalized covariance. Namely,

Theorem 5.3. S_t *is* f_* *mixing if and only if*

$$\lim_{\tau \to \infty} \rho_{\sigma,\eta}(\tau) = 0.$$

D. SUMMARY.

In this chapter we have introduced a type of dynamical behaviour, mixing, that leads to an evolution of densities that is more complicated than ergodicity. Mixing systems cause densities to evolve in phase space such that they are eventually supported on thready, fractal-like structures spread through the entire phase space. A slightly stronger type of behaviour than mixing, that displayed by K-systems, was also introduced.

We have shown (Theorem 5.1) that a necessary and sufficient condition for a dynamics S_t to be mixing is the weak convergence of $\{P^t f\}$ to a unique stationary density f_* for all initial densities f. However (Theorem 5.2), for reversible mixing dynamics the entropy is fixed at the value determined by the system preparation. Finally, in Theorem 5.3 we have shown that this weak convergence of $\{P^t f\}$ to a unique stationary density is completely equivalent to the eventual decay to zero of the correlation between any dynamical variables. Thus, in spite of this weak convergence and the decay of correlations, mixing by itself is not sufficient to ensure the convergence of system entropy to a maximum.

In the next chapter we introduce another dynamical property, asymptotic periodicity, which is sufficient for the evolution of system entropy to a local maximal value generally less than zero. Interestingly, the final thermodynamic state of an asymptotically periodic system depends, in general, on the initial state.

Figure 5.1. Iteration of 10^4 initial points under the action of a uniformly mixing transformation. Note the development of the thread-like structures.

Figure 5.2. Graphical illustration of the operation of the baker transformation. See the text for details.

Figure 5.3. The behaviour of an initial set B under backward (a) and forward (b) iteration by the uniformly mixing baker transformation, and the generation of the thready behaviour as seen in Figure 5.1. See the text for more discussion.

Figure 5.4. A graphical illustration of the behaviour of an initial nonuniform density for backward and forward iteration of the baker transformation. See the text for the behaviour of the entropy, and Example 8.1 for a discussion of the corresponding changes in the coarse grained entropy.

CHAPTER 6.
ASYMPTOTIC PERIODICITY AND ENTROPY EVOLUTION

In this chapter we turn to an investigation of the fascinating property of asymptotic periodicity in the evolution of densities. This behaviour is the statistical analog for densities of the more common periodicity found in some time series. The existence of asymptotic periodicity will allow us to prove a weak form of the Second Law in which the conditional entropy increases to (at least) a local maximum.

In Section A we introduce a class of Markov operators known as smoothing. Smoothing operators have three characteristics that are important for our ultimate understanding of the basis of the Second Law of thermodynamics. First, the sequence of densities evolving under the action of a smoothing Markov operator has the property of asymptotic (or statistical) periodicity. This is illustrated in Section B using the hat and quadratic maps. Second, any smoothing Markov operator has at least one stationary density thus ensuring that there is a state (perhaps not unique) of thermodynamic equilibrium. In Section C we show how, for asymptotically periodic systems, the entropy of the sequence of densities always increases to a maximum. This maximum, however, may only be relative and less than the maximum possible entropy value, thus corresponding to a metastable state. The relative maximum of entropy which asymptotically periodic systems approach usually depends on the initial density of the system (the way in which the system was prepared). In Section D we show that the correlation function for an asymptotically periodic system is made up of a stochastic component and a strictly periodic (nondecreasing) component.

A. ASYMPTOTIC PERIODICITY.

First, we define a smoothing Markov operator. A Markov operator P^t is said to be **smoothing** if there exists a set A of finite measure, and two positive constants $k < 1$ and $\delta > 0$ such that for every set E with $\mu_L(E) < \delta$ and every density f there is some integer $t_0(f, E)$ for which

$$\int_{E \cup (X \setminus A)} P^t f(x) \, dx \leq k \qquad \text{for } t \geq t_0(f, E).$$

This definition implies that any initial density, even if concentrated on a small region of the phase space X, will eventually be smoothed out by P^t and not end up looking looking like a delta function. Notice that if X is a finite phase space we can take $X = A$ so the smoothing condition looks simpler:

$$\int_{E} P^t f(x) \, dx \leq k \qquad \text{for } t \geq t_0(f, E).$$

Smoothing operators are important because of a theorem of Komornik and Lasota (1987), first proved in a more restricted situation by Lasota, Li, and Yorke (1984).

Theorem 6.1. *Spectral Decomposition Theorem (Komornik and Lasota, 1987). Let P^t be a smoothing Markov operator. Then there is an integer $r > 0$, a sequence of nonnegative densities g_i, a sequence of bounded linear functionals λ_i, $i = 1, \ldots, r$, and an operator $Q : L^1 \to L^1$ such that for all densities f, Pf has the form*

$$Pf(x) = \sum_{i=1}^{r} \lambda_i(f) g_i(x) + Qf(x). \tag{6.1}$$

The densities g_i and the transient operator Q have the following properties:

  (1) *The g_i have disjoint support (i.e. are mutually orthogonal and thus form a basis set), so $g_i(x)g_j(x) = 0$ for all $i \neq j$.*
  (2) *For each integer i there is a unique integer $\alpha(i)$ such that $Pg_i = g_{\alpha(i)}$. Furthermore, $\alpha(i) \neq \alpha(j)$ for $i \neq j$. Thus the operator P permutes the densities g_i.*
  (3) $\| P^t Qf \| \to 0$ *as $t \to \infty$,* $t \in N$.

Notice from equation (6.1) that $P^{t+1}f$ may be written in the form

$$P^{t+1}f(x) = \sum_{i=1}^{r} \lambda_i(f) g_{\alpha^t(i)}(x) + Q_t f(x), \qquad t \in N \tag{6.2}$$

where $Q_t = P^t Q$, $\| Q_t f \| \to 0$ as $t \to \infty$, and $\alpha^t(i) = \alpha(\alpha^{t-1}(i)) = \cdots$. The density terms in the summation of (6.2) are just permuted by each application of P. Since r is finite, the series

$$\sum_{i=1}^{r} \lambda_i(f) g_{\alpha^t(i)}(x) \tag{6.3}$$

must be periodic with a period $T \leq r!$. Further, as

$$\{\alpha^t(1), \ldots, \alpha^t(r)\}$$

is just a permutation of $1, \cdots, r$ the summation (6.3) may be written in the alternative form

$$\sum_{i=1}^{r} \lambda_{\alpha^{-t}(i)}(f) g_i(x),$$

where $\alpha^{-t}(i)$ is the inverse permutation of $\alpha^t(i)$.

This rewriting of the summation portion of (6.2) makes the effect of successive applications of P completely transparent. Each application of P simply permutes the set of scaling coefficients associated with the densities $g_i(x)$ [remember that these densities have disjoint support].

Since T is finite and the summation (6.3) is periodic (with a period bounded above by $r!$), and $\| Q_t f \| \to 0$ as $t \to \infty$, we say that for any smoothing Markov operator the sequence $\{P^t f\}$ is **asymptotically periodic** or, more briefly, that P is asymptotically periodic. Komornik (1991) has recently reviewed the subject of asymptotic periodicity.

One interpretation of equation (6.2) is that *any asymptotically periodic system is quantized from a statistical point of view*. Thus if t is large enough, which simply means that we have observed the system longer than its relaxation time so $\| Q_t f \|$ is approximately zero, then

$$P^{t+1} f(x) \simeq \sum_{i=1}^{r} \lambda_i(f) g_{\alpha^t(i)}(x).$$

Asymptotically, $P^t f$ is either equal to one of the basis densities g_i of the ith pure state, or to a mixture of the densities of these states, each weighted by $\lambda_i(f)$. It is important to also realize that the limiting sequence $\{P^t f\}$ is, in general, dependent on the choice of the initial density f.

How would the property of asymptotic periodicity be manifested in a continuous time system? If t is continuous, $t \in R^+$, then for every t we can find a positive integer m and a number $\theta \in [0, 1]$ such that $t + 1 = m + \theta$. Then, asymptotically

$$P^{t+1} f(x) = P^m(P^\theta f) \simeq \sum_{i=1}^{r} \lambda_{\alpha^m(i)}(P^\theta f) g_i(x).$$

Now, in the continuous time case we expect that there will be a periodic modulation of the scaling coefficients λ dependent on the initial density f, and the asymptotic limiting density will continue to display the quantized nature characteristic of the discrete time situation. This behaviour has been discovered and studied by Losson (1991) in differential delay equations.

Asymptotically periodic Markov operators always have at least one stationary density given by

$$f_*(x) = \frac{1}{r} \sum_{i=1}^{r} g_i(x), \tag{6.4}$$

where r and the $g_i(x)$ are defined in Theorem 6.1. It is easy to see that $f_*(x)$ is a stationary density, since by Property 2 of Theorem 6.1 we also have

$$P f_*(x) = \frac{1}{r} \sum_{i=1}^{r} g_{\alpha(i)}(x),$$

and thus f_* is a stationary density of P^t. Therefore, for any smoothing Markov operator the stationary density (6.4) is just the average of the densities g_i.

Our next theorem will be very useful in Chapter 10 when we study the entropy behaviour of discrete time systems placed in contact with a heat bath.

Theorem 6.2. *Let P be a Markov operator. If there exists an $h \in L^1$ and $\gamma < 1$ such that*

$$\limsup_{t \to \infty} ||(P^t f - h)^+|| \le \gamma \qquad for \quad f \in D, \tag{6.5}$$

then $\{P^t f\}$ is asymptotically periodic.

Proof. Let $\epsilon = \frac{1}{4}(1 - \gamma)$ and take $\mathcal{F} = \{h\}$. Since $\mathcal{F}$, which contains only one element, is evidently weakly precompact, then by WPC3 of Chapter 3 there exists a $\delta > 0$ such that

$$\int_E h(x) \, \mu(dx) < \epsilon \qquad for \quad \mu(E) < \delta. \tag{6.6}$$

Furthermore, there is a measurable set A of finite measure for which

$$\int_{X \setminus A} h(x) \, \mu(dx) < \epsilon. \tag{6.7}$$

Now fix $f \in D$. From (6.5) we may choose an integer $n_0(f)$ such that

$$|| (P^t f - h)^+ || \le \gamma + \epsilon \qquad for \quad t \ge t_0(f),$$

and, as a consequence

$$\int_C P^t f(x) \, \mu(dx) \le \int_C h(x) \, \mu(dx) + \gamma + \epsilon \qquad for \quad t \ge t_0(f) \tag{6.8}$$

for an arbitrary set C. Setting $C = E \cup (X \setminus A)$ in (6.8) and using (6.6) and (6.7) we have

$$\int_{E \cup (X \setminus A)} P^t f(x) \, \mu(dx) \le \int_E h(x) \, \mu(dx) + \int_{X \setminus A} h(x) \, \mu(dx) + \gamma + \epsilon$$
$$< 3\epsilon + \gamma = 1 - \epsilon \qquad for \quad t \ge t_0(f).$$

Thus P is smoothing. This, in conjunction with Theorem 6.1, completes the proof. $\square$

The interpretation of Theorem 6.2 is straightforward. Namely, for those regions where $P^t f > h$ for sufficiently large t, if the area of the difference between $P^t f$ and h is bounded above by $\gamma < 1$, then $\{P^t f\}$ is asymptotically periodic.

We close this section with the statement and proof of a necessary and sufficient condition for the ergodicity of a smoothing Markov operator.

Theorem 6.3. *Let P be an asymptotically periodic Markov operator in a normalized measure space. Then P is ergodic if and only if the permutation $\alpha(i)$ of the Spectral Decomposition Theorem 6.1 is cyclical.*

Proof. We start with the proof that when P is ergodic then $\alpha(i)$ must be a cyclical permutation. Suppose that the disjoint supports of the r densities $g_i(x)$ are labeled by A_i, $i = 1, \cdots, r$. Assume that $\alpha(i)$ is not cyclical so there is an invariant subset $I \in \{\alpha(i)\}$. As a consequence, there is at least one set A_i that is invariant, and since the supports of the densities $g_i(x)$ have positive measure we conclude that there is an invariant subset of the phase space X that is not trivial. This contradicts the definition of ergodicity, so when P is ergodic the permutation $\alpha(i)$ must be cyclical.

To prove the converse, that if $\alpha(i)$ is a cyclical permutation then P is ergodic, we first use the spectral decomposition of $P^t f$ given by equation (6.1) to write the system state density average (3.15a) as

$$A_t f(x) = \sum_{i=1}^r g_i(x) \frac{1}{t} \sum_{k=0}^{t-1} \lambda_{\alpha^{-k}(i)}(f) + \frac{1}{t} \sum_{k=0}^{t-1} Q_k f(x).$$

Now the limit

$$\bar{\lambda}_i(f) = \lim_{t \to \infty} \frac{1}{t} \sum_{k=0}^{t-1} \lambda_{\alpha^{-k}(i)}(f)$$

exists because the cyclicity of the permutation $\alpha(i)$ of the set $\{1, \cdots, r\}$ implies the periodicity of the $\lambda_{\alpha^{-k}(i)}(f)$. Furthermore, since every portion of this summation of length r consists of exactly the same set of numbers but in a different order for each different i, it is clear that the limit $\bar{\lambda}_i(f)$ is, in fact, independent of i. Call it $\bar{\lambda}(f)$. Thus, from the Spectral Decomposition Theorem 6.1, we have that

$$\lim_{t \to \infty} A_t f(x) = \bar{\lambda}(f) \sum_{i=1}^{r} g_i(x).$$

Since $\lim_{t \to \infty} A_t f$ is a density, integrating over the entire phase space X gives

$$\int_X \lim_{t \to \infty} A_t f(x)\, dx = r\bar{\lambda}(f) = 1,$$

so $\bar{\lambda}(f) = \frac{1}{r}$ and

$$\lim_{t \to \infty} A_t f(x) = \frac{1}{r} \sum_{i=1}^{r} g_i(x) \equiv f_*(x),$$

which is a stationary density of the asymptotically periodic Markov operator P. Thus, $\{P^t f\}$ is Cesàro convergent to a unique stationary density f_* and P is ergodic by Theorem 4.7. This finishes the proof. $\square$

This theorem tells us that for an asymptotically periodic system, cyclicity of the permutation $\alpha(i)$ is necessary and sufficient for the existence of a unique state of thermodynamic equilibrium characterized by the stationary density f_*.

B. ASYMPTOTIC PERIODICITY ILLUSTRATED.

Asymptotic periodicity may be either inherent to a dynamical system, or induced by stochastic perturbations of a system (Chapter 10). For dynamics described by maps on the unit interval, the following theorem (Lasota and Mackey, 1994) is sometimes useful in establishing the existence of inherent asymptotic periodicity.

Theorem 6.4. *Let $S : [0,1] \to [0,1]$ be a nonsingular transformation satisfying the following three conditions:*

(1) *There exists a partition $0 = b_0 < b_1 < \cdots < b_m = 1$ of $[0,1]$ such that for each integer $i = 1, \cdots, m$ the restriction of $S(x)$ to $[b_{i-1}, b_i]$ is a C^2 function.*

(2) *$|S'(x)| \geq \vartheta > 1$, $x \neq b_i$.*

(3) *There exists a real constant c such that $\frac{|S''(x)|}{|S'(x)|^2} \leq c < \infty$, $x \neq b_i$, $i = 0, 1, \cdots, m$.*

Further, let P be the Frobenius-Perron operator corresponding to S. Then for all densities f, the sequence $\{P^t f\}$ is asymptotically periodic.

Example 6.1. To examine the properties of an asymptotically periodic system, choose a generalization of the tent map (3.5),

$$S(x) = \begin{cases} ax & 0 \leq x < \frac{1}{2} \\ a(1-x) & \frac{1}{2} \leq x \leq 1, \end{cases} \tag{6.9}$$

where $1 < a < 2$ (see Provatas and Mackey, 1991a).

To investigate how the map (6.9) transforms densities, we must first derive an expression for the operator P that corresponds to this transformation. Proceeding as in Example 3.6 where the tent map with $a = 2$ was introduced, it is a simple calculation to show that the Frobenius-Perron operator corresponding to (6.9) is given by

$$Pf(x) = \frac{1}{a} \left[f\left(\frac{1}{a}x\right) + f\left(1 - \frac{1}{a}x\right) \right]. \tag{6.10}$$

For $1 < a \leq 2$, and for the partition $b_0 = 0 < b_1 = \frac{1}{2} < b_2 = 1$, the generalized hat map (6.9) satisfies the conditions of Theorem 6.4. Thus, the hat map is asymptotically periodic and the evolution of densities *via* the operator (6.10) can be expressed through the spectral decomposition (6.1).

Ito *et al.* (1979) have shown that the hat map is ergodic, thus possessing a unique invariant density f_* of the form (6.4). Its form has been derived in the parameter window $a_{n+1} = 2^{1/2^{1/(n+1)}} < a \leq 2^{1/2^{1/n}} = a_n$, $n = 1, 2, \cdots$ by Yoshida *et al.* (1983). Provatas and Mackey (1991a) have proved the asymptotic periodicity of (6.9) with period

$T = (n+1)$ for $2^{1/2^{1/(n+1)}} < a \leq 2^{1/2^{1/n}}$. Thus, for example, $\{P^t f\}$ has period 1 for $2^{1/2} < a \leq 2$, period 2 for $2^{1/4} < a \leq 2^{1/2}$, period 4 for $2^{1/8} < a \leq 2^{1/4}$, *etc.*

To analytically illustrate the eventual dependence of the sequence $\{P^t f\}$ on the initial density f for asymptotically periodic systems, pick $a = \sqrt{2}$ which is the upper boundary of the range of a values for which (6.9) is asymptotically periodic with period 2. For this value of a, the unique stationary density (6.4) satisfying $Pf_* = f_*$, where P is given by (6.10), takes the explicit form

$$f_*(x) = u 1_{J_1}(x) + v 1_{J_2}(x) \tag{6.11}$$

where $u = \frac{1}{2}[3 + 2\sqrt{2}]$, $v = \frac{1}{2}[4 + 3\sqrt{2}]$, and the sets J_1 and J_2 are defined by

$$J_1 = [\sqrt{2} - 1, 2 - \sqrt{2}] \qquad \text{and} \qquad J_2 = [2 - \sqrt{2}, \frac{1}{2}\sqrt{2}] \tag{6.12}$$

respectively (*cf.* Provatas and Mackey (1991a)). S maps the set J_1 into J_2 and *vice versa*.

It can be shown analytically that picking $f_*(x)$ given by (6.11) as an initial density simply results in a sequence of densities all equal to the starting density. This is quite different from what happens with an initially uniform density

$$f(x) = (2 + \sqrt{2}) 1_{J_1 \cup J_2}(x). \tag{6.13}$$

In this case, the first iterate $f_1 = Pf$ is given by

$$f_1(x) = (1 + \sqrt{2}) 1_{J_1}(x) + 2(1 + \sqrt{2}) 1_{J_2}(x) \tag{6.14}$$

and iteration of $f_1(x)$ leads, in turn to an $f_2(x) = f(x)$ and thus the cycling of densities repeats indefinitely with period 2 (*cf.* Figure 6.1a).

This effect of the choice of the initial density on the sequence of subsequent densities can be further illustrated by choosing an initial density

$$f(x) = [3 + 2\sqrt{2}] 1_{J_1}(x) \tag{6.15}$$

totally supported on the set J_1. In this case,

$$f_1(x) = Pf(x) = [4 + 3\sqrt{2}] 1_{J_2}(x), \tag{6.16}$$

and $f_2 = f$, $f_3 = f_1$, $\cdots$ so once again the densities cycle between f and f_1 with period 2 (*cf.* Figure 6.1b). Figure 6.1c illustrates the behaviour of $\{P^t f\}$ for an initially nonuniform density.•

Example 6.2. Sharkovski (1965) has shown that maps like (3.7),

$$S(x) = rx(1 - x) \tag{6.17}$$

with a single quadratic maximum display period doubling in the number of fixed points as the parameter r is increased. For example, with $0 \leq r < 1$ the single fixed point of (5.17) is $x^* = 0$, while for $1 < r \leq 3$, equation (6.17) has one stable fixed point given by $x^* = 1 - \frac{1}{r}$. For r between $3 < r \leq r_c \simeq 3.57 \cdots$ there is a cascade of parameters which sequentially give rise to 2 unstable fixed points, then 4, 8 *etc.* The periodicity in each of these intervals is equal to the number of fixed points. At r_c, also known as the accumulation point, there are an infinite number of unstable fixed points.

On the other side of the critical parameter, $r_c < r \leq 4$ the quadratic map (and maps like it with a single quadratic maximum) has a spectrum of parameter values, labeled by r_n, $n = 1, 2, \cdots$ where so-called "banded chaos" has been reported by Crutchfield *et al.* (1980), Lorenz (1980), and Grossman and Thomae (1977, 1981) based on numerical work. At these values the unit interval $X = [0, 1]$ partitions into 2^n subintervals, labeled J_l, $l = 1, 2, \cdots, 2^n$. These are such that $S^{2^n} : J_l \to J_l$ maps J_l *onto* J_l. As well each J_l is mapped cyclically through the whole sequence of $\{J_l\}$ after 2^n applications of S. The iterates of a time series are attracted to these J_l subsets, returning to any J_l every 2^n iterations. These iterates form an aperiodic sequence with a positive Liapunov exponent [Devaney, 1986]. The procedure whereby which one obtains the parameter values r_n at which 2^n banded chaos occurs is given by Grossman and Thomae (1981).

The Frobenius-Perron operator corresponding to the quadratic map (6.17) is

$$Pf(x) = \frac{1}{\sqrt{1 - \frac{4x}{r}}} \left[f\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - \frac{4x}{r}} \right) + f\left(\frac{1}{2} - \frac{1}{2}\sqrt{1 - \frac{4x}{r}} \right) \right]. \tag{6.18}$$

At values of $r = r_n$, the iterates of any initial density f supported on $[0, 1]$, acted on by (6.18), will eventually decompose so they are supported on disjoint sets J_l. Subsequent to the contraction of density supports onto the sequence of sets $\{J_l\}$, the evolution of the sequence $\{P^t f\}$ becomes periodic in time. At these values, the observed periodic evolution of ensemble densities, is, in fact, asymptotically periodic (Provatas and Mackey, 1991a).

The parameter values $r = r_n$ define a reverse sequence to the period doubling sequence for $r \leq r_c$. For the latter sequence, we talk of a period doubling in the number of unstable fixed points. When $r = r_n$ however, fixed points are replaced by "chaotic bands" and going from r_n to r_{n+1} involves a doubling in the number of bands.

As with the hat map of Example 6.1, the scaling coefficients $\lambda_1(f)$, $\lambda_2(f)$ can be analytically determined for period two asymptotic periodicity for the quadratic map when $r = r_1$, and the attracting phase space consists of the subsets J_1 and J_2. These are disjoint and connected at the fixed point of (6.17), and $S : J_1 \to J_2$, $S : J_2 \to J_1$. The coefficients $\lambda_1(f)$, $\lambda_2(f)$ may be obtained for any arbitrary initial density f supported on the phase space $X = [0, 1]$.

Figure 6.2 illustrates the period 2 asymptotic evolution of $\{P^t f\}$ after 20 transients, for $r = r_1$. In Figure 6.2a the initial density is uniform on the region of $J_1 \cup J_2$ given by $[0.7, 0.8]$. Figure 6.2b shows an asymptotic cycle of $\{P^t f\}$ with $f(x) = 200(x - 0.9)$ supported on $[0.9, 1]$. Figure 6.3a illustrates a period 4 cycle in $\{P^t f\}$ when $r = r_2$, with the initial density f uniform on $[0.5, 0.85]$. Figure 6.3b shows one period 4 cycle of $P^t f$ with $f(x) = 200(x - 0.91)$ supported on $[0.9, 1]$. All of the illustrated sequences are dependent on the initial density. •

C. THE WEAK FORM OF THE SECOND LAW.

The fact that asymptotically periodic Markov operators have a stationary density given by (6.4) does not guarantee the uniqueness of this stationary density. Regardless of whether or not asymptotically periodic systems have unique stationary densities, they have the important property that their conditional entropy is an increasing function that approaches a maximum. This result is formulated more precisely in

Theorem 6.5. *Let P be an asymptotically periodic Markov operator with stationary density f_*. Then as $t \to \infty$ the conditional entropy $H_c(P^t f | f_*)$ of $P^t f$ with respect to f_* approaches a limiting value $H_{max}(f | f_*) \leq 0$, where*

$$H_{max}(f | f_*) = -\sum_i \int_X \lambda_i(f) g_i(x) \log \left\{ \frac{1}{f_*(x)} \sum_i \lambda_i(f) g_i(x) \right\} dx. \tag{6.19}$$

Proof. Since P is asymptotically periodic, the representation of the Spectral Decomposition Theorem 6.1 is valid, and more precisely equation (6.2) for $P^t f$. Write equation (6.2) in the form

$$P^{t+1} f(x) = \Sigma_t(f, x) + Q_t f(x),$$

where $\Sigma_t(f, x)$ denotes the summation portion of (6.2). Remember that since P is asymptotically periodic, for large times t, $\| Q_t f \| \simeq 0$ and thus $P^{t+1} f(x) \simeq \Sigma_t(f, x)$, so the long time conditional entropy is given by

$$H_c(P^{t+1} f | f_*) \simeq - \int_X \Sigma_t(f, x) \log \left\{ \frac{\Sigma_t(f, x)}{f_*(x)} \right\} dx$$
$$= H_c(\Sigma_t(f) | f_*).$$

However, $\Sigma_t(f, x)$ is periodic with finite period T. Since by Theorem 3.1 we also know that $H_c(P^t f | f_*) \geq H_c(f | f_*)$ [the conditional entropy can never decrease], it follows that the approach of $H_c(P^t f | f_*)$ to $H_c(\Sigma_t(f) | f_*)$ must be uniform. Even though $\Sigma_t(f, x)$ is periodic with a finite period T, $H_c(\Sigma_t(f) | f_*)$ is a constant independent of t. In fact we have

$$H_c(\Sigma_t(f) | f_*) = - \int_X \sum_i \lambda_i(f) g_i(x) \log \left\{ \frac{1}{f_*(x)} \sum_i \lambda_i(f) g_i(x) \right\} dx$$
$$\equiv H_{max}(f | f_*) \leq 0$$

for large t. The nonpositivity of $H_{max}(f|f_*)$ is a consequence of the integrated Gibbs inequality (1.5). $\quad\square$

Note that if the stationary density f_* of P is given by (6.4), then the expression for $H_{max}(f|f_*)$ becomes even simpler. Namely, with

$$f_*(x) = \frac{1}{r}\sum_{i=1}^{r} g_i(x),$$

$H_{max}(f|f_*)$ as given by (6.19) becomes

$$H_{max}(f|f_*) = -\log r - \sum_{i=1}^{r} \lambda_i(f)\log\lambda_i(f) \tag{6.20}$$

when we use the orthogonality of the densities $g_i(x)$. Since $0 \le \lambda_i(f) \le 1$ for all i, we may also place a lower bound on $H_{max}(f|f_*)$:

$$-\log r \le H_{max}(f|f_*) \le 0.$$

This weak form of the Second Law of thermodynamics is the strongest result that we have yet encountered. It demonstrates that as long as the density evolves under the action of a Markov operator that is smoothing, the conditional entropy of that density converges to a maximum. There are two important facets of this evolution that should be recognized:

(1) The convergence of the entropy is due to the fact that $\| Q^t f \| \to 0$ as $t \to \infty$ in the representation (6.2) of Theorem 6.1.
(2) The maximum value of the entropy, $H_{max}(f|f_*)$, as made explicit by the notation, is generally dependent on the choice of the initial density f and, thus, the method of preparation of the system. This indicates that systems with asymptotically periodic dynamics may have a discrete or continuous spectrum of metastable states of thermodynamic equilibrium, each with an associated maximal entropy.

Example 6.3. To illustrate the evolution of the conditional entropy of an asymptotically periodic system we return to our example of the tent map (6.9) with $a = \sqrt{2}$. For this value of a, the stationary density f_* is given by equation (6.11). If we pick an initial density given by f_*, then the conditional entropy $H_c(P^t f_*|f_*) = 0$, its maximal value, for all t. However, if we pick an initially uniform density (6.13), $f(x) = (2+\sqrt{2})1_{J_1 \cup J_2}$, then it is straightforward to show that

$$H_c(f|f_*) = H_c(f_1|f_*) \simeq -0.01479,$$

where $f_1 = Pf$ is given by equation (6.14). Thus by choosing an initial density given by (6.13) or (6.14), the limiting conditional entropy approaches a value less than its maximal value of zero.

This effect of the choice of the initial density affecting the limiting value of the conditional entropy can be further illustrated by choosing an initial density

$$f(x) = [3 + 2\sqrt{2}]1_{J_1}(x)$$

totally supported on the set J_1. In this case, as we have shown,

$$f_1(x) = Pf(x) = [4 + 3\sqrt{2}]1_{J_2}(x),$$

and $f_2 = f$, $f_3 = f_1$, *etc.* so once again the densities cycle between f and f_1 with period 2. The limiting value of the conditional entropy is given by

$$H_c(f|f_*) = H_c(f_1|f_*) = -\log(2) \simeq -0.69316.$$

Thus, with three different choices of an initial density f we have shown that the conditional entropy of the asymptotically periodic system (6.9) may have at least three different limiting asymptotic values. $\bullet$

Example 6.4. The continuous functional dependence of $H_{max}(f|f_*)$ on the initial density f can be illustrated analytically for the maps (6.9) and (6.17) when they generate period 2 asymptotic periodicity. In particular consider a class of initial densities given by (*cf.* Provatas and Mackey, 1991a)

$$f(x) = \begin{cases} \frac{1}{\xi} & x \in [\gamma_1, \gamma_1 + \xi] \\ 0 & \text{otherwise,} \end{cases} \tag{6.21}$$

where γ_1 is the solution of $\gamma_1 = S^2(\gamma_1)$ and is given by

$$\gamma_1 = \frac{1}{a+1}$$

for the hat map and by

$$\gamma_1 = \frac{r_1^2}{4}\left(1 - \frac{r_1}{4}\right)$$

for the quadratic map.

A plot of $H_{max}(f|f_*)$ for the hat map is shown in Figure 6.4. A remarkable feature of Figure 6.4 is the existence of a sequence of ξ values at which the limiting conditional entropy values are equal. For these values of ξ the asymptotic decomposition of $P^t f$ is identical and the limiting conditional entropy is $H_{max}(f|f_*) \simeq -0.01479$ as we calculated in the previous example with an initial density given by (6.13). Note also the local minima in the limiting conditional entropy as the spreading parameter ξ increases.

A similar comparison of the limiting conditional entropy can be made for the asymptotic periodicity of the quadratic map at $r = r_1$. The same set of initial densities defined by (6.21) is considered. Figure 6.5 is the plot analogous to Figure 6.4 for the hat map. Note that for the quadratic map the maxima in the limiting conditional entropy do not define isoentropic points, although $H_{max}(f|f_*) \simeq -0.093$ as $\xi \to 1$. Moreover, a zig-zag pattern similar to Figure 6.4 emerges but on a much smaller scale, as shown by the insets. •

We close this section with the statement and proof of a sufficient condition for the weak form of the Second Law of thermodynamics.

Theorem 6.6. *Let P be a Markov operator in a normalized measure space, and assume that there is a stationary density $f_* > 0$ of P. If there is a constant $c > 0$ such that for every bounded initial density f*

$$H_c(P^t f|f_*) \geq -c$$

for sufficiently large t, then P^t is asymptotically periodic and

$$\lim_{t \to \infty} H_c(P^t f|f_*) = H_{max}(f|f_*) \leq 0.$$

This theorem assures us that if we are able to find some time t_1 such that the conditional entropy is bounded below for times $t > t_1$, then the entropy is evolving under the action of an asymptotically periodic Markov operator and, as a consequence of Theorem 6.5, the conditional entropy of $P^t f$ approaches a maximum that is generally dependent on the initial density with which the system was prepared.

Proof. Pick a subset E of the phase space X with nonzero Lebesgue measure $\mu_L(E)$. From the definition of the conditional entropy $H_c(P^t f|f_*)$ and our hypothesis, for all sufficiently large times t we have

$$H_c(P^t f|f_*) \equiv -\int_E P^t f(x) \log\left(\frac{P^t f(x)}{f_*(x)}\right)\, dx - \int_{X\setminus E} P^t f(x) \log\left(\frac{P^t f(x)}{f_*(x)}\right)\, dx$$
$$\geq -c.$$

Remembering the definition of the function η from equation (1.2), it follows that

$$\int_E P^t f(x) \log\left(\frac{P^t f(x)}{f_*(x)}\right)\, dx \leq c - \int_{X\setminus E} P^t f(x) \log\left(\frac{P^t f(x)}{f_*(x)}\right)\, dx$$
$$= c + \int_{X\setminus E} \eta\left(\frac{P^t f(x)}{f_*(x)}\right)\, \mu_*(dx)$$
$$\leq c + \eta_{max} \int_{X\setminus E} \mu_*(dx)$$
$$\leq c + \frac{\mu_*(X)}{e}.$$

Further specify the set E by

$$E = \left\{ x \in X : \left(\frac{P^t f(x)}{f_*(x)} \right) > N \right\},$$

where the constant N is selected to make $\mu_L(E) < \delta$. Then,

$$\log N \int_E P^t f(x)\, dx \leq \int_E P^t f(x) \log \left(\frac{P^t f(x)}{f_*(x)} \right) dx \leq c + \frac{\mu_*(X)}{e},$$

or

$$\int_E P^t f(x)\, dx \leq \frac{c + \frac{\mu_*(X)}{e}}{\log N} \equiv \epsilon.$$

Next, pick a second subset $A \subset X$ of nonzero measure so

$$\int_{X \setminus A} P^t f(x)\, dx = \int_X P^t f(x)\, dx - \int_A P^t f(x)\, dx = 1 - \mu_L(A).$$

Thus,

$$\int_{E \cup (X \setminus A)} P^t f(x)\, dx \leq 1 - \mu_L(A) + \epsilon \equiv k.$$

It is clear that we may always select the set A in such a way that $\epsilon < \mu_L(A) < 1$ and, hence, $0 < k < 1$. Therefore, P is smoothing by definition. The rest of the proof is a direct consequence of the Spectral Decomposition Theorem 6.1 and Theorem 6.5 concerning the convergence of the conditional entropy under the action of an asymptotically periodic Markov operator. $\square$

D. ASYMPTOTIC PERIODICITY AND CORRELATIONS.

In the previous chapter we showed that temporal correlations in mixing systems decay to zero in spite of the fact that entropy is absolutely constant when the system is invertible. Suppose that instead of a mixing transformation we have an asymptotically periodic transformation with a unique stationary density f_* of the corresponding Markov operator P, and, as a consequence, the system is ergodic. In this case the behaviour of the correlation function is quite different.

Since P is asymptotically periodic and Theorem 6.1 also holds for L^1 functions, we can choose $f = \eta$ to obtain

$$P^{\tau+1} \eta(x) = \sum_{i=1}^{r} \lambda_i(\eta) g_{\alpha^\tau(i)}(x) + Q_\tau \eta(x).$$

Further, because of the ergodicity of P we can write the correlation function as

$$R_{\sigma,\eta}(\tau + 1) = < P^{\tau+1} \eta, \sigma >$$

or, more explicitly,

$$R_{\sigma,\eta}(\tau + 1) = \sum_{i=1}^{r} \lambda_i(\eta) \int_X g_{\alpha^\tau(i)}(x) \sigma(x)\, dx + \int_X \sigma(x) Q_\tau \eta(x)\, dx. \tag{6.22}$$

Due to the asymptotic periodicity of P, the first term in (6.22) is periodic in τ with period $T \leq r!$. Furthermore, because of the convergence properties of the transient operator Q the second term will decay to zero as $\tau \to \infty$. Therefore, for asymptotically periodic dynamics the correlation function naturally separates into sustained periodic and decaying stochastic components.

This decoupling of the time correlation function into two independent components can be understood as follows. Asymptotically periodic systems have r disjoint attracting regions of their phase space X whose union is given by

$$\bigcup_{i=1}^{r} \text{supp}\,\{g_i\}.$$

Each of the regions supp$\{g_i\}$ map onto each other cyclically according to $\alpha(i)$. All ensembles of initial conditions will asymptotically map into these regions (*i.e.*, all densities will decompose). Thus a time series will also visit these supports periodically, and we expect a periodic component in the time correlation function. However, iterates of the time series which return into any one of the supp $\{g_i\}$, are described by a density g_i, and so there must exist a stochastic component of the correlation function (the second term of (6.22)).

Thus, asymptotically periodic systems have temporal correlations which are a combination of both periodic and stochastic elements and which never decay to constant values as $t \to \infty$ in spite of the fact that their conditional entropy does approach a local maximum as $t \to \infty$. This is to be compared with mixing systems whose entropy is forever fixed by the mode of preparation of the system, but which nevertheless show an approach of the correlations in the system to zero at long times. The contrasting nature of these two results indicates that there is no connection to be drawn between the limiting behaviour of entropy in a system and the limiting behaviour of temporal correlations.

E. SUMMARY.

In this chapter we have shown how the property of smoothing for Markov operators is equivalent to asymptotic periodicity of sequences of densities (Theorem 6.1), and that asymptotic periodicity is sufficient to guarantee the existence of at least one state of thermodynamic equilibrium (with density given by equation (6.4)) as well as the increase of the entropy to a maximum as time progresses (Theorem 6.5). Interestingly, the maximum entropy to which asymptotically periodic systems evolve in this circumstance (equation (6.19)) may be less than the absolute maximum value corresponding to equation (6.4), and usually depends on the initial density with which the system is prepared. Thus the entropy of the final thermodynamic state of an asymptotically periodic system depends, in general, on the initial state. Theorem 6.6 gives a sufficient condition for this behaviour in the form of the existence of a finite lower bound on the conditional entropy. Further, the behaviour of the entropy and correlations in asymptotically periodic systems is opposite to that of mixing systems, indicating that there is no connection to be drawn between entropy evolution and the limiting behaviour of correlations.

In the next chapter we introduce a dynamical property even stronger than asymptotic periodicity which is both necessary and sufficient for the evolution of system entropy to its unique maximal value of zero.

Figure 6.1. The evolution of $P^t f$ in the period two window under the action of the hat map, with $a = \sqrt{2}$. In (a) f is uniform over $J_1 \cup J_2$. Since the g_i are uniform over J_i, $i = 0, 1$, $P^t f$ sets into immediate oscillations without transients. In (b) f is uniform over the subspace J_1. Again $P^t f$ sets into immediate oscillations through the states g_1 and g_2. In (c) $f(x) = \frac{4(5+\sqrt{2})}{7}x$, restricted to $J_1 \cup J_2$. Now $P^t f$ evolves through two transient densities before settling into a periodic oscillation.

Figure 6.2. A numerical illustration of one periodic cycle of the asymptotic sequence $\{P^t f\}$ under the action of the quadratic map for the parameter $r = r_1 = 3.678573508$. A transient of 20 densities has been discarded, and the iterates $P^{21}f$, $P^{22}f$, and $P^{23}f$ are shown. Since $P^{21}f = P^{23}f$, the sequence $\{P^t f\}$ asymptotically repeats with period 2. In (a) the initial density f, shown in the inset, is uniform over $[0.7, 0.8]$. In (b), $f(x) = 200(x-0.9)$ over $[0.9, 1]$.

Figure 6.3. Two period 4 cycles of the asymptotic sequence $\{P^t f\}$ for the quadratic map when $r = r_2 = 3.592572184$. In this figure 40 transients have been discarded and the iterates $P^{41}f$, $P^{42}f$, $P^{43}f$, $P^{44}f$ and $P^{45}f$ are shown. Since $P^{41}f = P^{45}f$, the sequence $\{P^t f\}$ asymptotically repeats with period 4. In (a) the initial density (inset) f is uniform over $[0.5, 0.85]$. In (b) $f(x) = 200(x - 0.9)$ over $[0.9, 1]$.

Figure 6.4. The limiting conditional entropy, $H_{max}(f|f_*)$, versus the spreading parameter ξ for the hat map at $a = \sqrt{2}$. ξ is equal to the width of the support of an initial uniform density f. The local maxima in the figure correspond to equal limiting conditional entropy values.

Figure 6.5. A graph of the limiting conditional entropy $H_{max}(f|f_*)$ versus ξ for the quadratic map at $r = r_1$. The parameter ξ plays the same role as in Figure 6.4. Variations in $H_{max}(f|f_*)$ occur over a smaller ξ scale for the quadratic map. (ii) is a blow-up of the inset box in frame (i). (iii) is a blow-up of the inset box in (ii).

CHAPTER 7.
GLOBAL EVOLUTION OF ENTROPY

In Chapter 3 we have shown that invertible systems have absolutely constant entropy, namely $H_c(P^t f|f_*) = H_c(f|f_*)$ for all times t (Theorem 3.2), while for noninvertible systems the entropy may increase (Theorem 3.1) since $H_c(P^t f|f_*) \geq H_c(f|f_*)$. Thus, noninvertibility is absolutely necessary (though not necessarily sufficient) for the entropy of any system to increase from its initial value.

To this point we have introduced three types of dynamics that have important consequences for understanding thermodynamic behaviour. The first is ergodicity, introduced in Chapter 4, which is both necessary and sufficient for a unique state of thermodynamic equilibrium to exist (Theorem 4.5). In Chapter 5 mixing, an even stronger type of irregular behaviour, was introduced. In spite of the fact that mixing systems display weak convergence of $P^t f$ to a unique state of thermodynamic equilibrium regardless of the initial density (Theorem 5.1), when they are invertible the entropy of these systems is constant and equal to the initial entropy corresponding to the density with which the system is prepared (Theorem 5.2). Finally, in the last chapter we discussed asymptotic periodicity. Asymptotic periodicity is important since it ensures the existence of at least one state of thermodynamic equilibrium with stationary density f_*. It further guarantees the convergence of the conditional entropy to an extremum which is not only equal to or less than its maximal value of zero (corresponding to f_*) but also dependent on the choice of initial density (Theorem 6.5).

These observations indicate that attention should be focused on extensions of the concepts of ergodicity, mixing, and asymptotic periodicity that may only occur in noninvertible systems. Since we also know that increases in entropy need not culminate in the maximum value of the entropy (*e.g.* asymptotically periodic systems, Chapter 6), the essential question we now face is: **Under what circumstances will the entropy of a noninvertible system approach its maximum value of zero?**

To start to construct the answer, in Section A we introduce the concept of exactness, a new type of irregular behaviour that only irreversible transformations may display. Section B provides the complete answer to the question we posed above.

A. EXACTNESS.

To extend the catalog of irregular behaviors that transformations may exhibit, we make the following definition. If S_t is an f_* measure preserving transformation operating on a normalized phase space X, then S_t is said to be **f_* exact** if

$$\lim_{t \to \infty} \mu_*(S_t(A)) = 1$$

for all sets A of nonzero measure. If f_* is the uniform density, $f_* = 1$, then we say that S_t is **uniformly exact**.

To understand the nature of exactness, it is first important to realize that *invertible systems can not be exact*. To see this, note that for an invertible f_* measure preserving transformation S_t we have $\mu_*(S_t(A)) = \mu_*(S_t^{-1}(S_t(A))) = \mu_*(A)$. Thus the definition of exactness is violated.

Example 7.1. An example, similar to that for ergodicity and mixing, is helpful in showing how exact systems operate. Figure 7.1 shows the first six iterates of 10^4 points randomly distributed in $[0, \frac{1}{10}] \times [0, \frac{1}{10}]$ under the action of the uniformly exact transformation

$$S(x, y) = (3x + y, x + 3y) \qquad (\text{mod } 1). \tag{7.1}$$

It is clear that the behaviour is quite different from a mixing transformation. Under the action of an exact transformation an initial set A is quickly dispersed throughout the entire phase space X. If one interpreted this example in terms of many different particles moving with dynamics given by (7.1), and each with a different pair of initial conditions, then we would very soon find them uniformly dispersed throughout the phase space. •

Example 7.2. A second example of a uniformly exact transformation is given by the tent map (3.5). The tent map preserves the Lebesgue measure and if we start with an initial set $B = [0, b]$, then a simple geometric argument (try it!) suffices to show that after a finite number of iterations $\mu_L(S_t(B)) = 1$ and the transformation is uniformly exact. A more precise proof can be carried out using the behaviour of the evolution of densities by the Frobenius-Perron operator contained in Theorem 7.1 below. •

Example 7.3. Though not as well studied as discrete time systems, some noninvertible continuous time systems have been shown to be exact (Lasota and Mackey, 1994). Lasota (1979, 1981), Brunovský (1983), Brunovský and Komornik

(1984), Rudnicki (1985a,b; 1988) and Loskot (1985) have also considered the properties of the solutions $u(t,x)$ of the first order partial differential equation

$$\frac{\partial u}{\partial t} + c(x)\frac{\partial u}{\partial x} = f(x,u)$$

with the initial function

$$u(0,x) = v(x) \qquad \text{for} \quad x \in [0,1].$$

Both c and f are assumed to be continuously differentiable, and it is further assumed that

(1) $c(0) = 0, \quad c(x) > 0 \qquad$ for $\qquad x \in [0,1]$;
(2) $f_u(0,u_0) < 0, \quad f(0,u)(u-u_0) < 0 \quad$ for $\quad u > 0, u \neq u_0,$; and
(3) $0 \leq f(x,0), \quad f(x,u) \leq k_1 u + k_2 \quad$ for $\quad x \in [0,1], u \geq 0$ with constant $k_1, k_2 > 0$ and $u_0 > 0$.

With these conditions, whenever the initial function $v(x)$ satisfies $v(0) = 0$ then the semidynamical system $S_t(v(x)) \equiv u(t,x)$ is f_* exact. f_* is the (Gaussian) density of the Wiener measure (see Lasota and Mackey, 1994) on the function space $V = \{v \in C_+([0,1]) : v(0) = 0\}$ and $C_+(A)$ is the set of all nonnegative continuously differentiable functions on A. •

Example 7.4. Some delay differential equations, which are also noninvertible, have been studied as examples of continuous time exact systems. an der Heiden (1985) has studied the delay differential equation

$$\frac{dx}{dt} = a[f(x(t-1)) - x(t)]$$

with a suitably defined initial function $\phi(t')$, $t' \in [-1,0]$. It is known that this equation with a mixed feedback function of the form $f(z) = z/(1+z^n)$, $n > 0$, has solutions that are stable, periodic, or chaotic [Mackey and Glass, 1977; an der Heiden and Mackey, 1982]. an der Heiden uses a piecewise constant mixed feedback function f of the form

$$f(z) = \begin{cases} 0 & z < 1 \\ c & 1 \leq z \leq b \\ d & b < z, \end{cases}$$

so the analytic solution $x_\phi(t)$ can be written as the sequential joining of exponential functions of t. He then identifies the sequence of times t_i such that $x_\phi(t_i) = 1$, and derives an analytic map S relating successive differences in crossing times, $\Delta_i = t_{2i} - t_{2i-1}$,

$$\Delta_{i+1} = S(\Delta_i).$$

He has proved that for some parameter values (a,b,c,d) the Frobenius- Perron operator P corresponding to S is either asymptotically periodic or f_* exact.

Peters (1980a,b; 1983) has considered the solution behaviour of the delay differential equation

$$\frac{dx}{dt} = g(x(t-1))$$

where

$$g(z) = \begin{cases} \alpha & z < -1 \\ 1 & -1 \leq z < 0 \\ -1 & 0 \leq z \leq 1 \\ -\alpha & 1 < z. \end{cases}$$

As in the system considered by an der Heiden the solutions $x_\phi(t)$, corresponding to an initial condition $\phi(t')$, $t' \in [-1,0]$, can be written analytically as piecewise linear functions of time. Again by considering sequences of solution crossing times he derived a map S_ϕ which, using techniques developed in Lasota and Mackey (1985), may be shown to be either asymptotically periodic or f_* exact. •

Exact systems are important for an understanding of how convergence to a stationary density f_* of the canonical ensemble may be reached in a way that is an extension of mixing. To be specific, we have:

Theorem 7.1. *If S_t is an f_* measure preserving transformation operating on a finite normalized phase space X and P^t is the associated Frobenius-Perron operator corresponding to S_t, then S_t is f_* exact if and only if*

$$\lim_{t \to \infty} \| P^t f - f_* \| = 0,$$

i.e., $\{P^t f\}$ is strongly convergent to f_*, for all initial densities f.

This theorem offers a necessary and sufficient condition for the exactness of S_t in complete analogy with the previously presented necessary and sufficient ergodicity (Theorem 4.7) and mixing (Theorem 5.1) conditions related to the convergence properties of $\{P^t f\}$.

Proof. We start by showing that the strong convergence of $\{P^t f\}$ to f_* implies f_* exactness. Pick a set A of nonzero μ_* measure and pick an initial density f_A supported entirely on A. We also define a sequence $\{r_t\}$ by $r_t = ||P^t f_A - f_*||$ so $\{r_t\}$ is convergent to zero by the assumed strong convergence property.

By writing the functional form of the measure $\mu_*(S_t(A))$ and using the definition of the Frobenius-Perron operator, we have

$$
\begin{aligned}
\mu_*(S_t(A)) &= \int_{S_t(A)} f_*(x)\, dx = \int_{S_t(A)} P^t f_A(x)\, dx - \int_{S_t(A)} [P^t f_A(x) - f_*(x)]\, dx \\
&\geq \int_{S_t(A)} P^t f_A(x)\, dx - \int_X [P^t f_A(x) - f_*(x)]\, dx \\
&= \int_{S_t(A)} P^t f_A(x)\, dx - r_t \\
&= \int_{S_t^{-1}(S_t(A))} f_A(x)\, dx - r_t.
\end{aligned}
$$

Since $A \subset S_t^{-1}(S_t(A))$, this entire sequence reduces to

$$\mu_*(S_t(A)) \geq 1 - r_t,$$

and since $\{r_t\}$ converges to zero the proof is complete. The proof that f_* exactness implies the strong convergence of $\{P^t f\}$ to f_* is accomplished by a reversal of the argument. $\square$

The f_* exactness of a transformation implies that it is f_* mixing. To show this it suffices to remember that, from the Cauchy-Holder inequality, for a sequence of functions $\{f_t\}$ we have

$$| < f_t - f, g > | \leq \| f_t - f \| \cdot \| g \|.$$

Thus the convergence of $\| f_t - f \|$ to zero implies that $< f_t - f, g >$ also converges to zero and strong convergence therefore implies weak convergence. As a consequence exactness implies mixing just as mixing implies ergodicity.

As with ergodicity and mixing, we extend the definition of exactness to Markov operators P^t with a stationary density f_*. Then we say P^t is $\mathbf{f_*}$ **exact** if $\{P^t f\}$ is strongly convergent to f_* for all initial densities f.[9] Since strong convergence implies weak convergence which, in turn, implies Cesàro convergence, for Markov operators P we have immediately that exactness implies mixing implies ergodicity.

We may draw a connection between the exactness of systems with either the density of the microcanonical or canonical ensembles as stationary densities through the following result.

Theorem 7.2. *Consider a Markov operator $\tilde{P}$ with the density of the microcanonical ensemble as a stationary density, $\tilde{P}1 = 1$, and a second Markov operator P defined by*

$$Pf = f_* \tilde{P} \left(\frac{f}{f_*} \right).$$

---

[9] Operators P^t that are f_* exact have been called strong Markov operators by Misra *et al.* (1979), and monotonic Markov operators by Goldstein *et al.* (1981).

Then P^t is f_* exact if and only if $\tilde{P}^t$ is uniformly exact.

Proof. First notice that $\tilde{P}1 = 1$ if and only if $Pf_* = f_*$. By induction it is clear that

$$P^t f = f_* \tilde{P}^t \left(\frac{f}{f_*} \right).$$

Furthermore,

$$\lim_{t \to \infty} \| P^t f - f_* \| = \lim_{t \to \infty} \left\| f_* \left[\tilde{P}^t \left(\frac{f}{f_*} \right) - 1 \right] \right\|$$

$$\leq \sup_x f_*(x) \lim_{t \to \infty} \left\| \tilde{P}^t \left(\frac{f}{f_*} \right) - 1 \right\|.$$

As a consequence, $\tilde{P}^t$ uniformly exact implies that P^t is f_* exact. A reversal of the argument completes the proof. □

Example 7.5. As an illustration of Theorem 7.1, consider the dyadic transformation

$$S(x) = 2x \qquad (\text{mod } 1) \tag{7.2}$$

which is a special case of the r-adic transformation $S(x) = rx \pmod 1$ when r is a positive integer. The dyadic transformation (7.2) is clearly not invertible. A short calculation shows that it preserves the Lebesgue measure so the constant density $f_* = 1$ is a stationary density. (In fact, this is the unique stationary density.) The counterimage of an interval $[0, x]$ under the action of the dyadic transformation is

$$S^{-1}([0, x]) = [0, \tfrac{1}{2}x] \cup [\tfrac{1}{2}, \tfrac{1}{2} + \tfrac{1}{2}x],$$

so the Frobenius-Perron operator corresponding to S is given by

$$P_S f(x) = \tfrac{1}{2}[f(\tfrac{1}{2}x) + f(\tfrac{1}{2} + \tfrac{1}{2}x)].$$

It is obvious that $P_S 1 = 1$. By an inductive argument, $P_S^t f$ can be written in the form

$$P_S^t f(x) = \frac{1}{2^t} \sum_{i=0}^{2^t - 1} f \left(\frac{i + x}{2^t} \right).$$

In the limit as $t \to \infty$, the right hand side of this expression becomes the Riemann integral of the density f over $[0, 1]$, *i.e.*

$$\lim_{t \to \infty} P_S^t f(x) = \int_0^1 f(x)\, dx = 1.$$

Therefore the dyadic transformation is uniformly exact, and precisely the same argument generalized in an obvious way extends to the r-adic transformation when $r > 2$ is an integer. •

We can use this same technique to show that the tent map (3.5) is uniformly exact. Further, the uniform exactness of the tent map implies the f_* exactness of the quadratic transformation (3.7) when $r = 4$, with f_* given by equation (3.9), through the following result for one dimensional maps. It also offers a constructive method to develop dynamics with any desired statistical property.

Theorem 7.3. *Let $T : [0,1] \to [0,1]$ be a nonsingular transformation, f_* be a positive density on (a, b), and $S : [a, b] \to [a, b]$ be a second transformation defined by $S = h^{-1} \circ T \circ h$ where*

$$h(x) = \int_a^x f_*(y)\, dy \qquad a < x < b.$$

Then T is uniformly exact if and only if S is f_* exact.

Proof. The hardest part of the proof is the calculation of the relation between the Frobenius Perron operators corresponding to S and T. We start by writing the definition of P_S and using the definition of S with a sequence of variable changes:

$$
\begin{aligned}
\int_a^y P_S f(x)\,dx &= \int_{S^{-1}([a,y])} f(x)\,dx \\
&= \int_{g^{-1}(T^{-1}([g(a),g(y)]))} f(x)\,dx \\
&= \int_{T^{-1}([g(a),g(y)])} f(g^{-1}(z)) \frac{dz}{f_*(g^{-1}(z))} \\
&= \int_{g(a)}^{g(y)} P_T\left(\frac{f(g^{-1}(z))}{f_*(g^{-1}(z))}\right)\,dz \\
&= \int_a^y \left\{ P_T\left(\frac{f(x)}{f_*(x)}\right) \right\} f_*(x)\,dx.
\end{aligned}
$$

Thus, P_S and P_T are related through

$$
P_S f = f_* P_T\left(\frac{f}{f_*}\right),
$$

and a straightforward application of Theorem 7.2 completes the proof. $\square$

At this point it is appropriate to note some convergence properties of exact systems. Suppose we have an exact system and wish to construct an approximation to f_* from the time series $\{S_t(x_0)\}_{t>0}$. Pick a small subset A of the phase space X with positive Lebesgue measure, say $\mu_L(A) = \Delta$, and take $g(x) = 1_A(x)$ in equation (4.20) to give

$$
\int_X 1_A(x) f_*(x)\,dx = \int_A f_*(x)\,dx = \lim_{t\to\infty} \frac{1}{t} \sum_{k=0}^{t-1} 1_A(S_k(x)).
$$

By the Mean Value Theorem for integrals, this can be written, for $x \in A$, as

$$
f_*(x) \simeq \frac{1}{\Delta} \lim_{t\to\infty} \frac{1}{t} \sum_{k=0}^{t-1} 1_A(S_k(x)),
$$

showing that the convergence of the series to the desired value of f_* goes as t^{-1}. This illustrates the necessity of using long time series to numerically approximate densities.

The situation is quite different when we are given an initial density f and examine the convergence properties of the sequence $\{P^t f\}$ to f_* when P is f_* exact. Jabloński *et al.* (1985) [see also Jabloński and Malczak, 1983; 1985] have shown that for large classes of exact transformations the convergence of $\{P^t f\}$ to f_* is exponential, *i.e.*, goes as $e^{-\alpha t}$ with $\alpha > 0$. This convergence of iterates to f_* is significantly faster than is the convergence of the time series approximation to f_*, as can be easily shown using the hat map (3.5) or the quadratic transformation (3.7) as examples.

We close this section with three theorems related to exactness. The first is a sufficient condition for the exactness of asymptotically periodic Markov operators.

Theorem 7.4. *Let P be an asymptotically periodic Markov operator in a phase space X. If $r = 1$ in the spectral decomposition (5.1) of $P^t f$, then P is exact.*

Proof. Since, by hypothesis, $r = 1$ in (6.2) we may write

$$
P^t f(x) = \lambda(f) g(x) + Q_t f(x)
$$

and thus

$$
\lim_{t\to\infty} P^t f(x) = \lambda(f) g(x).
$$

Both f and g are densities, so integration over the entire phase space X gives $\lambda(f) \equiv 1$ and thus $\{P^t f\}$ is strongly convergent to g, and exactness follows by Theorem 7.1. $\square$

This theorem shows, for example, that the generalized hat map (6.9) is in fact f_* exact for $2^{1/2} < a \leq 2$. Our second result is

Theorem 7.5. *Let P be an asymptotically periodic Markov operator. Assume that there is a subset A of the phase space X with positive measure such that for every density f there is an integer $t_1(f)$ such that $P^t f(x) > 0$ for all $t \geq t_1(f)$ and almost all points x in A. Then $\{P^t f\}$ is exact.*

Proof. Since P is asymptotically periodic, we know that the expansion (6.1) of Theorem 6.1 is valid. If we can show that $r = 1$ in this expansion, then Theorem 7.4 will complete the proof.

Assume the contrary, that $r > 1$, and choose an integer i_0 such that the subset A is not contained in the support of $g_{i_0}(x)$. Pick a density given by $f(x) = g_{i_0}(x)$ and let τ be the period of the permutation α. Then it follows that $P^{t\tau} f(x) = g_{i_0}(x)$, so that $P^{t\tau} f$ is not positive on A since A is not contained in the support of g_{i_0}. This is in contradiction to the assumption of the theorem, and thus we must have $r = 1$. Hence $\{P^t f\}$ is exact by Theorem 7.4. $\square$

The final result requires the introduction of the notion of a lower bound function for a sequence of densities $\{P^t f\}$. We say that an L^1 function h is a **lower bound function** for a Markov operator P if, for every density f,

$$\lim_{t \to \infty} ||(P^t f - h)^-|| = 0.$$

This condition could be written in the alternate form

$$P^t f \geq h - \epsilon_t$$

where $||\epsilon_t|| \to 0$ as $t \to \infty$, illustrating that a lower bound function is such that successive iterates of a density f by a Markov operator P^t are eventually above it. Further, h is a **nontrivial lower bound function** if $h \geq 0$ and $||h|| > 0$.

With these concepts, we can now state the following result that will be of use in our examination of the behaviour of entropy in later chapters.

Theorem 7.6. *P^t is an exact Markov operator if and only if P^t has a nontrivial lower bound function.*

The original proof of this theorem by Lasota and Yorke (1982) was quite long. The proof that is given here (Lasota and Mackey, 1991) is considerably shorter.

Proof. First observe that if P^t is exact then the existence of a lower bound function is easy since we may take $h = f_*$.

Conversely, assume P has a nontrivial lower bound function. Pick a density f and choose a number $t_0(f)$ such that

$$||(P^t f - h)^-|| \leq \frac{1}{4}||h|| \qquad \text{for} \quad t \geq t_0(f).$$

From $|a - b| = a - b + 2(a - b)^-$ we have

$$||(P^t f - h)^+|| \leq ||P^t f - h|| \leq ||P^t f|| - ||h|| + 2||(P^t f - h)^-||,$$

and since $||P^t f|| \equiv 1$ this becomes

$$||(P^t f - h)^+|| \leq 1 - \frac{1}{2}||h|| \qquad \text{for} \quad t \geq t_0(f).$$

Thus by Theorem 6.2 we know that the operator P is asymptotically periodic and we may use the decomposition formula (6.1).

We now show that $r = 1$ by necessity. Assume the contrary and take $r \geq 2$. Consider two basis functions g_1 and g_2 in the decomposition (6.1). From $Pg_i = g_{\alpha(i)}$ we have $P^{tm} g_i = g_i$ for $m = r!$. However from the definition of the lower bound function it also follows that

$$P^{tm} g_i \geq h - \epsilon_{tm}^i, \qquad i = 1, 2,$$

so $g_i \geq h - \epsilon_{tm}^i$ for $i = 1, 2$. This then implies that $g_1 g_2 > 0$ which contradicts the orthogonality of the g_i required by Theorem 6.1. We are led to a contradiction and therefore must have $r = 1$. Thus Theorem 7.4 implies the exactness of $\{P^t f\}$ with $f_* = g_1$ and the proof is compete. $\square$

B. THE STRONG FORM OF THE SECOND LAW.

The main result of this chapter is a necessary and sufficient condition for the Second Law of thermodynamics to operate in its strong form. We consider a Markov operator P that has a stationary density f_* which is not necessarily constant, thus corresponding to the density of the canonical ensemble, and give a necessary and sufficient condition for the conditional entropy to go to its absolute maximal value of zero. Namely we have:

Theorem 7.7. *Let P^t be a Markov operator operating in a phase space X. Then the conditional entropy of $P^t f$ with respect to a density f_* goes to its maximal value of zero as $t \to \infty$,*

$$\lim_{t \to \infty} H_c(P^t f | f_*) = 0,$$

if and only if P^t is f_* exact.

Proof. We give the proof in the case that $f_* > 0$ and for densities f that are bounded. The result holds in the general case.

We first prove that $\lim_{t \to \infty} H_c(P^t f | f_*) = 0$ implies that P^t is f_* exact. Since f is assumed to be bounded, there must exist a lower bound constant such that

$$H_c(P^t f | f_*) \geq -c.$$

By Theorem 6.6, this implies that P^t is asymptotically periodic, so the spectral decomposition (6.1) is valid and P^t has a stationary density $f_*(x) = \frac{1}{r} \sum_{i=1}^r g_i(x)$. We will show that $r = 1$ and therefore, by Theorem 7.4, P^t is f_* exact.

As usual, let the sets $A_i \subset X$ be the supports of the densities $g_i(x)$. Remember that $\mu_*(A_i) > 0$, and select an initial density

$$f(x) = \frac{1_{A_i}(x)}{\mu_*(A_i)} g_i(x).$$

If T is the period of the asymptotically periodic sequence $\{P^t f\}$, then

$$P^{tT} f(x) = \frac{1_{A_i}(x)}{\mu_*(A_i)} g_i(x).$$

By our hypothesis, $\lim_{t \to \infty} H_c(P^t f | f_*) = 0$ for *all* initial densities f, so

$$H_c \left(\frac{1_{A_i}(x)}{\mu_*(A_i)} g_i(x) \,\middle|\, f_* \right) = 0.$$

By the elementary properties of the conditional entropy discussed in Chapter 3, this implies that

$$f_*(x) = \frac{1_{A_i}(x)}{\mu_*(A_i)} g_i(x),$$

so $r = 1$ and P^t is f_* exact by Theorem 7.4.

To prove the converse, that when P^t is f_* exact we have $\lim_{t \to \infty} H_c(P^t f | f_*) = 0$, first realize that since f is assumed to be bounded and $f_* > 0$ by assumption, there must be a constant $\gamma > 1$ such that for some x

$$\frac{P^t f}{f_*} < \gamma.$$

Define a subset $B_t \subset X$ by

$$B_t = \left\{ x \in X : 1 < \frac{P^t f(x)}{f_*(x)} \leq \gamma \right\}.$$

Then,

$$
\left| \int_{B_t} \eta\left(\frac{P^t f(x)}{f_*(x)}\right) \mu_*(dx) \right| = \int_{B_t} \left| \eta\left(\frac{P^t f(x)}{f_*(x)}\right) - \eta(1) \right| \mu_*(dx)
$$

$$
= \int_{B_t} \left| \int_1^{\frac{P^t f(x)}{f_*(x)}} \frac{d\eta}{du}\, du \right| \mu_*(dx)
$$

$$
\leq \sup_{1 \leq u \leq \frac{P^t f}{f_*}} \eta'(u) \int_{B_t} \left| \frac{P^t f(x)}{f_*(x)} - 1 \right| \mu_*(dx)
$$

$$
\leq \sup_{1 \leq u \leq \frac{P^t f}{f_*}} \eta'(u) \int_X |P^t f(x) - f_*(x)|\, dx
$$

$$
= \sup_{1 \leq u \leq \frac{P^t f}{f_*}} \eta'(u) \, \|P^t f - f_*\|.
$$

Since P^t is f_* exact by assumption, Theorem 7.1 tells us that

$$
\lim_{t \to \infty} \left| \int_{B_t} \eta\left(\frac{P^t f(x)}{f_*(x)}\right) \mu_*(dx) \right| = 0.
$$

This, in conjunction with

$$
0 \geq H_c(P^t f | f_*) \equiv \int_X \eta\left(\frac{P^t f(x)}{f_*(x)}\right) \mu_*(dx) \geq \int_{B_t} \eta\left(\frac{P^t f(x)}{f_*(x)}\right) \mu_*(dx),
$$

completes the proof that the f_* exactness of P^t implies the global convergence of the conditional entropy. $\square$

Example 7.6. An illustration of this theorem is given by the quadratic map (3.7) with $r = 4$, which is f_* exact by Theorem 7.3 and the uniform exactness of the tent map (3.5). Both have a smooth increase of the conditional entropy to zero at long times irrespective of the initial system density. •

Theorem 7.7 sets forth *necessary and sufficient criteria for the operation of the strong form of the Second Law of thermodynamics*, namely for the entropy of a system to globally converge to its maximal value regardless of the way in which the system was prepared. The only requirement that the system must satisfy is that *the density must evolve under the action of an exact Markov operator*. If this operator is a Frobenius Perron operator then the dynamics must be f_* exact. Since f_* exactness implies f_* ergodicity, the state of thermodynamic equilibrium characterized by the density f_* is unique

There is a corollary to Theorem 7.7 concerning the behaviour of the Boltzmann Gibbs entropy of systems operating in a finite normalized phase space when the stationary density is that of the microcanonical ensemble, $f_* = 1$.

Corollary 7.8. *If P is a Markov operator operating in a finite normalized phase space X, then the Boltzmann-Gibbs entropy of $P^t f$ approaches its maximal value of zero as $t \to \infty$, i.e.,*

$$
\lim_{t \to \infty} H(P^t f) = 0,
$$

if and only if P is uniformly exact.

Thus, the Boltzmann-Gibbs entropy will converge to its maximal value of zero if and only if the density of the microcanonical ensemble is a stationary density and the system evolves under the action of a uniformly exact Markov operator P. As before, *ergodicity of P guarantees that the uniform density of the microcanonical ensemble is the unique state of thermodynamic equilibrium, while the uniform exactness of P guarantees that the entropy will approach its maximum value of zero regardless of the way in which the system is prepared.* Both the r-adic transformation, when r is an integer (Example 7.5), and the tent map (3.5) are uniformly exact by our previous observations, and thus display a smooth evolution of their Boltzmann-Gibbs entropy to zero for all initial system states.

Thus, for finite normalized spaces:

$$P^t \text{ is uniformly exact} \Leftrightarrow \lim_{t \to \infty} H(P^t f) = 0,$$

while in general

$$P^t \text{ is } f_* \text{ exact} \Leftrightarrow \lim_{t \to \infty} H_c(P^t f | f_*) = 0.$$

These results point out a very important property of the entropy *vis a vis* the common notion that maximal entropy should be associated with maximal disorder, or minimal structure. Experimentally, what we *measure* is that the entropy of a system evolving in time goes to a maximum. Further, in the course of any experiment the *dynamics* are the ultimate selector of the proper f_* with respect to which the conditional entropy is "computed" during the system evolution. This state of maximal entropy, in turn, corresponds to a state of thermodynamic equilibrium, and in no way makes a judgment about whether this state is totally structureless (f_* uniform) or highly ordered. Any apparent inconsistency between a state of maximal entropy and a nonuniform f_* comes exclusively from the erroneous identification of $f_* = 1$ as the preferred state of thermodynamic equilibrium. This partially stems from the long historical preoccupation of trying to find a rational foundation for thermodynamics in the statistical mechanics of Hamiltonian systems which preserve the Lebesgue measure and for which the attendant density $f_* = 1$ is a stationary density.

C. SUMMARY.

With the results of this chapter giving necessary and sufficient conditions for the approach of system entropy to a maximum, one might think that our quest for the dynamical foundations of thermodynamics and the functioning of the second law was at an end. This is far from the reality of the situation as a moments reflection reveals.

Here it has been demonstrated that it is only through the operation of *noninvertible* f_* exact systems that the entropy will increase to its maximal value (Theorem 7.7). Further, given the observation that dynamics are the ultimate determinant of the stationary density f_*, that this corresponds to a state of thermodynamic equilibrium, and that since states of thermodynamic equilibrium depend on a variety of parameters (temperature, pressure, *etc.*), we must conclude that the corresponding f_* must also depend on these parameters *as must the underlying dynamics.*

Given these results we are now faced with another problem since all of the laws of physics are framed in terms of invertible dynamical (as opposed to noninvertible semidynamical) systems which are independent of these external parameters.

This dilemma seems to have at least two solutions. Either:

(1) The laws of physics are at present incorrectly formulated. R. Penrose (1979, 1989) has argued quite lucidly and simply for this point of view, basing his thesis on CPT violation in K° meson decay. Fer (1977) makes a similar point, basing his argument on the neglect of time delays in the usual formulations of physical laws. Gal-Or (1974, 1981) and Davies (1974) have examined possible sources of time asymmetry in physics, primarily from a cosmological and electromagnetic perspective; or

(2) There is some effect, neglected to this point in our considerations, which alters the behaviour of a dynamical system to give rise to the experimentally observed behaviour.

The next four chapters are devoted to an exploration of the second of these possibilities, as the first involves a drastic restructuring of the entire formulation of classical and quantum physics.

In the next chapter we examine the concept of coarse graining, and in Chapter 9 we consider traces. These two concepts are closely linked. Coarse graining, in spite of the fascination that it has held for decades as a potential source of irreversible thermodynamic behaviour, is unable to stand as a viable candidate because it induces an increase in entropy to its maximal value of zero regardless of the direction of time (forward or backward)! A more extreme form of coarse graining, known as a trace and implying the existence of hidden variables, is able to induce truly irreversible thermodynamic behaviour.

Figure 7.1. The behaviour of an initial 10^4 points under the action of the exact transformation (7.1). Note in particular how rapidly these points spread throughout the phase space without developing the thread-like structures seen in Figure 6.1 for a mixing transformation.

PART III.
POSSIBLE, BUT IMPROBABLE, SOLUTIONS

CHAPTER 8.
COARSE GRAINING

To this point, in studying entropy behavior it has been assumed that the dynamical variables are known with infinite precision. As a consequence, the density f corresponding to a given thermodynamic state would also be known precisely. While this is the situation when an analytic form for the density is available, in the world of experiment the reality is that the density f (or, more usually, some functional of f) is either measured or estimated with some associated error.

Perhaps the most obvious way in which this situation might arise is that due to errors (arising, for example, from measurement impreciseness) f will not be known exactly but will be known only to some level of accuracy. Alternately, it is entirely possible that Nature herself may have introduced an inherent graininess to phase space, rendering the absolute determination of dynamical variables, and thus densities, impossible. Many have suggested that there is an elementary fundamental volume in position-momentum space whose measure corresponds to Planck's constant. This would be entirely in keeping with other apparently fundamental indivisible units in the real world.

In this chapter we examine the consequences of lack of knowledge of the specific values of dynamical variables by studying the properties of the coarse grained entropy. In Section A we define the coarse grained entropy, and in Section B we prove that for a mixing system the coarse grained entropy always approaches zero for long times but that this behaviour is independent of the direction (positive or negative) with which time is allowed to increase. Finally, in Section C we consider the effect of observing or sampling a continuous time process at a set of discrete times which might be likened to a temporal coarse graining.

A. COARSE GRAINED ENTROPY.

To examine the effect of imprecision in our knowledge of dynamical variables on entropy calculations, we introduce the entropy of a coarse grained density, or more briefly, the **coarse grained entropy**. This concept seems to have been first qualitatively discussed by Gibbs (1902), and quantified by Ehrenfest and Ehrenfest (1959). Denbigh and Denbigh (1985) have considered aspects of the effects of coarse graining on the behaviour of entropy.

Coarse graining is carried out by first partitioning the phase space X (finite and normalized) into discrete cells A_i that satisfy

$$\bigcup_i A_i = X \qquad \text{and} \qquad A_i \bigcap_{i \neq j} A_j = \emptyset. \tag{8.1}$$

Obviously, there is no unique way in which such a partition $\{A_i\}$ may be formed, but we require that the partition is **nontrivial** with respect to the Lebesgue measure μ_L so $0 < \mu_L(A_i) \leq \mu_L(X) = 1$ for all values of i. For every density f, within each cell A_i of this partition we denote the average of f over A_i by $< f >_i$,

$$< f >_i = \frac{1}{\mu_L(A_i)} \int_{A_i} f(x)\, dx, \tag{8.2}$$

so the density f coarse grained with respect to the partition A_i is given by

$$f^{cg}(x) = \sum_i < f >_i 1_{A_i}(x). \tag{8.3}$$

Thus, f^{cg} is constant within each cell A_i and $\sum_i < f >_i \mu_L(A_i) = 1$.

Therefore, given a partition A_i satisfying (8.1) (nontrivial with respect to Lebesgue measure), a density f, and a coarse grained density f^{cg} defined by (8.2)-(8.3), then the Boltzmann-Gibbs entropy of the coarse grained density f^{cg} is given by

$$H(f^{cg}) = -\sum_i < f >_i \mu_L(A_i) \log < f >_i .$$

The demonstration is direct since, from (8.3) and the definition of the entropy, we have

$$
\begin{aligned}
H(f^{cg}) &= -\int_X \left[\sum_i <f>_i 1_{A_i}(x) \right] \log \left[\sum_i <f>_i 1_{A_i}(x) \right] dx \\
&= -\sum_i <f>_i \int_X 1_{A_i}(x) \log \left[\sum_i <f>_i 1_{A_i}(x) \right] dx \\
&= -\sum_i <f>_i \int_{A_i} \log \left[\sum_i <f>_i 1_{A_i}(x) \right] dx \\
&= -\sum_i <f>_i \mu_L(A_i) \log <f>_i .
\end{aligned}
$$

It is noteworthy that for any density f, the Boltzmann-Gibbs entropy of the coarse grained density f^{cg} may be greater than the entropy of f, or more specifically:

Theorem 8.1. *For any density f and any nontrivial partition A_i of the phase space X, $H(f) \leq H(f^{cg})$.*

Proof. This is quite straightforward to prove using the integrated form of the Gibbs inequality (1.5). First, by use of the indicator function $1_A(x)$ we may write

$$
\begin{aligned}
H(f) &\equiv -\int_X f(x) \log f(x) \, dx \\
&= -\sum_i \int_X f(x) 1_{A_i}(x) \log f(x) \, dx \\
&\leq -\sum_i \int_X f(x) 1_{A_i}(x) \log g(x) \, dx,
\end{aligned}
$$

for $g(x)$ an integrable density. Pick $g(x) = <f>_i$ so

$$
\begin{aligned}
H(f) &\leq -\sum_i \log <f>_i \int_X f(x) 1_{A_i}(x) \, dx \\
&= -\sum_i \log <f>_i \int_{A_i} f(x) \, dx \\
&= -\sum_i <f>_i \mu_L(A_i) \log <f>_i \\
&= H(f^{cg}),
\end{aligned}
$$

and the assertion is proved. $\square$

Thus, the effect of any error in the estimation of a density f characterizing a system, no matter what the origin, will be to either increase the entropy of the estimated (coarse grained) density $H(f^{cg})$ above its actual value $H(f)$, or leave it unchanged.

Precisely analogously to the way in which the entropy of the coarse grained density was derived, it is easy to show that the conditional entropy of f^{cg} with respect to a second density g, also coarse grained with respect to the partition A_i, is given by

$$
H_c(f^{cg}|g^{cg}) = -\sum_i <f>_i \mu_L(A_i) \log \left[\frac{<f>_i}{<g>_i} \right].
$$

It is equally easy to show that $H_c(f|g) \leq H_c(f^{cg}|g^{cg})$ for all densities f and g, and nontrivial partitions A_i of the phase space X.

Therefore, in general, *coarse graining of the phase space*, and the consequent coarse graining of a density, *will either increase the entropy or leave it equal to its value before coarse graining.*

Now assume that an initial density f evolves under the action of a Markov operator to give the sequence $\{P^t f\}$. In analogy with (8.3), the coarse grained $P^t f$ is given by

$$(P^t f(x))^{cg} = \sum_i < P^t f >_i 1_{A_i}(x)$$

where

$$< P^t f >_i = \frac{1}{\mu_L(A_i)} \int_{A_i} P^t f(x)\, dx.$$

It is important to realize that we are assuming that the Markov operator operates without any error on the density f, and that the coarse graining arises because of our inability to precisely measure dynamical variables, and consequently densities, for whatever reason. The converse situation in which we may measure densities with infinite precision, but the dynamics always work with some error are considered in Chapters 10 and 11 where we consider system interactions with a heat bath.

Example 8.1. An example is helpful in illustrating the effect of coarse graining, and we return to the baker transformation (5.2), illustrated in Figure 5.4, with f given by equation (5.6).

Consider first of all the situation with the partition $\{A_1, A_2\} = \{Y_1, Y_2\}$. Then we have $< f >_1 = < f >_2 = 1$ and thus $H(f^{cg,Y}) = 0$. Following one application of the baker transformation (Figure 5.4c), $H(f_1^{cg,Y}) \simeq -0.13$ and finally (Figure 5.4d), $H(f_2^{cg,Y}) = 0$. On the other hand, after one application of the inverse of the baker transformation (Figure 5.4a) we have $H(f_{-1}^{cg,Y}) = 0$.

Alternately, if we choose the partition to be $\{A_1, A_2\} = \{X_1, X_2\}$, then $H(f^{cg,X}) \simeq -0.13$ while $H(f_{-1}^{cg,X}) = H(f_1^{cg,X}) = H(f_2^{cg,X}) = 0$. •

These computations illustrate that coarse graining in this invertible mixing system:

(1) Induces the entropy of the coarse grained density to approach the equilibrium entropy for both positive and negative times;
(2) This approach may not be monotone (compare $H(f^{cg,Y})$ with $H(f_1^{cg,Y})$);
(3) The approach is not necessarily symmetric with respect to a reversal of time (compare $H(f_{-1}^{cg,Y})$ with $H(f_1^{cg,Y})$); and
(4) The approach may be dependent on the partition chosen (X *versus* Y).

B. COARSE GRAINING OF MIXING SYSTEMS.

Coarse graining has interested numerous authors since the concept was first introduced by Gibbs (1902, pp. 148-150) with the observation that coarse graining of a mixing system should lead to an increase in the entropy to its maximal value as we have just illustrated. To prove this, assume that P^t is an f_* mixing Markov operator and rewrite the definition (5.1) of an f_* mixing Markov operator in the equivalent integral form:

$$\lim_{t \to \infty} \int_X [P^t f(x)] g(x)\, dx = \int_X f_*(x) g(x)\, dx. \tag{8.4}$$

If we pick $g(x) = 1_{A_i}(x)/\mu_L(A_i)$, then equation (8.4) becomes

$$\lim_{t \to \infty} \frac{1}{\mu_L(A_i)} \int_X [P^t f(x)] 1_{A_i}(x)\, dx = \frac{1}{\mu_L(A_i)} \int_X 1_{A_i}(x) f_*(x)\, dx.$$

The left hand side of this equality is $< P^t f >_i$ while the right hand side is identically equal to $< f_* >_i$. Thus

$$\lim_{t \to \infty} < P^t f >_i = < f_* >_i$$

so

$$\lim_{t \to \infty} \sum_i < P^t f >_i 1_{A_i}(x) = \sum_i < f_* >_i 1_{A_i}(x).$$

Finally, from the definitions of $(P^t f)^{cg}$ and f_*^{cg} it follows that

$$\lim_{t \to \infty} (P^t f)^{cg} = f_*^{cg}.$$

Thus, nontrivial coarse graining of an invertible f_* mixing Markov operator causes it to become f_* exact. Finally, if P^t is also invertible (as for the baker transformation) we have proved the following.

Theorem 8.2. *If P^t is an invertible f_* mixing Markov operator with a unique stationary density f_*, and $\{A_i\}$ is a nontrivial partition of the phase space X, then*

$$\lim_{t \to \pm\infty} (P^t f)^{cg} = f_*^{cg}$$

for all initial densities f, where

$$f_*^{cg}(x) = \sum_i <f_*>_i 1_{A_i}(x).$$

As a consequence of this result and Theorem 7.7, we have

Theorem 8.3. *If P^t is an invertible f_* mixing Markov operator with a unique stationary density f_* and $\{A_i\}$ is a nontrivial partition of the phase space X, then*

$$\lim_{t \to \pm\infty} H_c((P^t f)^{cg} | f_*^{cg}) = 0$$

for all initial densities f.

For uniformly mixing systems operating in a normalized finite space, it is an easy consequence of these results that after coarse graining of the phase space, $\{P^t f\}$ will approach the uniform density of the microcanonical ensemble, and that the Boltzmann-Gibbs entropy will approach its maximum value of zero.

C. SAMPLING.

Consider a continuous time sequence of densities $\{P^t f\}_{t \geq 0}$ and the corresponding sequence $\{P^{t_n} f\}_{n=0}^\infty$ obtained by sampling at times t_n where $t_n \leq t_{n+1}$. For convenience we suppose that there is a basic sampling interval t_0 so $t_n = n t_0$, but this is not necessary for the conclusions that follow. Since $t_n = n t_0$ by assumption we may define $\tilde{P} = P^{t_0}$ so $P^{t_n} \equiv P^{n t_0} = \tilde{P}^n$, and the sampled sequence can be written $\{\tilde{P}^n f\}_{n=0}^\infty$.

With respect to sampling, the basic question we wish to address is whether this procedure can give rise to any entropy behaviour of the sampled sequence $\{\tilde{P}^n f\}_{n=0}^\infty$ that was not present in the original sequence $\{P^t f\}_{t \geq 0}$. As summarized in the following theorem, the answer is a definitive no.

Theorem 8.4. *Let P be a Markov operator with stationary density f_*, define a sequence of densities $\{P^t f\}_{t \geq 0}$, and let $\tilde{P} = P^{t_0}$ be the corresponding Markov operator obtained by sampling at times t_0 to generate the sequence $\{\tilde{P}^n f\}_{n=0}^\infty$. Then $\{\tilde{P}^n f\}_{n=0}^\infty$ is f_* exact (mixing) if and only if $\{P^t f\}_{t \geq 0}$ has the same property.*

Proof. The if part of this theorem, that exactness (mixing) of $\{P^t f\}_{t \geq 0}$ implies the same property for $\{\tilde{P}^n f\}_{n=0}^\infty$, is easily proved. We prove the converse only for the case of exactness as the proof for the mixing situation is similar.

Since, by assumption, $\{\tilde{P}^n f\}_{n=0}^\infty$ is f_* exact, we know that $\tilde{P}^n f_* = f_*$ for all n and

$$\lim_{n \to \infty} ||\tilde{P}^n f - f_*|| = 0 \qquad \text{for all} \quad f \in D.$$

We first show that $\tilde{P}^t f_* = f_*$ for all t follows by picking an arbitrary time t' and setting $f' = P^{t'} f_*$ (which is a density), and further noting that $f_* = \tilde{P}^n f_* \equiv P^{n t_0} f_*$. Thus,

$$||P^{t'} f_* - f_*|| = ||P^{t'}(P^{n t_0} f_*) - f_*||$$
$$= ||P^{n t_0} f' - f_*||$$
$$= ||\tilde{P}^n f' - f_*||$$

By assumption the right hand side converges to zero as $n \to \infty$ for all densities f', and since the left hand side is independent of n we must have $||P^{t'} f_* - f_*|| = 0$ for all t' and thus $P^{t'} f_* = f_*$.

Next we must show that $\lim_{t \to \infty} ||P^t f - f_*|| = 0$ for all densities f. By Property 4 of Markov operators, $||P^t f - f_*|| = ||P^t(f - f_*)|| \leq ||f - f_*||$ and since we have convergence to zero on a subsequence of nonincreasing functions, $\lim_{t \to \infty} ||P^t f - f_*|| = 0$. $\square$

The situation is not so straightforward if we are considering ergodicity in sampled systems, as the following example shows.

Example 8.2. Consider the transformation $S_t : [0, 1) \to [0, 1)$ defined by

$$S_t(x) = x + \omega t \qquad (\text{mod } 1),$$

which is a special case of the system considered in Example 4.3. From our comments there and in footnote 5 (Chapter 4), we know that S_t is ergodic if and only if ω is irrational.

Now suppose we sample S at an interval t_0 such that ωt_0 is rational. Then it is clear that the sampled system, for this particular value of t_0, is not ergodic. $\bullet$

This example illustrates that even though a sequence $\{P^t f\}_{t \geq 0}$ is ergodic, it may happen that the sampled sequence $\{\tilde{P}^n f\}_{n=0}^{\infty}$ will not be ergodic. The converse, however, is not true and is given by the following theorem.

Theorem 8.5. *Under the assumptions of Theorem 8.4, if $\{\tilde{P}^n f\}_{n=0}^{\infty}$ is ergodic, then $\{P^t f\}_{t \geq 0}$ is also.*

The proof proceeds much as for Theorem 8.4.

Thus we see from Theorems 8.4 and 8.5 that sampling a continuous sequence of densities $\{P^t f\}_{t \geq 0}$ at an interval t_0 cannot induce any new thermodynamic behaviour in the sampled sequence $\{\tilde{P}^n f\}_{n=0}^{\infty}$. The same conclusion holds if we consider an irregularly sampled sequence $\{\tilde{P}^{t_n} f\}_{n=0}^{\infty}$.

D. SUMMARY.

Here, we have introduced the concept of coarse graining and the coarse grained entropy. We have shown that the introduction of coarse graining of the phase space is sufficient to cause the entropy of an (invertible) mixing transformation to increase to its maximal value of zero irrespective of the direction of time.

Given the fact that the result of Theorem 8.3 was clearly known by Gibbs, though not proved with rigor, it is surprising that the effects of nontrivial coarse graining have had, and continue to have, so much attention as possible sources of irreversible thermodynamic behaviour.

Even setting aside the lack of invertibility of the behaviour of the coarse grained entropy, it is important to realize that the rate of convergence of the entropy of the coarse grained densities that Theorem 8.3 guarantees will, in general, depend on the way in which the coarse graining of the phase space is carried out. Experimentally, if entropy increases to a maximum only because we have invertible mixing dynamics but there is coarse graining due to measurement imprecision, then the rate of convergence of the entropy (and all other thermodynamic variables) to equilibrium should become slower as measurement techniques improve. Such phenomena have not been observed. Thus, it seems likely that nontrivial coarse graining plays no role in determining thermodynamic behaviour, even if the coarse graining is externally imposed by Nature in the form of an inherent graininess or unitary cellularity of phase space. The same conclusion relative to temporal coarse graining, or sampling, also holds.

CHAPTER 9.
TRACES AND FACTORS

As an alternative to the coarse graining of the previous chapter, we now explore the consequences of having an invertible dynamics in which not all dynamical variables are observable. Essentially this means that we have a dynamical system operating in an m-dimensional space, but are able to observe only $n < m$ of these variables. That is, we observe only a *trace* of its operation in an n-dimensional space because $(m-n)$ of the variables are hidden to us, *e.g.* because either we do not know about them, or do not have the technology to measure them.

A. TRACES.

To make these ideas more specific, we return to a brief consideration of dynamical systems which were first formally introduced in Chapter 1. If we have a dynamical system S_t operating in some phase space X, then only three possible types of limiting trajectories may be observed. Either:

(1) The trajectory is a single fixed point x_* such that $x_* = S_t(x_*)$ for all times t; or
(2) The trajectory of S_t is a nonintersecting curve, which we express as $S_{t'}(x) \neq S_{t''}(x)$ for all times t' and t'' that are not equal; or
(3) S_t has a periodic trajectory so $S_t(x) = S_{t+\omega}(x)$ for all times t and all points x in some subset A of the phase space X. In this case we say that the trajectory has period ω.

The only possible type of intersecting trajectory that a dynamical system may have is a periodic one. To demonstrate this, assume that for some point x in the phase space X we have $S_{t'}(x) = S_{t''}(x)$ for a time $t'' > t'$. Apply $S_{t-t'}$ to this relation, and use the definition of a dynamical system to obtain

$$S_{t-t'} \circ S_{t'}(x) = S_t(x) = S_{t-t'} \circ S_{t''}(x) = S_{t+(t''-t')}(x).$$

With $\omega = t'' - t' > 0$, we have arrived at $S_t(x) = S_{t+\omega}(x)$ for all times t.

However, we often observe (apparently) nonperiodic intersecting trajectories, and it is not terribly difficult to understand how they might arise. As an example, a periodic or aperiodic trajectory of a three dimensional oscillator might display an intersecting trajectory in a two dimensional projection of its phase space.

As alluded to earlier, this projection is called a trace, a concept that is made more precise by the following. Let X and Y be two (topological Hausdorff) phase spaces, $F : Y \to X$ a given continuous function, and $S_t : Y \to Y$ a dynamical system operating in the phase space Y. A function $h : R \to X$ is a **trace** of the dynamical system if there is a point y in the space Y such that $h(t) = F(S_t(y))$ for all times t.

One is naturally led to wonder under what circumstances a nonperiodic intersecting trajectory can be viewed as the trace of a higher dimensional dynamical system. It is actually easy to give a surprising answer to a much more general question. *Every continuous trajectory (function) in a space X is the trace of a* **single** *dynamical system operating in a higher dimensional phase space Y!* More precisely, we have the following result which I like to call the God Theorem because of an amusing conversation with my colleague A. Lasota in Katowice, Poland, in April, 1984. We had both enjoyed the fruits of an especially good Bulgarian vineyard.

Theorem 9.1 (God Theorem). *Let the phase space X be arbitrary. Then there is a second phase space Y, a dynamical system S_t operating in Y, and a continuous function $F : Y \to X$ such that every continuous trajectory $h : R \to X$ is the trace of S_t. That is, for every trajectory h there is a point y in the phase space Y such that $h(t) = F(S_t(y))$ for all times t.*

Proof. The proof can best be understood by using the following diagram.

$$
\begin{array}{ccc}
y(\tilde{t}) \in Y & \xrightarrow{S_t \circ y(\tilde{t})} & Y \ni y(t+\tilde{t}) \\
{\scriptstyle F \circ y(\tilde{t})} \downarrow & & \downarrow {\scriptstyle F \circ y(t+\bar{t})} \\
y(0) \in X & \xrightarrow[S_t \circ y(0)]{} & X \ni y(t)
\end{array}
$$

We let Y be the space of all continuous functions $y : R \to X$, and define a transformation S_t operating on Y by the simple shift

$$S_t \circ y(\tilde{t}) \equiv y(t + \tilde{t}).$$

(It is clear from the definitions of Chapter 1 that S_t is a dynamical system.) Furthermore, we define a projection $F : Y \to X$ by

$$F \circ y(\tilde{t}) \equiv y(0).$$

Now let $h : R \to X$ be an arbitrary and continuous trajectory. From our definitions it follows that $S_t \circ h(\tilde{t}) = h(t + \tilde{t})$ and $F \circ S_t \circ h(\tilde{t}) = h(t)$. Thus the trajectory $h(t)$ is the trace of the dynamical system S_t operating in the space Y that had $h(\tilde{t})$ as its initial function. $\square$

There are important consequences for the behaviour of the entropy when one is considering the trace of a dynamical system.

If we have a dynamical system S_t operating on Y, then the entropy is always identically equal to the entropy of the initial density since it is impossible for the entropy of an invertible system to change (Theorem 3.2.). This need not be the case for the entropy of a density evolving under the action of a trace of a dynamical system.

Example 9.1. To illustrate this point, again consider the baker transformation (5.2) which is a K-automorphism. We have shown directly that the entropy of the baker transformation is absolutely constant and equal to the value determined by the choice of the initial density. However, note that if we consider only the x portion of the baker transformation, it is identical to the dyadic transformation $T(x) = 2x \pmod 1$, introduced in Example 7.5, which is uniformly exact and whose entropy smoothly increases to zero.[10] •

This example illustrates that taking a trace of a dynamical system with time independent entropy may be sufficient to generate a system in which the entropy is increasing. Of course, in general we do not know what the limit of this increase may be, and the entropy may approach a limit considerably less than its maximal value if, for example, the trace is asymptotically periodic.

B. FACTORS.

This leads us to discuss specific types of traces for which much more can be said about the behaviour of the entropy. To see how this works, we introduce the notion of a factor of a transformation with the aid of the following diagram.

$$
\begin{array}{ccc}
Y & \xrightarrow{\;S_t\;} & Y \\
{\scriptstyle F}\big\downarrow & & \big\downarrow{\scriptstyle F} \\
X & \xrightarrow[\;T_t\;]{} & X
\end{array}
$$

Let X and Y be two different phase spaces with normalized measures μ_{f_*} and μ_{g_*} and associated densities f_* and g_* respectively, and $T_t : X \to X$ and $S_t : Y \to Y$ be two measure preserving transformations. If there is a transformation $F : Y \to X$ that is also measure preserving, i.e., if $\mu_{g_*}(F^{-1}(A)) = \mu_{f_*}(A)$ for all subsets A of the phase space Y, and such that $T_t \circ F = F \circ S_t$ (so the diagram commutes), then T_t is called a **factor** of S_t.

From this definition *a trace of the system S_t is a trajectory of the factor T_t*. In Example 9.1 the dyadic transformation is a factor of the baker transformation (5.2).

Example 9.2. As a second example of the effect of taking the factor of an invertible system, consider the quadratic baker transformation

$$S(x,y) = \begin{cases} (4x(1-x), \frac{1}{2}y) & 0 \le x \le \frac{1}{2} \\ (4x(1-x), \frac{1}{2} + \frac{1}{2}y) & \frac{1}{2} < x \le 1. \end{cases} \tag{9.1}$$

This system, like the original baker transformation, is invertible and in fact

$$S^{-1}(x,y) = \begin{cases} (\frac{1}{2} - \frac{1}{2}\sqrt{1-x}, 2y) & 0 \le y \le \frac{1}{2} \\ (\frac{1}{2} + \frac{1}{2}\sqrt{1-x}, 2y-1) & \frac{1}{2} < y \le 1. \end{cases}$$

Using this in conjunction with the observation that $J^{-1}(x,y) = 1/4\sqrt{1-x}$ and equation (4.5) gives an explicit form for the Frobenius Perron operator corresponding to (9.1):

$$Pf(x) = \frac{1}{4\sqrt{(1-x)}} \{f(\tfrac{1}{2} - \tfrac{1}{2}\sqrt{1-x}, 2y) + f(\tfrac{1}{2} + \tfrac{1}{2}\sqrt{1-x}, 2y-1)\}. \tag{9.2}$$

---

[10]Goldstein and Penrose (1981) have called this trace entropy a coarse grained entropy.

The density

$$f_*(x,y) = \frac{1_{[0,1]}(y)}{\pi\sqrt{x(1-x)}}$$

is the unique stationary density of (9.2), and in fact (9.1) is f_* mixing. As for the standard baker transformation (5.2) the conditional entropy satisfies $H_c(P^t f|f_*) \equiv H_c(f|f_*)$ for all initial densities f with which the system is prepared.

As in Example 9.1, if we assume we have access to only the x variable of (9.1) then we have a factor system given by $T(x) = 4x(1-x)$ which we know is f_* exact, with f_* given by (3.9), and consequently $\lim_{t\to\infty} H_c(P^t f|f_*) = 0$ for all initial system preparations. •

The formal connection between these concepts and the behaviour of the entropy is furnished by the following theorem due to Rochlin (1964). The proof may be found in Cornfeld *et al.* (1982).

Theorem 9.2. *(Rochlin, 1964). Every f_* exact transformation is the factor of a K-automorphism.*

The transformation F involved in our discussion of factors and traces is precisely what Misra *et al.* (1979) and Misra and Prigogine (1981) refer to as a projection operator in their work on the generation of noninvertible behaviour from invertible dynamics. The Rochlin Theorem 9.2 serves as the analytic link in their work between invertible K-automorphisms and f_* exact transformations (or strong or monotonic Markov operators).

As noted in Chapter 5, since K-automorphisms are invertible their entropy is forever fixed at its initial value by Theorem 3.2. On the other hand, by Theorem 7.7 and Corollary 7.8, we know that the entropy of an f_* exact transformation, which by the above theorem is the factor of a K- automorphism, increases smoothly to its maximum value of zero irrespective of the initial density with which the system was prepared.

C. COARSE GRAINING AND TRACES.

One way to view the connection between the effects of coarse graining the phase space and taking the trace of a dynamical system is as follows. In coarse graining, we lose *some* information about the exact values of the dynamical variables. One could easily imagine the situation in which we have m variables, of which n were measured with infinite precision, and $(m-n)$ of them were measured with some error. Thus the act of taking a trace is just a more extreme case of coarse graining in which we are not able to measure *any* of the $(m-n)$ variables.

Given a phase space in which the evolution of densities is governed by the generalized Liouville equation (3.2), it is partially this operation of taking a trace that leads to the Boltzmann equation and its successful predictions of the behaviour of dilute gases. The Boltzmann equation describes the behaviour of a density evolving under the action of a factor of the original dynamics. Thus there is an analogy between the dynamics of the Liouville equation and of the Frobenius-Perron operator for the baker transformation, while the dynamics of the Boltzmann equation are analogous to those of the Frobenius-Perron operator corresponding to the dyadic transformation:

$$
\begin{array}{ccc}
\text{Liouville equation} & \xrightarrow{\text{INVERTIBLE}} & \text{baker transformation} \\[2mm]
\text{Trace} \downarrow & & \downarrow \text{Trace} \\[2mm]
\text{Boltzmann equation} & \xrightarrow[\text{NONINVERTIBLE}]{} & \text{dyadic transformation}
\end{array}
$$

D. SUMMARY.

This and the previous chapter have presented two possible ways out of the clear problems associated with the necessity of noninvertible exact system dynamics for entropy to increase, and the fact that all of the laws of physics are formulated as invertible dynamical systems that are not exact.

Here we have introduced the concept of a trace, and shown that when a trace is a factor of a dynamical system, the entropy may increase. Even stronger results are available in some circumstances when the trace is taken from a K-automorphism, for then the trace may be f_* exact with an entropy that increases to its maximal value of zero.

CHAPTER 10.
OPEN DISCRETE TIME SYSTEMS.

To this point we have examined two situations in which the entropy of a reversible system may appear to increase. In the first (coarse graining, Chapter 8), we have a transformation operating precisely but are unable to measure the dynamical variables with perfect accuracy. The second situation (taking a trace, Chapter 9) assumed that we did not have access to all of the dynamical variables, but only to a subset of them. In both situations, the system is closed in that there are no external influences acting on the system.

This chapter examines the consequences of having a discrete time deterministic transformation experience a perturbation from an outside source. Thus we are starting to examine what could be considered as the mathematical analogue of the interaction between a system and a "heat bath", or an open system. These considerations are also important since in any numerical investigation of the dynamics of discrete time or continuous time systems, one is always dealing with finite difference schemes in which "noise" from roundoff error is present. Stochastically perturbed continuous time systems with dynamics described by ordinary differential equations are considered in the next chapter.

Assume that, in general, a system evolves according to a given transformation $S(x_t)$. The qualifying phrase 'in general' means that the transition $x_t \to x_{t+1} = S(x_t)$ occurs with probability $(1 - \epsilon)$. In addition, with probability ϵ, the value of x_{t+1} is uncertain. If $x_t = y$ is given, then, in this case, x_{t+1} may be considered as a random variable distributed with a density $K(x, y)$ which depends on y. In Section A we derive a density evolution equation for this process.

One interpretation of this process is that ϵ corresponds to the degree of coupling between the system under study and the heat bath. If this is the case, then the parameter ϵ can be thought of as a number related to the ratio of the fundamental frequency of operation of the basic deterministic system, F_D, to the frequency of the outside perturbation coming from the heat bath, F_P. Thus when $F_D \ll F_P$, $\epsilon \simeq 1$ and the system operates almost like a random walk, while with $F_D \gg F_P$, we have $\epsilon \simeq 0$ and the system evolves almost completely deterministically. We will refer to the situation when $0 < \epsilon < 1$ as 'loose coupling' (Section B). For $\epsilon = 1$, in which the influence of the external system is always experienced, we will speak of strong (or continuous) coupling (Section C). However, as will become clear in Section D, precisely the same formulation may be interpreted in a totally different fashion as arising from taking a trace. Sections E and F respectively consider the effects of additive and parametric perturbations in inducing weak and strong form Second Law behaviour. The chapter closes with Section G in which we consider the approximation of a Markov operator by a sequence of Frobenius Perron operators.

A. AN OPERATOR EQUATION.

The first step in the study of this process is the derivation of an equation for the operator P which gives the prescription for passing from the density f_t of x_t to the density f_{t+1} of x_{t+1}. Assume that the dynamics operate in a phase space X (with positive measure, of course) which is some measurable subset of R^d, and that the dynamics S are nonsingular.

If the density f_t of x_t is given, we wish to know the probability that some point x_{t+1} is in a subset A of the phase space. Clearly, x_{t+1} may be reached in only one of two ways: deterministically with probability $(1 - \epsilon)$ and stochastically with probability ϵ. In the deterministic case, $x_{t+1} = S(x_t)$ and

$$\text{Prob}_D(x_{t+1} \in A) = \text{Prob}_D(S(x_t) \in A). \tag{10.1}$$

(The index D denotes the deterministic situation.) From the definition of the Frobenius-Perron operator, the density of $S(x_t)$ is $P_S f_t$ and, as a result,

$$\text{Prob}_D(S(x_t) \in A) = \int_A P_S f_t(x) \, dx \tag{10.2}$$

If the stochastic perturbation occurs, and if $y = x_t$, then

$$\text{Prob}_P(x_{t+1} \in A | x_t = y) = \int_A K(x, y) \, dx.$$

(P denotes the perturbation). Since x_t is a random variable with density f_t, it is also the case that

$$\text{Prob}_P(x_{t+1} \in A) = \int_X \text{Prob}_P(x_{t+1} \in A | x_t = y) f_t(y) \, dy.$$

Combining this relation with the previous one gives

$$\text{Prob}_P(x_{t+1} \in A) = \int_A \left\{ \int_X K(x,y) f_t(y) \, dy \right\} dx \tag{10.3}$$

From equations (10.1) through (10.3), it follows that

$$\text{Prob}(x_{t+1} \in A) = (1-\epsilon)\text{Prob}_D(x_{t+1} \in A) + \epsilon\text{Prob}_P(x_{t+1} \in A)$$
$$= \int_A \left\{ (1-\epsilon) P_S f_t(x) + \epsilon \int_X K(x,y) f_t(y) \, dy \right\} dx.$$

Since A is an arbitrary subset of the phase space, the density f_{t+1} exists whenever f_t exists and is, in fact, given by

$$f_{t+1}(x) = (1-\epsilon) P_S f_t(x) + \epsilon \int_X K(x,y) f_t(y) \, dy.$$

Thus the full expression for the operator P describing the evolution of densities in this mixed system operating with both deterministic and perturbed elements is

$$Pf(x) = (1-\epsilon) P_S f(x) + \epsilon \int_X K(x,y) f(y) \, dy. \tag{10.4}$$

It is straightforward to show that the operator defined by (10.4) is a Markov operator.

Since $K(x,y)$ for fixed y is a density, it clearly satisfies

$$K(x,y) \geq 0 \qquad \text{and} \qquad \int_X K(x,y) \, dx = 1. \tag{10.5}$$

Conditions (10.5) in conjunction with the requirement that K is measurable means that K is a **stochastic kernel**. Further, we will always assume that for every $\eta > 0$ there is a $\delta(\eta) > 0$ such that

$$\int_E K(x,y) \, dx \leq \eta, \tag{10.6}$$

for every y in X and subset E of X with $\mu_L(E) \leq \delta$, *i.e.* K is uniformly integrable in x.

B. LOOSELY COUPLED SYSTEMS.

We are now in a position to state our first results concerning the behaviour of the entropy of a discrete time deterministic system coupled to a heat bath. In investigating the properties of the evolution of densities by the operator equation (10.4), and the consequent behaviour of the entropy of these densities, some mild restrictions on both the transformation S and the kernel K are required. First, assume that the deterministic transformation S satisfies

$$|S(x)| \leq a_0|x| + a_1 \tag{10.7}$$

throughout the phase space, where $a_0 < 1$ and a_1 are nonnegative constants. Secondly, it will be assumed that with $b_0 < 1$ and b_1 nonnegative constants,

$$\int_X |x| K(x,y) \, dx \leq b_0|y| + b_1. \tag{10.8}$$

This condition is automatically satisfied if the phase space X is bounded (finite), but if it is unbounded then (10.8) prevents divergence of the trajectories to infinity.

The first result guarantees the existence of at least one state of thermodynamic equilibrium and the evolution of the conditional entropy to a maximum, though not necessarily to zero, in the presence of noise. Thus the following result is equivalent to the weak form of the Second Law of thermodynamics.

Theorem 10.1. *If S is a nonsingular transformation that satisfies (10.7) and K is a uniformly integrable stochastic kernel satisfying (10.8), then for $0 < \epsilon \leq 1$ the operator P given by (10.4) is asymptotically periodic.*

Proof. Using (10.4) and (10.6) in conjunction with the Chebyshev inequality[11], it is moderately straightforward to find a constant $c > 0$ such that

$$\limsup_{t \to \infty} \int_{X \setminus A} P^t f(x) \, dx \leq \frac{\epsilon(1 - \eta)}{2},$$

where $A = \{x \in X : |x| \leq c\}$. Setting $k = 1 - \epsilon(1 - \eta)/2$ gives

$$\int_{E \cup (X \setminus A)} P^{t+1} f(x) \, dx \leq \frac{\epsilon(1 - \eta)}{2} + \int_E P^t f(x) \, dx$$

$$\leq \frac{\epsilon(1 - \eta)}{2} + (1 - \epsilon) \int_E P_S P^t f(x) \, dx + \epsilon \int_X P^t f(y) \, dy \int_E K(x, y) \, dx$$

$$\leq \frac{\epsilon(1 - \eta)}{2} + (1 - \epsilon) + \epsilon \eta = k < 1$$

for every density f and set E with $\mu_L(E) \leq \delta(\eta)$, and sufficiently large $t \geq t_0(f, E)$. Thus, by the definition in Chapter 6, P^t is smoothing. Application of the Spectral Decomposition Theorem 6.1 finishes the proof. $\square$

Therefore, for any closed system whose dynamics evolve through the action of a nonsingular transformation S satisfying (10.7), placing it in contact with a second system whose effect on the first is a perturbation characterized by a kernel K satisfying (10.8) leads automatically to a situation in which the resulting open system is asymptotically periodic *regardless of the nature of the original closed system S.* Further, since this procedure induces asymptotic periodicity we know that at least one state of thermodynamic equilibrium, characterized by a stationary density f_*, exists and the conditional entropy $H_c(P^t f | f_*)$ is an increasing function with a limiting value given by $H_{max}(f | f_*)$ as defined in (6.19) of Theorem 6.5.

Under certain circumstances involving loose coupling to a heat bath, there are even stronger results concerning the behaviour of the entropy, corresponding to the strong form of the Second Law of thermodynamics. One such case is as follows.

Assume that the value of the perturbation to the system S coming from the heat bath (when it occurs) at time $(t + 1)$ is independent of the value of x_t. Then the stochastic kernel $K(x, y)$ is independent of y and simply becomes $K(x, y) = g(x)$, where g is the density of the perturbations ξ_t. In this case, with the external perturbations independent of the state of the system S, the perturbations ξ_t could be interpreted as completely stochastic or as coming from another deterministic system. They could even be viewed as the trace of some deterministic system whose Frobenius-Perron operator has g as its unique stationary density. This is a slightly different situation from that explored in Chapter 9. There we considered the effect on the behaviour of the entropy of only examining the trace of a system. Now we are considering the situation which could be interpreted as the *perturbation of a system by the trace of another system.*

In this case, the operator equation (10.4) takes the form

$$Pf(x) = (1 - \epsilon) P_S f(x) + \epsilon g(x). \tag{10.10}$$

There are some surprising consequences of making the loose coupling independent of the state of the system S. Namely

---

[11]If $V : X \to R$ is an arbitrary nonnegative measurable function, and f is a density, set $E(V|f) = \int_X V(x) f(x) \, dx$. Define a set $A = \{x \in X : |x| \leq c\}$ with $c > 0$ so

$$E(V|f) \geq \int_{X \setminus A} V(x) f(x) \, dx \geq c \int_{X \setminus A} f(x) \, dx \geq c \left\{ 1 - \int_A f(x) \, dx \right\}$$

and the **Chebyshev inequality**

$$\int_A f(x) \, dx \geq 1 - \frac{1}{c} E(V|f) \tag{10.9a}$$

results. This can be written in the alternate form

$$\int_{X \setminus A} f(x) \, dx \leq \frac{1}{c} E(V|f). \tag{10.9b}$$

Theorem 10.2. *If P is the operator defined by (10.10), then $\{P^t f\}$ is f_* exact.*

Proof. Using the lower bound function Theorem 7.6, the proof is short. By the definition of P in equation (10.10) we have

$$P^t f = P(P^{t-1} f) \geq \epsilon g \int_X f(x)\, dx = \epsilon g$$

for all densities f. Thus ϵg is a nontrivial lower bound function for all $\epsilon > 0$, and $\{P^t f\}$ is f_* exact. $\square$

Thus, by loosely coupling a system to a heat bath such that the system experiences perturbations that are independent of the state of the system, there will be a unique state of thermodynamic equilibrium and the conditional entropy of the coupled system will globally converge to zero regardless of the nature of the original system S. In fact, it is even possible to write down the unique stationary density f_* of the operator P in equation (10.10), characterizing the thermodynamic equilibrium, as

$$f_* = \sum_{k=0}^{\infty} (1 - \epsilon)^k P^k g. \tag{10.11}$$

To show that this is the unique stationary density, note that since $\| (1 - \epsilon)^k P^k g \| \leq (1 - \epsilon)^k \| g \|$ by the contractive property of Markov operators, the series in f_* is absolutely convergent. Therefore, substitution of the expression for f_* into equation (10.10) gives $Pf_* = f_*$.

C. STRONGLY COUPLED SYSTEMS.

A much different interpretation of this perturbation at random times of a deterministically operating system is possible and related to strong coupling ($\epsilon = 1$) between a deterministic system and an external source of noise.

When $\epsilon = 1$ and $X = R^d$, then equation (10.4) takes the form

$$Pf(x) = \int_{R^d} K(x, y) f(y)\, dy. \tag{10.12}$$

In thinking about the interpretation of (10.12), consider the following. Take the quantities $\xi_0, \xi_1, \ldots$ to be d-dimensional random vectors and let the phase space X be R^d. Then for a given $\{\xi_t\}$ and a dynamics W of two variables, $W : R^d \times R^d \to R$, we may assume that the system goes from $x_t = y$ to $x_{t+1} = W(y, \xi_t)$. Let $K(x, y)$ be the density of $W(y, \xi_t)$. Then the density will always exist if $W(y, z)$ as a function of z is nonsingular. If this is the case, then equation (10.12) describes the evolution of the densities corresponding to

$$x_{t+1} = W(x_t, \xi_t). \tag{10.13}$$

We can make this more formal through the following theorem initially formulated and proved by A. Lasota, J. Traple, and J. Tyrcha.

Theorem 10.3. *Let $g : R^d \to R^d$ be a density and $K : R^d \times R^d \to R^d$ be a stochastic kernel. Then the (generally nonunique) function $W : R^d \times R^d \to R^d$ defined implicitly by*

$$\int_0^{W(y,z)} K(r, y)\, dr = \int_0^z g(u)\, du \tag{10.14}$$

defines a dynamical system

$$x_{t+1} = W(x_t, \xi_t)$$

where the ξ_t are independent random variables with density g. This system has an evolution of densities described by $f_{t+1} = P f_t$ where the operator P is given by

$$Pf(x) = \int_{R^d} K(x, y) f(y)\, dy.$$

Proof. Let $W^{-1}(y, z)$ be the inverse function of $z \to W(y, z)$ at fixed y. [This inverse always exists since with $y > 0$ we know that $\int_0^z g(u)\, du$ is strictly increasing and thus $W(y, z)$ is also strictly increasing.] Therefore, (10.14) can be written as

$$\int_0^x K(r, y)\, dr = \int_0^{W^{-1}(y,x)} g(u)\, du,$$

or

$$K(x,y) = g(W^{-1}(y,x)) \frac{\partial W^{-1}(y,x)}{\partial x}.$$

Next note that

$$
\begin{aligned}
\int_0^x f_{t+1}(z)\,dz &= \mathrm{Prob}\{x_{t+1} < x\} \\
&= \mathrm{Prob}\{W(x_t,\xi_t) < x\} \\
&= \iint_{W(y,u)<x} f_t(y)g(u)\,dy\,du \\
&= \int_{R^d} f_t(y)\,dy \int_0^{W^{-1}(y,x)} g(u)\,du \\
&= \int_{R^d} f_t(y)\,dy \int_0^x K(r,y)\,dr \\
&= \int_0^x dr \int_{R^d} f_t(y)K(r,y)\,dy.
\end{aligned}
$$

Differentiating both sides of this equality gives

$$f_{t+1}(x) = \int_{R^d} K(x,y)f_t(y)\,dy$$

and the proof is complete. $\square$

The perturbations, appearing through the $\{\xi_t\}$, could be entering the system (10.13) in a variety of ways. This could be additively like $x_{t+1} = S(x_t) + \xi_t$ which is the subject of the next section, or through fluctuations in coefficients in a multiplicative fashion like $x_{t+1} = \xi_t S(x_t)$, which we treat in Section F below. In actuality, one need not consider the perturbations ξ to be "noise", for they could also be coming from another system. Traple (1988) has shown, for example, that if in the system

$$x_{t+1} = \zeta_t S(x_t) + \xi_t$$

either ζ_t and/or ξ_t are the trace of an ergodic (mixing) system, then the sequence $\{x_t\}$ is ergodic (mixing).

Before explicitly considering the effects of additive or multiplicative perturbations, we close this section with three theorems concerning the eventual behaviour of $\{P^t f\}$ when P is the integral operator (10.12). For the first two of these we consider the operator

$$P^\tau f(x) = \int_X K_\tau(x,y)f(y)\,dy$$

obtained by τ applications of (10.12), and call K_τ the τth iterate of the stochastic kernel K.

The first result is

Theorem 10.4. *If there exists an integer τ and a density g such that*

$$K_\tau(x,y) \le g(x),$$

where $K_\tau(x,y)$ is the τth iterate of a stochastic kernel, then $\{P^t f\}$ is asymptotically periodic.

Proof. Since $K_\tau(x,y) \le g(x)$ we have

$$P^t f(x) = \int_X K_\tau(x,y)P^{t-\tau}f(y)\,dy \le g(x) \qquad \text{for} \quad t \ge \tau.$$

Use Theorem 6.2 with $h = g$ and $\gamma = 0$ so the sequence $\{P^t f\}$ is asymptotically periodic. $\square$

A slight restriction on $K_\tau(x,y)$ in Theorem 10.4 leads to our second result.

Theorem 10.5. *If there exists an integer τ and a density g such that*

$$K_\tau(x, y) \leq g(x),$$

where $K_\tau(x, y)$ is the τth iterate of a stochastic kernel, and there is a set $S \subset X$ with $\mu_L(S) > 0$ such that

$$0 < K_\tau(x, y) \qquad for \quad x \in S, \quad y \in X,$$

then the sequence $\{P^t f\}$ is f_* exact.

Proof. The proof is a direct consequence of the asymptotic periodicity of P from Theorem 10.4, the assumptions, and Theorem 7.5. $\square$

Before stating our last result, we introduce the notion of a Liapunov function. If $G \subset R^d$ is an unbounded measurable set and $K : G \times G \to R$ is a measurable stochastic kernel, then any continuous nonnegative function $V : G \to R$ is a **Liapunov function** if

$$\lim_{|x| \to \infty} V(x) = \infty.$$

Then we have the following theorem, proved in Lasota and Mackey (1991):

Theorem 10.6. *Let $K : G \times G \to R$ be a stochastic kernel and P be the corresponding Markov operator defined by (10.12). Assume that there is a nonnegative $\lambda < 1$ such that for every bounded $B \subset G$ there is a $\delta = \delta(B) > 0$ for which*

$$\int_E K(x, y) \, dx \leq \lambda \qquad for \quad \mu_L(E) < \delta, \quad y \in B, \quad E \subset B.$$

Assume further there exists a Liapunov function $V : G \to R$ such that for $f \in D$

$$\int_G V(x) P f(x) \, dx \leq \alpha \int_0^\infty V(x) f(x) \, dx + \beta \qquad 0 \leq \alpha < 1, \quad \beta \geq 0$$

holds. Then $\{P^t f\}$ is asymptotically periodic.

Note that it is sufficient to check the simpler condition

$$\int_G K(x, y) V(x) \, dx \leq \alpha V(y) + \beta.$$

since

$$\int_G V(x) P f(x) \, dx = \int_G \int_X V(x) K(x, y) f(y) \, dx \, dy$$
$$\leq \int_X [\alpha V(y) + \beta] f(y) \, dy = \alpha \int_X V(y) f(y) \, dy + \beta.$$

D. ASYMPTOTIC PERIODICITY AND ADDITIVE PERTURBATIONS.

In a commonly considered situation, the perturbations are additive, $W(y, z) = S(y) + z$, so (10.13) becomes

$$x_{t+1} = S(x_t) + \xi_t. \tag{10.15}$$

It is rather surprising that a dynamics of the form described by equation (10.15) may also appear as the consequence of taking a factor or trace (Lasota and Mackey, 1989).

Example 10.1. To illustrate this we once again return to the baker transformation introduced in equation (5.2). As pointed out in Example 9.1, the x portion of the baker transformation has a trajectory determined by $x_{t+1} = T(x_t)$ where $T(x) = 2x \pmod 1$. As a consequence, the baker transformation (5.2) can be rewritten in the equivalent form

$$
\begin{aligned}
x_{t+1} &= T(x_t) \\
y_{t+1} &= \frac{1}{2}y_t + \xi_t,
\end{aligned}
\tag{10.16}
$$

where $\xi_t = \frac{1}{2}1_{[\frac{1}{2},1]}(x_t)$. From classical results of Borel, the ξ_t defined in this way are independent random variables. As a consequence, if we take only the y factor of the baker transformation we end up with a dynamics described by an equation that is a special case of (10.15). Thus, taking a trace of a dynamical system in two different ways may yield results with quite different interpretations. •

If the sequence $\{\xi_t\}$ of random variables in (10.15) has a common density g, then from (10.14) it follows that $K(x,y) = g(x - S(y))$, and equation (10.12) becomes

$$
Pf(x) = \int_{R^d} f(y)g(x - S(y)) \, dy.
\tag{10.17}
$$

For the special case of additive noise, a comparison of equations (10.17) and (10.12) shows that (10.17) can be derived independent of any assumption concerning the nonsingularity of S. Furthermore, in this case the condition given by equation (10.8) reduces to

$$
m = \int_{R^d} |x|g(x) \, dx < \infty.
\tag{10.18}
$$

Thus we have an immediate corollary to Theorem 10.1 for systems with noise added as in (10.15).

Corollary 10.7. *(Lasota and Mackey, 1987). If S (nonsingular or not) is a transformation operating in the phase space R^d, satisfies inequality (10.7), and experiences an additive perturbation (as in equation 10.15) with a finite first moment, then the sequence $\{P^t f\}$, where P is the Markov operator defined by equation (10.17), is asymptotically periodic.*

A second result for asymptotic periodicity requiring the verification of a Liapunov function condition is contained in the next theorem.

Theorem 10.8. *Let the Markov operator P be defined by (10.17) and let g be a density. If there exists a Liapunov function $V : R^d \to R$ such that, with $\alpha < 1$ and β nonnegative,*

$$
\int_{R^d} g(x - S(y))V(x) \, dx \leq \alpha V(y) + \beta \qquad \text{for all} \quad y \in R^d
$$

then the sequence $\{P^t f\}$ is asymptotically periodic.

Proof. We will use Theorem 10.6 in the proof, noting that the stochastic kernel is explicitly given by $K(x,y) = g(x - S(y))$.

Since g is integrable, for every $\lambda > 0$ there is a $\delta > 0$ such that

$$
\int_A g(x) \, dx < \lambda \qquad \text{for} \quad \mu_L(A) < \delta.
$$

In particular

$$
\int_E K(x,y) \, dx = \int_E g(x - S(y)) \, dx = \int_{E - S(y)} g(x) \, dx < \lambda
$$

for $\mu_L(E - S(y)) = \mu_L(E) < \delta$. Thus the first condition of Theorem 10.6 holds.

Further, from (10.17) and the assumptions of the theorem we have

$$
\begin{aligned}
\int_{R^d} V(x)Pf(x) \, dx &= \int_{R^d} V(x) \, dx \int_{R^d} f(y)g(x - S(y)) \, dy \\
&\leq \alpha \int_{R^d} V(y)f(y) \, dy + \beta,
\end{aligned}
$$

so the second condition also holds. Thus $\{P^t f\}$ is asymptotically periodic. $\square$

As a consequence, for all situations in which perturbations are *added* to a transformation S, the effect is to induce asymptotically periodic behaviour regardless of the nature of the original unperturbed dynamics S (remember that S may even be singular). Because of this, we also know that *perturbations induce at least one state of thermodynamic equilibrium*, whose stationary density is given by equation (6.4), *and guarantee the approach of the conditional entropy to a maximum* (Theorem 6.5).

It would be of interest to know how the period of $\{P^t f\}$ depends on the perturbations to the system. Though this cannot be answered in full generality, for the case of additive perturbations as in (10.15) some insight is possible. For example, if the sequence $\{x_t\}$ is generated by (10.15) and the space is finite so we may consider the system on the unit circle T^1, then

$$P^t f(x) = \int_{T^1} g(x - S(y)) P^{t-1} f(y) \, dy$$
$$\leq \gamma \int_{T^1} P^{t-1} f(y) \, dy = \gamma,$$

where $\gamma = \sup g$. In particular, if $f = g_i$ where g_i is one of the basis densities in the spectral decomposition (5.1), then $P^t f = g_{\omega^t(i)}$ so $g_i \leq \gamma$. Furthermore, since the g_i have disjoint supports it follows that

$$r = \int_{T^1} \sum_{i=0}^{r} g_i(x) \, dx \leq \gamma,$$

and the asymptotic period of the densities is less than or equal to γ!. If the amplitude of the perturbation is small, then $\sup g$ is large and *vice versa* so large amplitude perturbations correspond to shorter periods of the asymptotically periodic sequence of densities. In particular, if $\gamma < 2$ then since r must be an integer we have $r = 1$ and the sequence $\{P^t f\}$ will be f_* exact.

For some transformations, the induction of asymptotic periodicity by the addition of perturbations would not be at all surprising, *e.g.* the addition of a stochastic perturbation to a transformation with an exponentially stable periodic orbit gives asymptotic periodicity.

Example 10.2. This phenomenon is easy to illustrate by considering

$$x_{t+1} = S(x_t) \pmod{1}, \tag{10.19}$$

where $S(x) = \alpha x + \lambda$, $0 < \alpha < 1$ and $0 < \lambda < 1$. This map is an example of a class of transformations considered by Keener (1980). The Keener map (10.19) can be shown to have orbits of period r in the trajectories $\{x_t\}$ whenever

$$\lambda = \lambda_{per}(r) = \left(\sum_{i=0}^{r} \alpha^i \right)^{-1} = \frac{1 - \alpha}{1 - \alpha^{r+1}}. \tag{10.20}$$

Further, Provatas and Mackey (1991b) have proved that the noise perturbed Keener map

$$x_{t+1} = (S(x_t) + \xi_t) \pmod{1}$$
$$= (\alpha x_t + \lambda + \xi_t) \pmod{1}, \tag{10.21}$$

where the ξ_t are random numbers uniformly distributed on $[0, \theta]$, has a sequence of densities $\{P^t f\}$ that is asymptotically periodic with period r whenever $\lambda = \lambda_{per}(r)$ and the noise amplitude θ satisfies

$$0 < \theta \leq \theta_{crit}(r) = \alpha^r (1 - \alpha) \lambda_{per}(r). \tag{10.22}$$

This behaviour is illustrated for $(\alpha, r, \theta_{crit}(r)) = (\frac{1}{2}, 2, \theta_{crit}(2))$ and $(\frac{1}{2}, 3, \theta_{crit}(3))$ in Figure 10.1. As in the case of the inherent asymptotic periodicity of the hat map illustrated in Chapter 6, the initial density may have a profound

effect on the eventual limiting behaviour of $H_c(P^t f | f_*)$ given by equation (6.19) , as shown in Figure 10.2 for $r = 2$ and Figure 10.3 when $r = 3$. There, as for the hat and quadratic map Examples 6.3 and 6.4, an initial density

$$f(x) = \frac{1}{\xi} 1_{[0,\xi]}(x) \tag{10.23}$$

was chosen and $H_{max}(f | f_*)$ is plotted as a function of ξ.

The monotone increasing nature of $H_{max}(f | f_*)$ with ξ indicates that as the initial preparation of the system includes ever larger portions of the available phase space there is a progressive increase in the eventual maximal entropy. This contrasts with the behaviour of the limiting entropy of the hat and quadratic maps as a function of ξ shown in Figures 6.4 and 6.5.

While this is partially true, $e.g.$ when $\mathrm{supp}\{f\} \subset \mathrm{supp}\{g_i\}, i = 1, \cdots, r$, it need not be true in general. For example, take $r = 2$ and assume that given a value of α we pick $\lambda = \lambda_{per}(2)$ and a noise level $\theta \leq \theta_{crit}(2)$. If $\mathrm{supp}\{f\} \subset [0, \lambda_{per}(2) + \theta + \alpha - 1]$ or $\mathrm{supp}\{f\} \subset [\lambda_{per}(2), 1]$, then $P^t f$ will cycle between the g_1 and g_2 of the spectral decomposition (6.1) as shown in Figure 10.4a. Alternately, if

$$\mathrm{supp}\{f\} \subset \left[\frac{1 - \lambda_{per}(2) - \theta}{\alpha}, \lambda_{per}(2) \right],$$

then regardless of how localized the support of f, $P^t f$ will always contain two components, one supported on $\mathrm{supp}\{g_1\}$ and the other on $\mathrm{supp}\{g_2\}$, and the sequence $\{P^t f\}$ will always contain both the g_1 and g_2 states ($cf.$ Figure 10.4b). As a consequence, with this support for f the sequence $\{P^t f\}$ will have a larger limiting entropy than the situation in which the $\mathrm{supp}\{f\}$ leads to cycling between two quantized states. This is the origin of the sharp break in the function $H_{max}(f | f_*)$ versus ξ in Figure 10.3, which occurs precisely when ξ exceeds the level $\lambda_{per}(2) + \theta + \alpha - 1$ which is the right hand endpoint of $\mathrm{supp}\{g_1\}$. Similar reasoning explains the sequences of densities shown in Figure 10.5 for $\alpha = \frac{1}{2}$ and $r = 3$. •

As an example of perturbation induced asymptotic periodicity, this example is not especially surprising. The surprising content of Theorem 10.1 (and Corollary 10.7) is that even in a transformation that has aperiodic limiting behavior, additive perturbations will result in asymptotic periodicity.

Example 10.3. This is again easy to illustrate using the Keener map as has been done by Lasota and Mackey (1987). From the results for general Keener transformations, there exists an uncountable set Λ such that for each $\lambda \in \Lambda$ the rotation number corresponding to the transformation (10.19) is irrational. For each such λ the sequence $\{x_t\}$ is not periodic and the invariant limiting set

$$\bigcap_{k=0}^{\infty} S^k([0,1]) \tag{10.24}$$

is a Cantor set. The proof of Keener's general result offers a constructive technique for numerically determining values of λ that approximate elements of the set Λ.

The transformation (10.19) satisfies the conditions of Corollary 10.7 and is, therefore, an ideal candidate to illustrate the induction of asymptotic periodicity by noise in a transformation whose limiting behavior is quite erratic in the absence of noise. Lasota and Mackey (1987) picked $\alpha = \frac{1}{2}$ and used the results of Keener to show that $\lambda = \frac{17}{30}$ is close to a value in the set Λ for which the invariant limiting set (10.24) should be a Cantor set. They illustrated asymptotic periodicity by studying the perturbed Keener map (10.21) with noise uniformly distributed on $[0, \frac{1}{15}]$ and these values of α and λ, and found asymptotic periodicity with period 3. •

E. EXACTNESS AND ADDITIVE PERTURBATIONS.

The fact that additive perturbations in a system strongly coupled to its environment can induce asymptotic periodicity is important for the understanding of how coupling a system to a heat bath may cause the entropy to become an increasing function of time. Under certain circumstances there are even stronger results concerning the effects of additive perturbations. Namely, additive perturbations may induce exactness with a consequent increase in the conditional entropy to its maximal value of zero corresponding to the strong form of the Second Law of thermodynamics.

Theorem 10.8 also implies that P has a stationary density f_* since this is a consequence of the Spectral Decomposition Theorem 6.1. This does not, of course, guarantee the uniqueness of f_*, but a simple assumption concerning the positivity of g will not only ensure uniqueness of f_* but also the exactness of $\{P^t f\}$. More specifically we have the following result.

Theorem 10.9. *If P given by (10.17) satisfies the conditions of Theorem 10.8, and $g(x) > 0$ then $\{P^t f\}$ is exact.*

Proof. Note first that for every fixed x the product $g(x - S(y))P^{t-1}f(y)$, considered as a function of y, does not vanish everywhere. As a consequence

$$P^t f(x) = \int_{R^d} g(x - S(y))P^{t-1}f(y)\, dy > 0 \qquad \text{for all} \quad x \in R^d, t \geq 1, f \in D$$

The f_* exactness of $\{P^t f\}$ is proved by applying Theorem 7.5. $\square$

Example 10.4. We can use this theorem to show that the stochastically perturbed Keener map (10.21) is exact whenever $\lambda = \lambda_{per}(r)$ and $\theta_{crit}(r) < \theta \leq 1$. This was proved using different techniques in Provatas and Mackey (1991b). Noise induced exactness is illustrated in Figure 10.6 for $r = 2$ and Figure 10.7 when $r = 3$. •

F. PARAMETRIC PERTURBATIONS.

As a second example of the situation described by (10.13), consider the case when $W(y, z) = zS(y)$ and $S > 0$, so

$$x_{t+1} = \xi_t S(x_t). \tag{10.25}$$

Once again, using the form for $K(x, y)$ derived from (10.14), it is straightforward to show that the operator (10.12) takes the explicit form

$$Pf(x) = \int_{R^d} f(y)g\left(\frac{x}{S(y)}\right)\frac{dy}{S(y)}. \tag{10.26}$$

Horbacz (1989a,b) has considered the behaviour of the system (10.25) when $S : R^+ \to R^+$. The flavor of her results are summarized in the following two theorems.

Theorem 10.10. *Let the Markov operator P be defined by (10.26). Assume that g is a density,*

$$0 < S(x) \leq \alpha x + \beta, \tag{10.27}$$

and

$$\alpha m < 1 \qquad with \qquad m = \int_0^\infty xg(x)\, dx, \tag{10.28}$$

where α and β are nonnegative constants. Then the sequence $\{P^t f\}$ is asymptotically periodic.

Proof. Once again we employ Theorem 10.6 in the proof.

We first show that with the Liapunov function $V(x) = x$ the second condition of Theorem 10.6 is satisfied. We have

$$\int_0^\infty xPf(x)\, dx = \int_0^\infty x\, dx \int_0^\infty g\left(\frac{x}{S(y)}\right)\frac{1}{S(y)}f(y)\, dy$$
$$= \int_0^\infty f(y)\, dy \int_0^\infty g\left(\frac{x}{S(y)}\right)\frac{x}{S(y)}\, dx.$$

Using the change of variables $z = x/S(y)$ and then (10.27) we obtain

$$\int_0^\infty xPf(x)\, dx = \int_0^\infty f(y)S(y)\, dy \int_0^\infty zg(z)\, dz$$
$$= m\int_0^\infty f(y)S(y)\, dy \leq \alpha m \int_0^\infty yf(y)\, dy + \beta m.$$

Thus the second condition of Theorem 10.6 is satisfied.

We next show that the kernel K given by (10.26) satisfies the first criteria of Theorem 10.6. Fix an arbitrary positive $\lambda < 1$ and choose a bounded set $B \subset R^+$. Since g is uniformly integrable there must be a $\delta_1 > 0$ such that

$$\int_F g(x)\, dx \leq \lambda \qquad \text{for} \quad \mu_L(F) < \delta_1.$$

Define

$$\delta = \frac{\delta_1}{\sup_{y \in B} S(y)}.$$

Then for $\mu_L(E) < \delta$ we have $\mu_L(S(y)E) < \delta_1$ and

$$\int_E K(x,y)\,dx = \int_E g\left(\frac{x}{S(y)}\right)\frac{1}{S(y)}\,dx$$
$$= \int_{S(y)E} g(x)\,dx \leq \lambda \qquad \text{for} \quad y \in B \quad \text{and} \quad \mu_L(E) < \delta,$$

and all of the conditions of Theorem 10.6 are satisfied. Thus $\{P^t f\}$ is asymptotically periodic. $\square$

We close with a second theorem concerning f_* exactness induced by multiplicative perturbations.

Theorem 10.11. *If the Markov operator P defined by (10.26) satisfies the conditions of Theorem 10.10 and, in addition, $g(x) > 0$ then $\{P^t f\}$ is f_* exact.*

Proof. Note that, for fixed x, the quantity

$$g\left(\frac{x}{S(y)}\right)\frac{1}{S(y)}P^{t-1}f(y),$$

as a function of y, does not vanish everywhere. Consequently,

$$P^t f(x) = \int_0^\infty g\left(\frac{x}{S(y)}\right)\frac{1}{S(y)}P^{t-1}f(y)\,dy > 0 \qquad \text{for all} \quad x \in R^+, t \geq 1, f \in D,$$

and Theorem 7.5 finishes the proof of the f_* exactness of $\{P^t f\}$. $\square$

Theorems 10.10 and 10.11 illustrate the behaviors that may be induced by multiplicative perturbations in discrete time systems. A number of other results concerning asymptotic periodicity and exactness induced by multiplicative perturbations may be proved, but the reader is referred to Horbacz (1989a,b).

G. MARKOV OPERATORS AND DETERMINISTIC PROCESSES.

On several occasions we have emphasized that the interpretation of a given dynamics is not necessarily clear cut, *e.g.* in Examples 9.1 and 10.1 where the baker transformation was considered. Furthermore, we have also seen how one can *construct* any transformation with the property of f_* exactness by the use of Theorem 7.3.

In fact, given any Markov operator P it is always possible to construct a sequence of deterministic transformations $\{S_n\}$ such that the limiting value of $\{P_{S_n}^t f\}$ approximates $\{P^t f\}$ as closely as one likes. Results along this line have been published by Brown (1966) and Kim (1968, 1972a,b), but we state and prove our main result of this section in the spirit of an unpublished result of Lasota.

Theorem 10.12. *Let P be a given Markov operator operating in a finite normalized space $X = [0,1)$. Then there is a sequence of transformations $S_n : X \to X$ with corresponding Frobenius-Perron operators P_{S_n} such that*

$$\lim_{n \to \infty} ||P_{S_n} f - Pf|| = 0. \tag{10.29}$$

Proof. The proof divides naturally into two parts. We first construct the transformations S_n, and then prove that P_{S_n} satisfies (10.29).

For any integer $n \geq 1$ we make a partition of $[0,1)$ and define

$$A_{n,i} = \left[\frac{i-1}{2^n}, \frac{i}{2^n}\right) \qquad i = 1, \cdots, 2^n.$$

We further set

$$q_{n,i,j} = \int_{A_{n,j}} P 1_{A_{n,i}}(x)\,dx$$

and

$$r_{n,i,j} = \frac{i-1}{2^n} + \sum_{k=1}^{j} q_{n,i,k}$$

for $1 \leq i, j \leq 2^n$, with the convention that $r_{n,i,0} = (i-1)/2^n$.

Since P is a Markov operator, it is contractive so we always have

$$[r_{n,i,j-1}, r_{n,i,j}) \subset A_{n,i}.$$

Furthermore, if $q_{n,i,j} = 0$ then

$$[r_{n,i,j-1}, r_{n,i,j}) = \emptyset.$$

As a consequence, the function

$$\rho_n(x) = \frac{1}{2^n q_{n,i,j}} \qquad \text{for} \quad x \in [r_{n,i,j-1}, r_{n,i,j}) \tag{10.30}$$

is defined on the set

$$\Delta_n = \bigcup_{i,j=1}^{2^n} [r_{n,i,j-1}, r_{n,i,j}) \subset [0, 1.$$

We now define the transformations S_n by

$$S_n = \int_{r_{n,i,0}}^{x} \rho_n(s)\, ds \qquad \text{for} \quad x \in A_{n,i} \cap \Delta_n. \tag{10.31}$$

Having constructed the sequence $\{S_n\}$ of transformations given a Markov operator P, we now show that the corresponding P_{S_n} satisfies (10.29). First define an operator Q_n by

$$Q_n f(x) = 2^n \sum_{i=1}^{2^n} 1_{A_{n,i}}(x) \int_{A_{n,i}} f(y)\, dy. \tag{10.32}$$

It is easy to show that Q_n is a Markov operator with at least n stationary densities f_{*m}, $m = 1, \cdots, n$, of the form

$$f_{*m}(x) = \sum_{i=1}^{2^n} \alpha_i 1_{A_{m,i}}(x), \qquad 1 \leq m \leq n,$$

where the α_i's are nonnegative coefficients. Also, from (10.32) if $x \in A_{n,j}$ then

$$Q_n f(x) = 2^n 1_{A_{n,j}}(x) \int_{A_{n,j}} f(y)\, dy.$$

If we restrict f to be given by $f(x) = P 1_{A_{n,i}}(x)$, then for $x \in A_{n,j}$

$$Q_n f(x) = 2^n q_{n,i,j}.$$

Next, note that by definition the Frobenius-Perron operator P_{S_n} corresponding to S_n is given by

$$P_{S_n} f(x) = \frac{d}{dx} \int_{S_n^{-1}([0,x))} f(y)\, dy,$$

so using (10.31) and, again, taking $f(x) = P 1_{A_{n,i}}(x)$ we have

$$P_{S_n} f(x) = P_{S_n} P 1_{A_{n,i}}(x) = 2^n q_{n,i,j} = Q_n P 1_{A_{n,i}}(x) \qquad \text{for} \quad x \in A_{n,j}.$$

For any density f and $\epsilon > 0$ we can always find a stationary density f_{*m} such that $||f - f_{*m}|| \leq \epsilon$. From the above,

$$||Q_n f - f|| \leq ||Q_n f - Q_n f_{*m}|| + ||Q_n f_{*m} - f_{*m}|| + ||f_{*m} - f||$$
$$\leq (||Q_n|| + 1)\, ||f_{*m} - f|| \leq 2\epsilon$$

for $n \geq m$, so $Q_n f$ is strongly convergent to f. By (10.30) it follows that

$$||P_{S_n} f - Pf|| \leq ||P_{S_n} f - P_{S_n} f_{*m}|| + ||P_{S_n} f_{*m} - Pf_{*m}|| + ||Pf_{*m} - Pf||$$
$$\leq 2||f - f_{*m}|| + ||P_{S_n} f_{*m} - Pf_{*m}||$$
$$\leq 2||f - f_{*m}|| + ||Q_n Pf_{*m} - Pf_{*m}||$$

for any density f and stationary density f_{*m} with $n \geq m$. Since $Q_n Pf_{*m}$ converges to Pf_{*m} and $||f - f_{*m}||$ may be made arbitrarily small, we have shown that $P_{S_n} f$ converges to Pf. $\quad \square$

The consequences of this theorem are extremely far reaching, for it tells us that *any Markov operator*, whether it arises from the influence of random or deterministic perturbations on a totally deterministic system or through the action of a completely unperturbed deterministic system, *can always be approximated by a totally deterministic system to any degree of accuracy.* In fact, the proof of the theorem offers a constructive way of finding this approximating system.

H. SUMMARY.

In this chapter we have explored the effects of outside perturbations acting on a deterministic system with discrete time dynamics, and we have interpreted this as the coupling of the system to a "heat bath".

These outside perturbations can be viewed as perturbations coming from another deterministic system, from the trace of a deterministic system, or as stochastic perturbations. Whatever their source, we have shown in a variety of situations that the effect of these perturbations is to either induce asymptotic periodicity or exactness. It is significant that asymptotic periodicity or exactness may be induced in systems that had absolutely no remarkable behaviour, including statistical behaviour, before they experienced the outside influences. Under certain circumstances it is not even necessary that the original system be nonsingular.

Thus, the effect of perturbing systems in this way has a very powerful influence on the behaviour of their entropy. If the perturbation induces asymptotic periodicity, then the entropy will increase to a local maximum whose value depends in a complicated way on the initial preparation of the system (Theorem 6.5). If, on the other hand, exactness is induced, then the entropy will increase to its absolute maximal value of zero (Theorem 7.7).

In the next chapter we turn our attention to the effects of perturbations on continuous time dynamics.

Figure 10.1. Noise induced asymptotic periodicity in the Keener map. In (a), $\theta = \theta_{crit}(2)$, $\alpha = \frac{1}{2}$ and $\beta = \frac{1}{\alpha+1}$. A transient of 30 densities has been discarded, and $P^{31}f$, $P^{32}f$, $P^{33}f$ are shown. Since $P^{31}f = P^{33}f$, the sequence $\{P^t f\}$ repeats with period 2. The initial density, shown in the inset, was uniform over $[0.4, 0.7]$. For (b), $\theta = \theta_{crit}(3)$, $\alpha = \frac{1}{2}$ and $\beta = \frac{1}{\alpha^2+\alpha+1}$. A transient of 80 densities has been discarded and $P^{81}f$, $P^{382}f$, $P^{83}f$ and $P^{84}f$ are shown. Since $P^{81}f = P^{84}f$, the sequence $\{P^t f\}$ repeats with period 3. The initial density, shown in the inset, is uniform on $[0.3, 0.9]$.

Figure 10.2. The limiting conditional entropy $H_{max}(f|f_*)$ versus the spreading parameter ξ (see equation 10.23) for the noise perturbed Keener system with $\alpha = \frac{1}{2}$, $\beta = \frac{1}{\alpha+1}$ and $\theta = \theta_{crit}(2)$. Note the sudden increase in $H_{max}(f|f_*)$ when ξ increases past the top boundary of g_1.

Figure 10.3. A graph of $H_{max}(f|f_*)$ versus ξ, where ξ is as in Figure 10.2. $\alpha = \frac{1}{2}$, $\beta = \frac{1}{\alpha^2+\alpha+1}$, and $\theta = \theta_{crit}(3)$. Although for period 3 asymptotic periodicity $H_{max}(f|f_*)$ still is uniformly increasing with ξ, note the plateau that develops in the region of $\xi = 0.5$.

Figure 10.4. A numerical simulation of a period 2 cycle of noise induced asymptotic periodicity of $\{P^t f\}$ showing the effect of the initial density f. $\beta = \frac{1}{\alpha+1}$, $\alpha = \frac{1}{2}$ and $\theta = 0.14 < \theta_{crit}(2)$. The initial density f, shown in the inset, is uniform over $[0, 0.2]$ in (a), and over $[0.2, 0.6]$ in (b). In (c), $f(x) = 12.5(x - .2)$ for $x \in [.2, .6]$.

Figure 10.5. Numerical simulation of period 3 noise induced asymptotic periodicity of $\{P^t f\}$. $\beta = \frac{1}{\alpha^2 + \alpha + 1}$, $\alpha = \frac{1}{2}$ and $\theta = 0.068 < \theta_{crit}(3)$. f was uniform over $[0.6, 0.7]$ for (a), over $[0.2, 0.6]$ in (b), and $f(x) = \frac{50}{9}(x - .2)$ over $[0.2, 0.8]$ for (c). Note how a slight change in f changes the number of components in the decomposition of $P^t f$.

Figure 10.6. Numerical illustration of the strong convergence of $P^t f$ to a stationary density f_*. $\alpha = \frac{1}{2}$, $\beta = \frac{1}{\alpha+1}$ and $\theta = 0.24 > \theta_{crit}(2)$.

Figure 10.7. Another numerical illustration of the strong convergence of $P^t f$ to a stationary density f_*. $\alpha = \frac{1}{2}$, $\beta = \frac{1}{\alpha^2+\alpha+1}$ and $\theta = 0.14 > \theta_{crit}(3)$.

CHAPTER 11.
OPEN CONTINUOUS TIME SYSTEMS.

In the previous chapter we have shown how the perturbation of systems with discrete time dynamics may lead the entropy to increase to either a relative or absolute maximum. This behaviour may occur even in systems which have no exceptional behaviour in the absence of these perturbations, and has been likened to placing the system in contact with a heat bath.

Given these results for discrete time dynamics, it is natural to wonder if the perturbation of systems with continuous time dynamics will yield analogous results concerning the entropy. Though we do not treat this problem in its most general possible form, the effect of perturbations on the entropy of systems with dynamics described by sets of ordinary differential equations forms the heart of this chapter.

We start by first defining a Wiener process in Section A, and then consider the perturbation of a flow defined by a system of ordinary differential equations by a white noise term that is the derivative of a Wiener process. This leads naturally to the introduction of stochastic differential equations. We then consider the existence and uniqueness of solutions of stochastic differential equations, and demonstrate how approximating sums (the Euler–Bernstein relations) may be used to construct these solutions.

Following this, in Section B we derive the (parabolic) partial differential equation that describes the evolution of a density under the action of a stochastically perturbed flow. This equation, known as the Fokker–Planck equation, has a solution that is a Markov operator. This solution defines the evolution of densities and may, under certain circumstances, correspond to an evolution toward a unique state of thermodynamic equilibrium (Section C). It is possible to define sufficient conditions for a unique state of thermodynamic equilibrium to exist, characterized by a unique stationary density f_*.

In Section D we give sufficient conditions for stochastically perturbed continuous time systems to be f_* exact. Under these conditions we know, from the considerations of Chapter 7, that the conditional entropy will approach its maximal value of zero.

Sections E and F illustrate, through a series of examples, how additive and parametric perturbations can lead to bifurcations reminiscent of 1st and 2nd order phase transitions.

A. WIENER PROCESSES AND STOCHASTIC DIFFERENTIAL EQUATIONS.

In Chapter 3, Section B, we showed that there is no change in the entropy of densities evolving under the action of flows governed by the system of ordinary differential equations

$$\frac{dx_i}{dt} = F_i(x) \qquad i = 1, \ldots, d \tag{3.1}$$

operating in a region of R^d with initial conditions $x_i(0) = x_{i,0}$. Here we examine the behaviour of the stochastically perturbed analog

$$\frac{dx_i}{dt} = F_i(x) + \sum_{j=1}^{d} \sigma_{ij}(x)\xi_j, \qquad i = 1, \ldots, d \tag{11.1}$$

with the same initial conditions, where $\sigma_{ij}(x)$ is the amplitude of the stochastic perturbation and $\xi_j = \frac{dw_j}{dt}$ is a "white noise" term that is the derivative of a Wiener process. Without going into the details, the reader is cautioned that in this chapter it is always assumed that the Itô calculus, rather that the Stratonovich calculus, is used. For a discussion of the differences see Lasota and Mackey (1994), Horsthemke and Lefever (1984), and van Kampen (1981). In particular, if the σ_{ij} are independent of x then the two approaches yield identical results.

To fully interpret (11.1), we must carefully define what the properties of the ξ are when they are derived from a Wiener process. We say that a continuous process $\{w(t)\}_{t>0}$ is a one dimensional **Wiener process** if:

(1) $w(0) = 0$; and
(2) For all values of s and t, $0 \le s \le t$ the random variable $w(t) - w(s)$ has the Gaussian density

$$g(t - s, x) = \frac{1}{\sqrt{2\pi(t-s)}} \exp\left[-\frac{x^2}{2(t-s)}\right]. \tag{11.2}$$

In a completely natural manner this definition can be extended to say that the d dimensional vector

$$w(t) = \{w_1(t), \cdots, w_d(t)\}_{t>0}$$

is a **d-dimensional Wiener process** if its components are one dimensional Wiener processes. Because of the independence of the increments, it is elementary that the joint density of $w(t)$ is

$$g(t, x_1, \cdots, x_d) = g(t, x_1) \cdots g(t, x_d) \tag{11.3}$$

and thus

$$\int_{R^d} g(t, x)\, dx = 1, \tag{11.4}$$

that

$$\int_{R^d} x_i g(t, x)\, dx = 0, \qquad i = 1, \cdots, d \tag{11.5}$$

and

$$\int_{R^d} x_i x_j g(t, x)\, dx = \delta_{ij} t \qquad i, j = 1, \cdots, d. \tag{11.6}$$

In (11.6),

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

is the Kronecker delta. Therefore the average of a Wiener variable is zero by equation (11.5), while the variance increases linearly with time according to (11.6).

Equation (11.1) is a stochastic differential equation. As in the case of a nonperturbed system of ordinary differential equations, if the functions $F_i(x)$ and $\sigma_{ij}(x)$ satisfy Lipschitz conditions

$$|F_i(x) - F_i(y)| \leq \gamma |x - y|, \qquad x, y \in R^d, \quad i = 1, \ldots, d$$
$$|\sigma_{ij}(x) - \sigma_{ij}(y)| \leq \gamma |x - y|, \qquad x, y \in R^d, \quad i, j = 1, \ldots, d,$$

where $\gamma > 0$, then (11.1) has a unique solution (Gikhman and Skorokhod, 1969).

Approximating solutions to equation (11.1) can be generated in several ways, but for our purposes in the following section the most useful is based on a linear Euler extrapolation formula. Suppose that the solution $x(t)$ to equation (11.1) is given on some interval $[0, t_0]$. Then for small values of Δt, we may approximate x at time $t_0 + \Delta t$ using x at time t_0 with

$$x(t_0 + \Delta t) \simeq x(t_0) + F(x(t_0))\Delta t + \sigma(x(t_0))\Delta w \tag{11.7}$$

where we have written Δw for $w(t_0 + \Delta t) - w(t_0)$. We can use this same approach for any interval $[0, T]$ on which we have constructed a partition

$$0 = t_0 < t_1 < \cdots < t_{n-1} < t_n = T.$$

To do this we define

$$\Delta x(t_i) = F(x(t_{i-1}))\Delta t_i + \sigma(x(t_{i-1}))\Delta w_i, \tag{11.8}$$

where $\Delta x(t_i) = x(t_i) - x(t_{i-1})$, $\Delta t_i = t_i - t_{i-1}$, $\Delta w_i = w(t_i) - w(t_{i-1})$, and $x(t_0) = x_0$, the initial vector. The two formulae (11.7) and (11.8) are known as the **Euler-Bernstein equations** because of the use of the Euler approximation by Bernstein in his original work on stochastic differential equations.

B. THE FOKKER PLANCK EQUATION.

The previous section defined a Wiener process and introduced the stochastic differential equation (11.1) that results when an ordinary differential equation is perturbed by the derivative of a Wiener process. Now we turn to a consideration of the equation that governs the evolution of the density function of the process $x(t)$ generated as the solution to the stochastic differential equation (11.1).

This density, denoted by $f(t, x)$, is defined by

$$\text{prob} \quad (x(t) \in B) = \int_B f(t, s)\, ds. \tag{11.9}$$

To guarantee the existence and differentiability of $f(t, x)$, first note that if we set

$$a_{ij}(x) = \sum_{k=1}^{d} \sigma_{i,k}(x)\sigma_{j,k}(x), \qquad (11.10)$$

then it is obvious that $a_{ij} = a_{ji}$ and thus the quadratic form

$$\sum_{k=1}^{d} a_{ij}(x)\lambda_i\lambda_j \qquad (11.11)$$

is symmetric and nonnegative. We will assume a stronger condition, known as the **uniform parabolicity condition**:

$$\sum_{i,j=1}^{d} a_{ij}(x)\lambda_i\lambda_j \geq \rho \sum_{i=1}^{d} \lambda_i^2 \qquad (11.12)$$

where $\rho > 0$. If the $a_{ij}(x)$ satisfy the uniform parabolicity condition (11.12) and if they and the $F_i(x)$ are continuous and C^3, then $u(t, x)$ exists and is differentiable.

In deriving the evolution equation for $f(t, x)$ it is technically required that σ_{ij} and b_i are C^2, they and their derivatives up to second order are continuous for $t > 0$ and all $x \in R^d$, and that they and their first derivatives are bounded. We only sketch the derivation of the evolution equation here, and Lasota and Mackey (1994) can be consulted for the full derivation.

We start with the Euler–Bernstein equation (11.7), letting $t_0 > 0$ be arbitrary and assuming that $x(t)$ is the solution of equation (11.1) between 0 and t_0. Pick an $\epsilon > 0$ and define $x(t)$ on the interval $[t_0, t_0 + \epsilon]$ by

$$x(t_0 + \Delta t) = x(t_0) + F(x(t_0))\Delta t + \sigma(x(t_0))\Delta w(t_0), \qquad (11.13)$$

where $0 \leq \Delta t \leq \epsilon$ and $\Delta w(t_0) = w(t_0 + \Delta t) - w(t_0)$.

Consider a function $h : R^d \to R^d$ that, aside from being C^3 and having compact support, is arbitrary. We are going to calculate the expected value of $h(x(t_0 + \Delta t))$. To do this, make the assumption that $x(t)$ has a density $f(t, x)$ for $0 \leq t \leq t_0 + \Delta t$ and that $f_t(t, x)$ exists at $t = t_0$. Then by (11.13) we know that $x(t_0 + \Delta t)$ has a density $f(t_0 + \Delta t, x)$ and the expected value of $h(x(t_0 + \Delta t))$ is

$$E(h(x(t_0 + \Delta t))) = \int_{R^d} h(x)f(t_0 + \Delta t, x)\, dx. \qquad (11.14)$$

Note, however, that the Euler–Bernstein equation (11.7) allows us to write

$$h(x(t_0 + \Delta t)) = h(Q(x(t_0)), \Delta w(t_0))) \qquad (11.15)$$

where

$$Q(x, y) = x + F(x)\Delta t + \sigma(x)y.$$

Since the two random variables $x(t_0)$ and $\Delta w(t_0)$ are independent for all Δt satisfying $0 \leq \Delta t \leq \epsilon$, the random pair $(x(t_0), \Delta w(t_0))$ has the density

$$f(t_0, x)g(\Delta t, y),$$

where g is the density (11.3) of a d-dimensional Wiener process. Thus we may once again calculate the expected value of $h(x(t_0 + \Delta t))$ from (11.15) to yield

$$\int_{R^d} h(x)f(t_0 + \Delta t, x)\, dx = \int_{R^d} \int_{R^d} h(x + F(x)\Delta t + \sigma(x)y)f(t_0, x)g(\Delta t, y)\, dx\, dy.$$

Expanding h in a Taylor series, using equations (11.4) through (11.6), dividing throughout by Δt and then taking the limit as $\Delta t \to 0$ allows us to rewrite the last expression as

$$\int_{R^d} h(x)\frac{\partial f}{\partial t}\, dx = \int_{R^d} \left\{ \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2 h}{\partial x_i \partial x_j}a_{ij}(x) + \sum_{i=1}^{d} \frac{\partial h}{\partial x_i}F_i(x) \right\} f(t_0, x)\, dx.$$

Since h was assumed to have compact support, the right hand side of this last expression may be integrated by parts and the result rewritten as

$$\int_{R^d} h(x) \left\{ \frac{\partial f}{\partial t} + \sum_{i=1}^{d} \frac{\partial [F_i(x)f]}{\partial x_i} - \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2 [a_{ij}(x)f]}{\partial x_i \partial x_j} \right\} dx = 0.$$

The term within the braces must be identically zero (h was assumed to be C^3), and thus the evolution equation for the density $f(t,x)$ is given by

$$\frac{\partial f}{\partial t} = -\sum_{i=1}^{d} \frac{\partial [F_i(x)f]}{\partial x_i} + \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2 [a_{ij}(x)f]}{\partial x_i \partial x_j}. \tag{11.16}$$

This evolution equation is known variously as the **Fokker-Planck equation** or the **forward Kolmogorov equation**, and will be the foundation for our investigations into the effects of perturbations on the evolution of densities in systems whose dynamics are described by ordinary differential equations. The first term on the right hand side is usually called a **drift term**, while the second is known as a **diffusion term**. Had the Stratonovich calculus been used in deriving (11.16) rather than the Itô calculus, the result would have been

$$\frac{\partial f}{\partial t} = -\sum_{i=1}^{d} \frac{\partial [F_i(x)f]}{\partial x_i} + \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial}{\partial x_i} \left\{ a_{ij} \frac{\partial [a_{ij}(x)f]}{\partial x_j} \right\}.$$

Equation (11.16) can also be written in the equivalent form

$$\frac{\partial f}{\partial t} = L^+ f \tag{11.17}$$

where the operator L^+ is given by

$$L^+ = -\sum_{i=1}^{d} \frac{\partial}{\partial x_i} F_i(x) + \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2}{\partial x_i \partial x_j} a_{ij}(x). \tag{11.18}$$

The **backward Kolmogorov equation** is

$$\frac{\partial f}{\partial t} = -L^- f \tag{11.19}$$

where the operator

$$L^- = \sum_{i=1}^{d} F_i(x) \frac{\partial}{\partial x_i} + \frac{1}{2} \sum_{i,j=1}^{d} a_{ij}(x) \frac{\partial^2}{\partial x_i \partial x_j}. \tag{11.20}$$

is adjoint to L^+.[12]

C. SOLUTIONS OF THE FOKKER PLANCK EQUATION.

If the stochastic differential equation (11.1) has an initial condition $x(0)$ and an an associated initial density f, then the solution $f(t,x)$ of the Fokker-Planck equation satisfies $f(0,x) = f(x)$. Further, if the solution of the Fokker-Planck equation (11.16) can be written in the form

$$f(t,x) = \int_{R^d} \Gamma(t,x,s) f(s) \, ds \tag{11.21}$$

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[12]Remember that for any two L^1 functions u and v, if the operators L^+ and L^- are adjoint to one another they satisfy

$$\int_{R^d} v(L^+ u) \, dx = \int_{R^d} u(L^- v) \, dx.$$

where the kernel Γ is independent of the initial density $f(0, x) = f(x)$ and $\lim_{t \to 0} f(t, x) = f(0, x) \equiv f(x)$, then $f(t, x)$ is said to be a **generalized solution** of the Fokker-Planck equation.

Under some standard regularity conditions on the coefficients of the Fokker-Planck equation the generalized solution is unique. Since f is a density, the generalized solution corresponds to the evolution of the system to a unique thermodynamic state. To develop this, rewrite the Fokker–Planck equation in the form

$$\frac{\partial f}{\partial t} = -\sum_{i=1}^{d} b_i(x) \frac{\partial f}{\partial x_i} + \frac{1}{2} \sum_{i,j=1}^{d} a_{ij}(x) \frac{\partial^2 f}{\partial x_i \partial x_j} + c(x)f \tag{11.22}$$

where

$$b_i(x) = -F_i(x) + \sum_{i=1}^{d} \frac{\partial a_{ij}(x)}{\partial x_j},$$

and

$$c(x) = \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2 a_{ij}(x)}{\partial x_i \partial x_j} - \sum_{i=1}^{d} \frac{\partial F_i(x)}{\partial x_i}.$$

We now state, without proof, a condition for the solution $f(t, x)$ of the Fokker–Planck equation to be unique, corresponding to the evolution to a unique state of thermodynamic equilibrium. See Lasota and Mackey (1994) for the proof.

Theorem 11.1. *If $a_{ij}(x)$, $b_i(x)$, and $c(x)$ are all C^3, the a_{ij} satisfy the uniform parabolicity condition (11.12), and if there exists a positive constant M such that*

$$|a_{ij}(x)| \leq M, \quad |b_i(x)| \leq M(1 + |x|), \quad |c(x)| \leq M(1 + |x|^2),$$

then there exists a unique generalized solution $f(t, x)$ (11.21) to (11.22) for every initial density $f(x)$ that satisfies $|f(x) \leq c \exp(\alpha |x|^2)$ with $c > 0$ and $\alpha > 0$. Furthermore, the kernel Γ is strictly positive and satisfies the inequalities

$$\begin{aligned} 0 &< \Gamma(t, x, y) \leq \varphi(t, x - y) \\ |\Gamma_t| &\leq \varphi(t, x - y) \\ |\Gamma_{x_i}| &\leq \varphi(t, x - y) \\ |\Gamma_{x_i x_j}| &\leq \varphi(t, x - y), \end{aligned} \tag{11.23}$$

where

$$\varphi(t, z) = \frac{k}{t^{\frac{1}{2}(n+2)}} \exp\left[-\frac{Rz^2}{t}\right]$$

and k and R are constants.

These properties of the kernel Γ are useful in proving properties of functionals of $f(t, x)$. To see why, let g be a continuous function with bounded support in some ball $B_r = \{x : |x| \leq r\}$ and $f(t, x)$ the unique solution of the Fokker–Planck equation. Then from (11.21) and (11.23) we have

$$|f(t, x)| \leq \int_{B_r} \Gamma(t, x, s) g(s) \, ds \leq M \int_{B_r} \varphi(t, x - s) \, ds,$$

where $M = \max_s |g|$. Moreover, with $|x - s|^2 \geq \frac{1}{2} x^2 - r^2$ for $|s| \leq r$ we have

$$\int_{B_r} \varphi(t, x - s) \, ds \leq \frac{k}{t^{\frac{1}{2}(n+2)}} \exp\left[\frac{-R\left(\frac{1}{2}|x|^2 - r^2\right)}{t}\right]$$

so

$$|f(t, x)| \leq \frac{K}{t^{\frac{1}{2}(n+2)}} \exp\left[-\frac{R|x|^2}{t}\right]$$

with $K = kM|B_r|\exp(Rr^2)$. Analogous inequalities given by

$$|f|, \quad |f_t|, \quad |f_{x_i}|, \quad |f_{x_i x_j}| \leq \frac{k}{t^{\frac{1}{2}(n+2)}} \exp\left[-\frac{Rz^2}{t}\right] \tag{11.24}$$

may also be derived. These are of use in that they allow us to multiply the Fokker–Planck equation by any function that increases more slowly than $\exp(-R|x|^2)$ decreases, and then integrate to calculate various moments of the density $f(t, x)$.

From the expression (11.21) for the generalized solution, a family $\{P^t\}_{t \geq 0}$ of integral operators can be defined by

$$P^0 f(x) = f(x), \qquad P^t f(x) = \int_{R^d} \Gamma(t, x, s) f(s) \, ds, \tag{11.25}$$

where $f(0, x) = f(x)$. If the generalized solution is unique, *i.e.* if it satisfies all of the conditions of Theorem 11.1, then the operator P is a Markov operator.

To show this, first realize that the linearity of P is immediate since P is defined as a linear integral operator. Further, we also have that $P^t f \geq 0$ for $f \geq 0$ because of the positivity of the kernel Γ. To show that P^t preserves the norm, *i.e.* $||P^t f|| = ||f||$ for $f \geq 0$, is slightly more difficult. Multiply the Fokker–Planck equation by a continuous bounded C^2 function $h(x)$ with compact support, integrate over R^d, and then integrate a second time by parts to give

$$\int_{R^d} h(x) \frac{\partial f}{\partial t} \, dx = \int_{R^d} \left\{ \frac{1}{2} \sum_{i,j=1}^{d} a_{ij} \frac{\partial^2 h}{\partial x_i \partial x_j} + \sum_{i=1}^{d} b_i \frac{\partial h}{\partial x_i} \right\} f \, dx.$$

Picking $h = 1$ then gives $\frac{d||f||}{dt} = 0$ for $t > 0$ since $P^t f \geq 0$ for $f \geq 0$. Also, inequality (11.16) in conjunction with the continuity of $f(t, x)$ as $t \to 0$ imply that $||P^t f||$ is continuous at $t = 0$ and therefore that $||P^t f||$ is constant for all $t \geq 0$.

Thus the operator P^t defined by equation (11.25) is a Markov operator. It is instructive to compare the dynamical equations for densities evolving under the action of continuous flows in the perturbed and unperturbed situations. For the continuous time closed system in Chapter 4, the evolution of the Frobenius-Perron operator P^t is determined by the partial differential equation (4.14), the generalized Liouville equation. When the system is subject to external white noise perturbations, then the evolution of the Markov operator $P^t f$ is governed by the Fokker-Planck equation (11.16) which is just equation (4.14) with the addition of the diffusion term.

D. THE BEHAVIOUR OF ENTROPY.

In Example 3.8 we showed directly that the entropy of a closed continuous time system with dynamics described by ordinary differential equations was absolutely constant and equal to the entropy of the initial density with which the system was prepared. As pointed out, this result is not surprising since dynamics described by ordinary differential equations are invertible, and Theorem 3.2 shows that the entropy is constant for all reversible systems.

With the material of the previous sections, we are now in a position to examine the effects of perturbations on the entropy behaviour of these continuous time invertible systems.

In presenting our first result, we extend the concept of a Liapunov function, introduced in the previous chapter, by requiring that a Liapunov function V have the following properties:

(1) $V(x) \geq 0$ for all x;
(2) $\lim_{|x| \to \infty} V(x) = \infty$;
(3) V_{x_i} and $V_{x_i x_j}$ are continuous for $i, j = 1, \ldots, d$; and
(4) The growth conditions

$$V(x), \quad |V_{x_i}(x)|, \quad |V_{x_i x_j}(x)| \leq Ke^{M|x|}, \tag{11.26}$$

where K and M are positive constants, hold.

The existence of a Liapunov function V which satisfies the differential inequality

$$\sum_{i,j=1}^{d} a_{ij}(x) \frac{\partial^2 V}{\partial x_i \partial x_j} + \sum_{i=1}^{d} F_i(x) \frac{\partial V}{\partial x_i} \leq -\alpha V(x) + \beta, \tag{11.27}$$

where α and β are positive constants, is involved with a sufficient condition stating that the evolution of densities by the Fokker-Planck equation is described by an f_* exact Markov operator. Specifically we have the strong form of the Second Law:

Theorem 11.2. *Assume that there is a unique generalized solution of the Fokker-Planck equation and that there exists a Liapunov function V satisfying (11.27). Then the Markov operator P^t (11.25) defined by the generalized solution of the Fokker-Planck equation is f_* exact and the conditional entropy $H_c(P^t f | f_*)$ approaches its maximal value of zero as $t \to \infty$.*

Proof. Pick a continuous initial density f with compact support and consider the expectation of V with respect to the generalized solution (11.21) of the Fokker–Planck equation with initial condition $f(0, x) = f(x)$. We have

$$E(V|f) = \int_{R^d} V(x) f(t, x) \, dx. \tag{11.28}$$

From inequalities (11.24) and (11.26), Vf and Vf_t are both integrable, so differentiation of (11.28) with respect to t, use of the Fokker–Planck equation, integration by parts, using the fact that fV, f_x, V, and fV_x all vanish exponentially as $|x| \to \infty$, and then using the differential inequality (11.27), we finally obtain

$$\frac{dE(V|f)}{dt} \leq -\alpha E(V|f) + \beta.$$

This differential inequality is easily solved by multiplying by $e^{\alpha t}$, integrating, and then using the fact that at $t = 0$, $E(V|f) = E(V|f)$ to give

$$E(V|f) \leq e^{-a\,t} E(V|f) + \frac{\beta}{\alpha} \left[1 - e^{-\alpha t}\right].$$

Since $E(V|f)$ is finite, there will always exist a time $t_0 = t_0(f)$ such that

$$E(V|f) \leq 1 + \frac{\beta}{\alpha} \qquad \text{for} \qquad t \geq t_0.$$

Now let $G_q = \{x : V(x) \leq q\}$. Using the Chebyshev inequality (10.9a) we obtain

$$\int_{G_q} f(t, x) \, dx \geq 1 - \frac{1}{q} E(V|f)$$

so pick $q > 1 + \beta/\alpha$ to give

$$\int_{G_q} f(t, x) \, dx \geq 1 - \frac{1}{q} \left[1 + \frac{\beta}{\alpha}\right] \equiv \epsilon > 0$$

for $t \geq t_0$. Now since, by definition, $V(x) \to \infty$ as $|x| \to \infty$, there must be a positive constant r such that $V(x) > q$ for $|x| > r$ so the set G_q is entirely contained in the ball B_r defined in the derivation of the inequalities (11.24). As a result we may write

$$f(t, x) = \int_{R^d} \Gamma(1, x, y) f(t - 1, y) \, dy \geq \inf_{|y| \leq r} \Gamma(1, x, y) \int_{B_r} f(t - 1, y) \, dy$$
$$> \epsilon \inf_{|y| \leq r} \Gamma(1, x, y) \equiv h(x). \tag{11.29}$$

Since the kernel Γ is positive, the function $h(x)$ defined above is also positive and in fact we have shown that

$$P^t f(x) \equiv f(t, x) \geq h(x) \qquad \text{for} \quad t \geq t_0 + 1,$$

so that the sequence $\{P^t f\}$ has a nontrivial lower bound function. Thus by Theorem 7.6 we know that the Markov operator P^t is f_* exact. An application of Theorem 7.7 completes the proof that the conditional entropy increases to its maximal value of zero. $\square$

The unique stationary density f_* defined by

$$\lim_{t \to \infty} P^t f(x) = f_*(x)$$

that this theorem guarantees the existence of is given by the solution of the elliptic equation

$$-\sum_{i=1}^{d} \frac{\partial [F_i(x) f_*]}{\partial x_i} + \frac{1}{2} \sum_{i,j=1}^{d} \frac{\partial^2 [a_{ij}(x) f_*]}{\partial x_i \partial x_j} = 0. \tag{11.30}$$

It may not be the case that the solution of equation 11.30 is a density, even though it may be a unique solution (see Examples 11.3 and 11.4 below). When the solution is normalizable so it is a density, then another result giving a strong version of the Second Law may be established. This is given in

Theorem 11.3. *Assume that there is a unique generalized solution (11.21) to the Fokker-Planck equation (11.16), and that there is a unique stationary density*

$$\lim_{t \to +\infty} f(t, x) = \lim_{t \to +\infty} P^t f(x) = f_*(x),$$

that satisfies (11.30). Then

$$\lim_{t \to +\infty} H_c(P^t f | f_*) = 0.$$

Proof. From equations (3.14) and (11.17), and the adjointness of L^+ and L^- we may write

$$\frac{dH_c}{dt} = - \int_{R^d} f \left[L^- \log \left(\frac{f}{f_*} \right) \right] \, dx.$$

It is easy to show that

$$L^- \log \left(\frac{f}{f_*} \right) = \frac{f_*}{f} L^- \left(\frac{f}{f_*} \right) - \frac{1}{2} \left(\frac{f_*}{f} \right)^2 \sum_{i,j=1}^d a_{ij}(x) \frac{\partial}{\partial x_i} \left(\frac{f}{f_*} \right) \frac{\partial}{\partial x_j} \left(\frac{f}{f_*} \right).$$

Again using the adjointness of L^+ and L^-, and the fact that since f_* is a stationary density it satisfies (11.30), or $L^+ f_* \equiv 0$, we finally have

$$\frac{dH_c}{dt} = \frac{1}{2} \int_{R^d} \left(\frac{f_*^2}{f} \right) \sum_{i,j=1}^d a_{ij}(x) \frac{\partial}{\partial x_i} \left(\frac{f}{f_*} \right) \frac{\partial}{\partial x_j} \left(\frac{f}{f_*} \right) \, dx.$$

Since the a_{ij} satisfy the uniform parabolicity condition (11.12), we have

$$\frac{dH_c}{dt} \ge 0$$

with the equality holding if and only if $f = f_*$.

If we write $a_{ij} = \sigma^2 h(x)$ where $0 \le h(x) \le 1$, then

$$\frac{dH_c}{dt} = \sigma^2 I,$$

where $I \ge 0$, indicating that the rate of convergence of the conditional entropy to zero is proportional to the square σ^2 of the noise amplitude.

E. PHASE TRANSITIONS AND ADDITIVE PERTURBATIONS.

In this section we first make some general observations concerning the case when $d = 1$ and give a necessary and sufficient condition for the f_* exactness of the Markov operator (11.25) in this case. This, of course, is directly related to the behaviour of the entropy. We then illustrate this behaviour through two examples that show how additive white noise perturbations can lead to behaviour similar to that noted in 1st and 2nd order phase transitions.

If we are dealing with a one dimensional system, $d = 1$, then the stochastic differential equation (11.1) becomes

$$\frac{dx}{dt} = F(x) + \sigma(x)\xi, \tag{11.31}$$

where again ξ is a (Gaussian distributed) perturbation with zero mean and unit variance, and $\sigma(x)$ is the amplitude of the perturbation. The corresponding Fokker-Planck equation (11.16) becomes

$$\frac{\partial f}{\partial t} = - \frac{\partial [F(x)f]}{\partial x} + \frac{1}{2} \frac{\partial^2 [\sigma^2(x)f]}{\partial x^2}. \tag{11.32}$$

The Fokker-Planck equation can also be written in the equivalent form

$$\frac{\partial f}{\partial t} = - \frac{\partial S}{\partial x} \tag{11.33}$$

where

$$S = -\frac{1}{2}\frac{\partial[\sigma^2(x)f]}{\partial x} + Ff \tag{11.34}$$

is called the *probability current*.

When stationary solutions of (11.32), denoted by $f_*(x)$ and defined by $P_t f_* = f_*$ for all t, exist they are given as the generally unique (up to a multiplicative constant) solution of (11.30) in the case $d = 1$:

$$-\frac{\partial[F(x)f_*]}{\partial x} + \frac{1}{2}\frac{\partial^2[\sigma^2(x)f_*]}{\partial x^2} = 0. \tag{11.35}$$

Integration of equation (11.35) by parts with the assumption that the probability current S vanishes at the integration limits, followed by a second integration yields the solution

$$f_*(x) = \frac{K}{\sigma^2(x)}\exp\left[\int^x \frac{2F(z)}{\sigma^2(z)}\,dz\right]. \tag{11.36}$$

This stationary solution f_* will be a density if and only if there exists a positive constant $K > 0$ such that f_* can be normalized.

Rudnicki (1991) has recently proved a necessary and sufficient condition for exactness, and consequent existence of Second Law behaviour in its strong form. We extend his result to the behaviour of the conditional entropy without proof.

Theorem 11.4. *Assume that Theorem 11.1 holds so (11.32) has a unique generalized solution. Then the Markov operator P^t whose evolution is governed by equation (11.32) is f_* exact, and the corresponding conditional entropy $H_c(P^t f|f_*)$ approaches its maximal value of zero as $t \to \infty$, if and only if*

$$\int_{-\infty}^{+\infty}\exp\left[-\int^x \frac{2F(z)}{\sigma^2(z)}\,dz\right]\,dx = +\infty.$$

Systems like (11.31) may have behaviour reminiscent of 1st and 2nd order phase transitions as a parameter is varied [Mackey *et al.* (1990)].

Example 11.1. As an example of how 2nd order phase transition behaviour may occur, consider the two dimensional oscillator system

$$\frac{dr}{dt} = r(c - r^2)$$
$$\frac{d\theta}{dt} = 2\pi \tag{11.37}$$

in (r, θ) space. The system (11.37) is an example of a system with a supercritical Hopf bifurcation. For $c < 0$ the origin $r_* = 0$ is the globally stable steady state, while for $c > 0$ all solutions are attracted to the limit cycle defined by $r = \sqrt{c}$. Following Mackey *et al.* (1990) we consider the effects of perturbations in the analogous one dimensional system

$$\frac{dx}{dt} = x(c - x^2), \tag{11.38}$$

obtained by ignoring the angular coordinate θ in equations (11.37). For equation (11.38), sometimes known as the Landau equation, when $c < 0$ all solutions are attracted to the single steady state $x_* = 0$. Further, when $c > 0$ the steady state $x_* = 0$ is unstable and $x(t) \to \sqrt{c}$ if $x(0) = x_0 > 0$, while $x(t) \to -\sqrt{c}$ for $x_0 < 0$.

In the presence of additive perturbations, the stochastic differential equation corresponding to (11.38) is

$$\frac{dx}{dt} = x(c - x^2) + \sigma\xi, \tag{11.39}$$

so there is always a positive probability that $x(t)$ may take on negative values starting from a positive position and *vice versa*. Therefore it is natural to consider this problem for $x \in R$.

The Fokker-Planck equation corresponding to (11.39) is

$$\frac{\partial f}{\partial t} = -\frac{\partial[x(c-x^2)f]}{\partial x} + \frac{1}{2}\sigma^2\frac{\partial^2 f}{\partial x^2}, \tag{11.40}$$

and has a stationary solution

$$f_*(x) = Ke^{\beta x^2(2c-x^2)/4c}, \tag{11.41}$$

where $\beta = 2c/\sigma^2$. The normalization constant K always exists and thus the $f_*(x)$ defined by (11.41) is a stationary density.

To examine the question of exactness for this system, we use Theorem 11.2. Let $V(x) = x^2$ so V is a Liapunov function. Inequality (11.27) becomes

$$2\sigma^2 + (2c+\alpha)x^2 - 2x^4 \leq \beta.$$

This is clearly satisfied for all c with arbitrary fixed $\alpha > 0$ and sufficiently large $\beta > 0$, thus proving the exactness of the generalized solution of the Fokker-Planck equation (11.40) corresponding to (11.39) for additive perturbations applied to the system (11.38). As a consequence of this we also know that the effect of the additive perturbations has been to induce the conditional entropy to approach its maximal value of zero.

In Figure 11.1 we graph the location of the maxima of the stationary density given in equation (11.41) as a function of the parameter c. As might be expected on intuitive grounds, for $c < 0$ the stationary density $f_*(x)$ has a single maximum centered at $x = 0$, the location of the globally stable steady state of the unperturbed system (11.38). Once $c > 0$, the stationary density $f_*(x)$ shows two maxima centered at $x = \pm\sqrt{c}$, the locally stable steady states of (11.38), and a local minimum at the unstable steady state $x = 0$. Thus, if we were to calculate various system averages and plot them as a function of the parameter c a qualitatively similar pattern would emerge. If, for example, the parameter c were to be viewed as related to system temperature or pressure, the resulting graph has the characteristics of a 2nd order phase transition (Horsthemke and Lefever, 1984). It is important to realize that this appearance is exclusively due to the presence of the additive noise in the system. $\bullet$

Perturbations to continuous time systems may result in different types of behaviour similar to those found in 1st order phase transitions. This is illustrated by the next example.

Example 11.2. Consider a system

$$\begin{aligned}\frac{dr}{dt} &= r(c + 2r^2 - r^4) \\ \frac{d\theta}{dt} &= 2\pi\end{aligned} \tag{11.42}$$

which has a subcritical Hopf bifurcation at $c = -1$. As in the previous example, we examine the effects of perturbations on the one dimensional system

$$\frac{dx}{dt} = x(c + 2x^2 - x^4). \tag{11.43}$$

The solutions of equation (11.43) have the following behaviour. For $c < -1$ all solutions $x(t) \to 0$ regardless of the initial condition x_0. However, for $-1 < c < 0$ there is a tristability in that

$$x(t) \to \begin{cases} -\sqrt{1+\sqrt{1+c}}, & \text{for } x_0 < -x_*^+ \\ 0, & \text{for } -x_*^- < x_0 < x_*^- \\ \sqrt{1+\sqrt{1+c}}, & \text{for } x_*^+ < x_0. \end{cases}$$

where $x_*^+ = \sqrt{1+\sqrt{1+c}}$ and $x_*^- = \sqrt{1-\sqrt{1+c}}$. For $c > 0$, the steady state $x_* = 0$ becomes unstable and this tristable behaviour gives way to a bistability such that

$$x(t) \to \begin{cases} -\sqrt{1+\sqrt{1+c}}, & \text{for } x_0 < 0 \\ \sqrt{1+\sqrt{1+c}}, & \text{for } x_0 > 0. \end{cases}$$

With additive perturbations, the stochastic differential equation corresponding to (11.43) is

$$\frac{dx}{dt} = x(c + 2x^2 - x^4) + \sigma\xi. \tag{11.44}$$

As before, we consider this problem for $x \in R$. The Fokker-Planck equation corresponding to the stochastic differential equation (11.44) is

$$\frac{\partial f}{\partial t} = -\frac{\partial[x(c + 2x^2 - x^4)f]}{\partial x} + \frac{1}{2}\sigma^2\frac{\partial^2 f}{\partial x^2}, \tag{11.45}$$

and has the corresponding stationary solution

$$f_*(x) = Ke^{\beta x^2(3c + 3x^2 - x^4)/6c} \tag{11.46}$$

where $\beta = 2c/\sigma^2$ and K always exists. Therefore, $f_*(x)$ is a stationary density. Furthermore, the use of either Theorem 11.2 or Theorem 11.4 proves the convergence of the conditional entropy to zero for all values of the parameters.

The differences between the behaviour of the systems (11.39) and (11.44) immediately become apparent in Figure 11.2, which again shows the location of the maxima of the stationary density (11.46). For $c < -1$, the stationary density $f_*(x)$ has a single maximum located at $x = 0$, the globally stable steady state of the unperturbed system (11.43). For $-1 < c < 0$, where the tristable behaviour occurs, the stationary densities still have an absolute maximum at $x = 0$ but also display maxima at $x = \pm\sqrt{1 + \sqrt{1 + c}}$ that become progressively more prominent as c increases. Finally, for $c > 0$ the stationary density has absolute maxima located at $x = \pm\sqrt{1 + \sqrt{1 + c}}$ and a local minimum at $x = 0$. Translated into the language of a phase diagram, this behaviour is precisely what is found in 1st order phase transitions.•

F. PARAMETRIC PERTURBATIONS AND PHASE TRANSITIONS.

Both systems (11.38) and (11.43) of the previous section contain a single parameter c. In this section we investigate the effects of perturbations to this parameter by replacing c with

$$c + \sigma\xi,$$

where $\sigma > 0$ is a constant.

Example 11.3. With parametric noise of this type in (11.38), the stochastic differential equation (11.39) is replaced by

$$\frac{dx}{dt} = x(c - x^2) + \sigma x\xi. \tag{11.47}$$

The Fokker-Planck equation corresponding to (11.47) is given by

$$\frac{\partial f}{\partial t} = -\frac{\partial[x(c - x^2)u]}{\partial x} + \frac{1}{2}\sigma^2\frac{\partial^2[x^2 f]}{\partial x^2}, \tag{11.48}$$

and has a stationary solution $f_*(x)$ given by

$$f_*(x) = Kx^\gamma e^{-x^2/\sigma^2}, \tag{11.49}$$

where $\gamma = (2c/\sigma^2) - 2$.

To determine the normalization coefficient K in (11.49), we must specify the space on which we are working. From equation (11.47) it is clear that $x(t) = 0$ is always a solution. Therefore, for any $x_0 > 0$ the solution $x(t)$ will always be positive. For $x_0 < 0$ we will have $x(t) < 0$. Therefore, no trajectory can cross the $x = 0$ boundary.

We thus consider the situation in which $x \in R^+$. In this case, a stationary density will not exist for some parameter values. In order that f_* is a density, it must be integrable on R^+, and from (11.49) this is only possible if $\gamma > -1$, or

$$c > \frac{1}{2}\sigma^2. \tag{11.50}$$

Thus, in contrast to the results for additive noise, for parametric noise a stationary density $f_*(x)$ in the supercritical case exists for only a limited range of values of the parameter c as defined by inequality (11.50).

For $(\sigma^2/2) < c < \sigma^2$ the stationary density $f_*(x)$ given by equation (11.49) has a single maximum at $x = 0$. Once $c > \sigma^2$, the stationary density $f_*(x)$ has a local minimum at $x = 0$ and a maximum at $x = \sqrt{c - \sigma^2}$. Thus, with parametric perturbations there is not only a shift in the value of the parameter c at which there is a transition between the stationary density having a maximum at $x = 0$ and a nonzero value of x, but there is also a shift in the nonzero location of the maximum in the stationary density below that of the globally stable steady state in the absence of noise

$(x = \sqrt{c})$ toward zero. It is only as c becomes large that the location of the density maximum starts to approximate $\sqrt{c}$. This is once again similar to the behaviour seen in 1st order phase transitions, with the added crucial difference of the dependence (shift) of the bifurcation point on both c and σ^2.

In trying to prove that the Markov operator for this problem is exact, we no longer have available the Liapunov function technique that we were able to apply so easily with additive perturbations. This is because the coefficient $(\sigma^2 x^2/2)$ in (11.48) vanishes at $x = 0$ and the uniform parabolicity condition (11.12) is violated at $x = 0$. This fact is crucial.

However, by a straightforward change of variables, we may transform the Fokker-Planck equation (11.48) to circumvent this problem, and then again apply the Liapunov function argument. (This procedure may always be carried out.) Define a new variable $y = \ln x$ and a new density $\tilde{f}$ by

$$\tilde{f}(t,y) = e^{2y} f(t, e^y). \tag{11.51}$$

With these changes, the Fokker-Planck equation (11.43) takes the form

$$\frac{\partial \tilde{f}}{\partial t} = -\frac{\partial [(c - \frac{1}{2}\sigma^2 - e^{2y})\tilde{f}]}{\partial y} + \frac{1}{2}\sigma^2 \frac{\partial^2 \tilde{f}}{\partial y^2}. \tag{11.52}$$

As in the previous case, the uniform parabolicity condition is now satisfied and further $y(c - \frac{1}{2}\sigma^2 - e^{2y}) < 0$ for sufficiently large y whenever $c > \sigma^2/2$, which is the range of concern here. Thus if we are able to find a Liapunov function V which satisfies (11.27), the exactness of the Markov operator whose evolution is described by (11.52) will be demonstrated.

Set $q = 2\alpha/(c - \sigma^2/2)$, where $\alpha > 0$ is the same as in inequality (11.27). Clearly $c > \sigma^2/2$ whenever a stationary density of (11.52) exists, so take $q > 0$. It is evident that

$$V(y) = \cosh(qy)$$

is a Liapunov function. It is easy to show by a straightforward calculation that there are $\alpha > 0$ and $\beta > 0$ such that (11.27) is satisfied in the new variable y. Thus by Theorem 11.2 we know the stationary solution of (11.52) is f_* exact which, by the change of variables (11.51), in turn implies the f_* exactness of (11.43).•

Example 11.4. If we consider the effect of perturbations on the parameter c in equation (11.43), then it is straightforward to show that the corresponding Fokker Planck equation has a stationary density given by

$$f_*(x) = Kx^\gamma e^{-x^2(4-x^2)/\sigma^2}, \tag{11.53}$$

where γ is as before. As in the previous example, f_* is a stationary density if and only if

$$c > \frac{1}{2}\sigma^2.$$

Using the same Liapunov function of Example 11.3, we can also prove the f_* exactness of the parametrically perturbed system whenever $c > \sigma^2/2$. •

G. SUMMARY.

Here we have continued our investigations of the previous chapter into the effects of outside perturbations on system entropy by considering systems with continuous time dynamics that are perturbed by an (idealized) Wiener process. We have given several criteria that allows one to determine when perturbation by a Wiener process will lead to exactness and the consequent increase of system entropy to zero which is characteristic of the strong form of the Second Law. Furthermore, we have shown how the addition of noise in continuous time systems can lead to parametric dependence of the system stationary density like that observed in 1st and 2nd order phase transitions.

Figure 11.1. The stationary density (11.41) and (insert) locations in the (c, x) plane of the maxima (solid lines) and minima (dashed lines) in this density for the system (11.39). The behaviour as a function of the parameter c is analogous to that in 2nd order phase transitions.

Figure 11.2. The stationary density (11.46) and (insert) locations of the maxima (solid lines) and minima (dashed lines) in this density for the system (11.44). The behaviour as a function of the parameter c is like that seen in 1st order phase transitions.

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