

**THE SECOND LAW OF THERMODYNAMICS:  
COMMENTS FROM ERGODIC THEORY.**

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**ABSTRACT.** Recent results from ergodic theory are used to examine the possible dynamical foundations of nonequilibrium thermodynamics. Though ergodicity is necessary and sufficient to establish a unique state of thermodynamic equilibrium, much stronger dynamical properties (asymptotic periodicity and exactness) are needed to ensure that system entropy will change from its initial level. Asymptotic periodicity allows system entropy to evolve to a relative state of thermodynamic equilibrium in which the final entropy depends on system preparation. Exactness, a property that only irreversible (noninvertible) systems may have, is both necessary and sufficient for entropy to go to zero. Since all physical laws are formulated in terms of reversible dynamics, these results present a clear problem. Coarse graining, traces, factors, and perturbations are examined as possible sources of the experimentally observed behaviour of entropy.

Typeset by  $\mathcal{A}\mathcal{M}\mathcal{S}$ - $\mathcal{T}\mathcal{E}\mathcal{X}$

## 0. INTRODUCTION.

The mathematical discipline of ergodic theory developed in response to mathematical questions raised by the seminal work of Boltzmann<sup>[1]</sup> and Gibbs<sup>[11]</sup> at the turn of the century. Though the first few decades of this century saw extensive interaction between ergodic theorists and statistical mechanicians, the fields have diverged somewhat in recent years leaving a number of important physical questions unanswered. This paper outlines a reconvergence of these two fields. A more extensive discussion of the issues raised here and examples of various points, as well as a proof of all results, can be found elsewhere<sup>[22,25,25a]</sup>.

The central goal of this paper is to examine the primary issues that any successful statistical mechanics must address in deriving an understanding of the origin of the Second Law of thermodynamics. 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. To make matters explicit, we distinguish four versions. Let  $S_{TD}(t)$  denote the thermodynamic entropy at time  $t$ .

The weakest form of the Second Law is the

**0<sup>th</sup> order Second Law.**  $S_{TD}(t) = S_{TD}(t')$  for all times  $t, t'$ , so the entropy difference  $\Delta S = S_{TD}(t') - S_{TD}(t)$  satisfies  $\Delta S \equiv 0$ .

In this form, the system entropy remains forever fixed at the value with which the system is prepared, be it by Nature or by an investigator.

The next strongest form is called the

**1<sup>st</sup> order Second Law.**  $S_{TD}(t) \geq S_{TD}(t')$  for all times  $t > t'$  Thus, with this form the system entropy may increase and  $\Delta S \leq 0$ .

Following the 1<sup>st</sup> order form we have the stronger assertion

**2<sup>nd</sup> order Second Law.**  $S_{TD}(t) \geq S_{TD}(t')$  for all times  $t > t'$  and at least one  $\lim_{t \rightarrow +\infty} S_{TD}(t) = S_{TD}^*$  exists. Thus  $\Delta S(t) = S_{TD}(t) - S_{TD}^* \leq 0$  and  $\lim_{t \rightarrow +\infty} \Delta S(t) \leq 0$ .

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 final, and strongest, form of the Second Law of thermodynamics is the most interesting.

**3<sup>rd</sup> order Second Law.**  $S_{TD}(t) \geq S_{TD}(t')$  for all times  $t > t'$  and there is a unique  $\lim_{t \rightarrow +\infty} S_{TD} = S_{TD}^*$  for all initial system preparations. Under these circumstances,  $\lim_{t \rightarrow +\infty} \Delta S(t) = 0$ .

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

## 1. PRELIMINARIES.

In this section we introduce some basic concepts.

### 1.1. Thermodynamic Systems and Measure Spaces.

We first start with a set  $X$  which is going to be the **phase space** on which all of our dynamics operates. Whatever  $X$  is we are going to assume that it does not have any pathological properties. We let  $\mathcal{A}$  denote a  $\sigma$ -**algebra** on  $X$ , and  $\mu$  be a **measure** defined on the  $\sigma$ -algebra  $\mathcal{A}$ .

With the three concepts of a phase space  $X$ , a  $\sigma$ -algebra  $\mathcal{A}$ , and a measure  $\mu$  we call the triple  $(X, \mathcal{A}, \mu)$  a **measure space**. All of the measure spaces we consider will be  $\sigma$ -finite, and we associate a thermodynamic system with a  $\sigma$ -finite measure space through the following postulate.

**POSTULATE A. A thermodynamic system is equivalent to a measure space.**

### 1.2. Dynamics.

Consider a general 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.*,  $S_t : X \rightarrow X$ , 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 ( $t \in R$ ) or discrete (integer valued,  $t \in Z$ ).

Two types of dynamics will be important in our considerations. First we introduce 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  $t, t' \in R$ . Dynamical systems are **invertible** or **reversible** since they may be run either forward or backward in time. All of the laws of classical and quantum physics are invertible and describe the behaviour of reversible systems.

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  $N$ ). In sharp contrast to dynamical systems, semidynamical systems are **noninvertible** or **irreversible** and may not be run backward in time in an unambiguous fashion.

It is important not to confuse the issue of reversibility (or invertibility), which is a purely mathematical question, with the issue of dissipativeness, which is a physical question. 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.

### 1.3. Thermodynamic States and Densities.

In keeping with the ergodic theory approach adopted here we 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. 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  $f \in \{f \in L^1 : f \geq 0, \|f\| = 1\}$ . 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**  $\mu_f(A)$  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  $\mu_f$ . 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  $\mu_L(dx) = dx$ .

Both Boltzmann and Gibbs, in their treatments of statistical mechanics, assumed 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 basic phase space to be a  $2s$  dimensional space which is usually called  $\mu$  **space**. He then considered the evolution of a large number  $N$  of identical particles, each with the same dynamics, in  $\mu$  space.  $N$  is large and typically on the order of Avagadro's number,  $6 \times 10^{23}$ . The limiting case of  $N \rightarrow \infty$  is the **thermodynamic limit** in which case the Boltzmann approach considers the evolution of a density in  $\mu$  space.

Gibbs also considered  $N$  identical particles operating with these  $2s$  dimensional dynamics in a phase space (commonly called the  $\Gamma$  **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.

### 1.4. Boltzmann-Gibbs Entropy.

In his 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. He then introduced 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 ( $\mu$  space) and for Gibbs ( $\Gamma$  space). The Boltzmann Gibbs entropy is just the expectation of the negative of the index of probability, and is the only reasonable candidate for a theoretical analog of the empirical thermodynamic entropy. This is because the only function for the index of probability 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.

## 2. MAXIMAL ENTROPY PRINCIPLES.

### 2.1. Microcanonical Ensembles.

We may immediately understand the origin of the classical Gibbs microcanonical ensemble as reflecting a simple 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*

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

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

Notice that in this theorem there is 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 (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.

### 2.2. Canonical Ensembles.

Even more interesting consequences can emerge from the extremal properties of entropy that offer insight into the basic foundation of thermodynamics of both classical and quantum systems. Namely,

**Theorem 2.2.** Assume that a nonnegative measurable function  $\alpha(x)$  is given as well as the average  $\langle \alpha \rangle$  of that function over the entire space  $X$ , weighted by the density  $f$ :

$$\langle \alpha \rangle = \int_X \alpha(x) f(x) dx. \quad (2)$$

(Note that  $\langle \alpha \rangle$  is nonnegative and may be time dependent.) Then the maximum of the entropy  $H(f)$ , subject to the constraint (2), occurs for the density

$$f_*(x) = Z^{-1} e^{-\nu\alpha(x)} \quad (3)$$

where  $Z$  is defined by

$$Z = \int_X e^{-\nu\alpha(x)} dx, \quad (4)$$

and  $\nu$  is implicitly determined from  $\langle \alpha \rangle = Z^{-1} \int_X \alpha(x) e^{-\nu\alpha(x)} dx$ .

The choice of notation in (3) and (4) was intentional to draw the connection with the density of the Gibbs canonical ensemble, especially that  $Z$  corresponds to the partition function. It is quite easy to state and prove an obvious generalization of Theorem 2.2 that is applicable to systems in which there are multiple known averages  $\langle \alpha_i \rangle$ .

### 2.3. The Thermodynamic Connection.

All of conventional equilibrium thermodynamics can be deduced from the density (3), by a proper association with thermodynamic quantities<sup>[25,25a]</sup>, if we admit the fundamental assumption of thermodynamics that

**POSTULATE C. There exists a one to one correspondence between states of thermodynamic equilibrium and states of maximum entropy.**

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 (3<sup>rd</sup> order 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** (2<sup>nd</sup> order Second Law).

### 3. REVERSIBLE AND IRREVERSIBLE SYSTEMS.

From the perspective of the previous section, 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 section we start our investigation of this question.

### 3.1. 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 either the linear Markov or Frobenius-Perron 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 operator, introduced in Section 4, is the most useful 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 permits the accurate specification of a system state at any point in time.

The Frobenius-Perron operator is a special case of the more general Markov operator which may be used in the description of both deterministic and stochastic systems. Since the first results on reversibility and irreversibility that are of importance to an understanding of thermodynamics can be stated for Markov operators, we start with them.

Any linear operator  $P^t : L^1 \rightarrow L^1$  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. Any density  $f_*$  that satisfies  $P^t f_* = f_*$  for all  $t$  is said to be a **stationary density** of the Markov operator  $P$ .

In precise analogy with the definitions of dynamical and semi-dynamical systems in the last section, we may discuss reversible and irreversible Markov operators. Given a Markov operator  $P^t$ , then  $P^t$  is a **reversible Markov operator** if: (1)  $P^0 f = f$ ; and (2)  $P^t(P^{t'} f) = P^{t+t'} f$  for all  $t, t' \in R$  or  $Z$ . Clearly, allowing  $t, t' \in R$  or  $Z$  is the origin of the reversibility. However, if property (2) of a reversible Markov operator is replaced by (2')  $P^t(P^{t'} f) = P^{t+t'} f$  for all  $t, t' \in R^+$  or  $N$ , then  $P^t$  is an **irreversible Markov operator**.

### 3.2. Conditional Entropy.

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

$$H_c(f|g) = - \int_X f(x) \log \left[ \frac{f(x)}{g(x)} \right] dx. \quad (5)$$

The conditional entropy is always defined, *i.e.*  $H_c$  is finite or equal to  $-\infty$ . As is evident from the defining equation (5),  $H_c(f|g)$  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, it can be shown that  $H_c(f|g) \leq 0$ . It is only when  $f = g$  that the equality holds; and (2) If  $g$  is the constant density of the microcanonical ensemble,

i.e.  $g = 1/\mu(X)$  throughout the phase space  $X$ , then  $H_c(f|g) = H(f) - \log \mu(X)$ . 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 it follows that  $H_c(f|g) = H(f) + \int_X f(x) \log g(x) dx$ . An elementary calculation using property (1) of  $H_c(f|g)$  shows that the second term in the rewritten form of  $H_c(f|g)$ , with  $f = g = f_*$ , is just  $-H(f_*)$  and that  $H_c(f|f_*) = 0$  when  $f = f_*$ . These observations, in conjunction with our formulations of the 2<sup>nd</sup> and 3<sup>rd</sup> order forms of the Second Law, immediately suggest that the conditional entropy  $H_c$  can be interpreted as the entropy difference  $\Delta S$ . For example, under the conditions of Theorem 2.2, the Boltzmann-Gibbs entropy  $H(f)$  is maximized by the density  $f_*$  given by equation (3) and  $H(f_*) = \log Z + \nu < \alpha >$ . Thus, within the context of Theorems 2.1 and 2.2 we conclude that the conditional entropy will be zero whenever the Boltzmann-Gibbs entropy is at its maximum value.

With only the few tools developed so far and our identification of  $H_c$  with  $\Delta S$ , the behaviour of the entropy of a sequence of densities  $\{P^t f\}$  evolving under the action of a Markov operator may be examined. The first result is a weak (1<sup>st</sup> order) form of the Second Law of thermodynamics stating that the conditional entropy is never decreasing. More precisely<sup>[32]</sup>,

**Theorem 3.1.** *If  $P^t$  is a Markov operator, then  $H_c(P^t f|P^t g) \geq H_c(f|g)$  for and all densities  $f$  and  $g$ .*

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  $t \rightarrow \infty$ , though more information about  $P^t$  is required to define the limiting value.

The conclusions of Theorem 3.1 seem to be precisely the same as those reached by Boltzmann<sup>[1]</sup> 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 reversibility or irreversibility of the Markov operator  $P^t$  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 a reversible Markov operator is constant and determined by the way in which the system is prepared.

**Theorem 3.2.** *If  $P^t$  is a reversible 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  $t$ .*

From this theorem, in any system whose evolution of densities is described by a reversible 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<sup>[24]</sup> in his *Umkehrwand* (objection based on time reversal) argument against the Boltzmann approach to statistical mechanics.

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

Based on much more specific assumptions, this result concerning the necessity of irreversibility was well known to Clausius<sup>[3]</sup> and Boltzmann<sup>[1]</sup>, 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 (reversible) Hamiltonian dynamics? Both he and Clausius tried to circumvent this clear problem [the use of reversible (Hamiltonian) dynamics] by the addition of their *Stosszahlansatz* (molecular chaos) *postulate*. This reduces, quite simply, to a *postulate of irreversibility*.

#### 4. ERGODICITY.

In the last section we asserted the necessity of irreversibility for increases in entropy to take place. However, 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 section provides a necessary and sufficient criterion for the existence of a unique state of thermodynamic equilibrium as characterized by a unique stationary density  $f_*$ .

##### 4.1. The Frobenius Perron Operator.

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  $\mu_*$ , 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  $P^t : L^1 \rightarrow L^1$  defined by

$$\int_A P^t f(x) dx = \int_{S_t^{-1}(A)} f(x) dx \quad (6)$$

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

If  $f$  is a density, then equation (6) defining the Frobenius-Perron operator has a simple 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  $P^t f$ .

Given a density  $f$  and associated measure  $\mu_f$ , 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  $\mu_f$  is **invariant** with respect to the transformation  $S_t$  if  $S_t$  is  $f$  measure preserving.

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 4.1.** *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  $\mu_*(A) = \int_A f_*(x)dx$  is invariant with respect to  $S_t$ .*

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.

#### 4.2. Ergodicity.

We are ready to begin consideration of the characteristics  $S_t$  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, given, as usual, dynamics described by a transformation  $S_t$ . 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**.

The following result establishes a one to one correspondence between the uniqueness of a state of thermodynamic equilibrium and ergodicity.

**Theorem 4.2.** *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  $f_*$  ergodic.*

What does this result, in conjunction with Theorem 4.1, 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 4.2 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 characterized by maximal entropy*. 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.

To conclude we state one last theorem concerning conditions for the  $f_*$  ergodicity of a transformation  $S_t$  and thus, by our comments following Theorem 4.2, for the existence of a unique state of thermodynamic equilibrium.

**Theorem 4.3.** *Let  $S_t$  be a nonsingular transformation and  $P^t$  the corresponding Frobenius Perron operator with stationary density  $f_* > 0$  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  $\lim_{t \rightarrow \infty} \frac{1}{t} \sum_{k=0}^{t-1} \langle P^k f, g \rangle = \langle f_*, g \rangle$  in the discrete time case, or if  $\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \langle P^t f, g \rangle dt = \langle f_*, g \rangle$  in the continuous time case, for all bounded measurable functions  $g$ .*

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

## 5. ASYMPTOTIC PERIODICITY.

In this section 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 implies a  $2^{n^d}$  order form of the Second Law.

### 5.1. Asymptotic Periodicity.

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  $\int_{E \cup (X \setminus A)} P^t f(x) dx \leq k$  for  $t \geq t_0(f, E)$ . This definition of smoothing just means that any initial density, no matter how small a region of the phase space  $X$  it is concentrated on, will eventually be smoothed out by  $P^t$ .

Smoothing operators are important because of the following result<sup>[19]</sup>.

**Theorem 5.1.** *Let  $P^t$  be a smoothing Markov operator. Then there is an integer  $r > 0$ , a sequence of nonnegative densities  $g_i$  and a sequence of bounded linear functionals  $\lambda_i$ ,  $i = 1, \dots, r$ , and an operator  $Q : L^1 \rightarrow L^1$  such that for all densities  $f$ ,  $Pf$  has the form*

$$Pf(x) = \sum_{i=1}^r \lambda_i(f) g_i(x) + Qf(x). \quad (7)$$

The densities  $g_i$  and the operator  $Q$  have the following properties: (1) The  $g_i$  have disjoint support (i.e. are mutually orthogonal), 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  $g_i$ ; and (3)  $\|P^t Qf\| \rightarrow 0$  as  $t \rightarrow \infty$ ,  $t \in N$ , so  $Q$  can be viewed as a transient operator.

Notice from equation (7) that  $P^{t+1}f$  may be immediately written in the form

$$P^{t+1}f(x) = \sum_{i=1}^r \lambda_i(f) g_{\alpha^t(i)}(x) + Q_t f(x), \quad t \in N \quad (8)$$

where  $Q_t = P^t Q$ ,  $\|Q_t f\| \rightarrow 0$  as  $t \rightarrow \infty$ , and  $\alpha^t(i) = \alpha(\alpha^{t-1}(i)) = \dots$ . The terms in the summation of (8) are just permuted by each application of  $P$ . Since  $r$  is finite, the sum  $\sum_{i=1}^r \lambda_i(f) g_{\alpha^t(i)}(x)$  must be periodic with a period  $T \leq r!$ . Further, as  $\{\alpha^t(1), \dots, \alpha^t(r)\}$  is just a permutation of  $1, \dots, r$  this summation takes 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 (8) makes the effect of successive applications of  $P$  completely transparent. Each operation of  $P$  permutes the set of scaling coefficients associated with the densities  $g_i(x)$  [remember that these densities have disjoint support]. Since the summation portion of (8) is periodic (with a period bounded above by  $r!$ ), and  $\|Q_t f\| \rightarrow 0$  as  $t \rightarrow \infty$ , we say that for any smoothing Markov operator the sequence  $\{P^t f\}$  is **asymptotically periodic**.

One of the interesting interpretations of equation (8) 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  $\|Q_t f\| \simeq 0$ , 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  $i^{\text{th}}$  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  $f$ .

Asymptotically periodic Markov operators always have at least one stationary density given by

$$f_*(x) = \frac{1}{r} \sum_{i=1}^r g_i(x), \quad (9)$$

where  $r$  and the  $g_i(x)$  are as in the Komornik-Lasota Theorem 5.1. It is easy to see that  $f_*(x)$  is a stationary density, since by Property (2) of Theorem 5.1 we also have  $Pf_*(x) = \frac{1}{r} \sum_{i=1}^r g_{\alpha(i)}(x)$ , and thus  $f_*$  is a stationary density of  $P^t$ . Hence, for any smoothing Markov operator the stationary density (9) is just the average of the densities  $g_i$ .

We close with a necessary and sufficient condition for the  $f_*$  ergodicity of a smoothing Markov operator.

**Theorem 5.2.** *Let  $P$  be a smoothing, and thus asymptotically periodic, Markov operator working in a normalized measure space. Then  $P$  is ergodic if and only if the permutation  $\alpha(i)$  of the Spectral Decomposition Theorem 5.1 is cyclical.*

Thus, 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  $f_*$ .

## 5.2. Local Evolution of Entropy.

The fact that asymptotically periodic Markov operators have a stationary density given by (9) 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.

**Theorem 5.3.** *Let  $P$  be an asymptotically periodic Markov operator with stationary density  $f_*$ . Then 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*

$$H_{max}(f, f_*) = - \sum_i \int_X \lambda_i(f)g_i(x) \log \left\{ \frac{1}{f_*(x)} \sum_i \lambda_i(f)g_i(x) \right\} dx. \quad (10)$$

Note that if the stationary density  $f_*$  of  $P$  is given by (9), then the expression for  $H_{max}(f, f_*)$  becomes even simpler. Namely,  $H_{max}(f, f_*) = -\log r - \sum_{i=1}^r \lambda_i(f) \log \lambda_i(f)$  when we use the orthogonality of the densities  $g_i(x)$ . Since

$0 \leq \lambda_i(f) \leq 1$  for all  $i$ , we may also place a lower bound on  $H_{max}(f, f_*)$  with  $-\log r \leq H_{max}(f, f_*) \leq 0$ .

This 2<sup>nd</sup> order form of the Second Law of thermodynamics is the strongest result that we have yet encountered. It demonstrates that as long as the density in a discrete time system evolves under the operation of a Markov operator that is smoothing, the conditional entropy of that density converges to a maximum. However, there are two important facets of this evolution that should be recognized: (1) The convergence of the entropy is due to the fact that  $\|Q_t f\| \rightarrow 0$  as  $t \rightarrow \infty$  in the representation (8) of Theorem 5.1; and (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.

## 6. MIXING.

In this section, we consider systems with irregular dynamical behaviors that are stronger than ergodic. Namely, we consider with dynamics described by  $f_*$  measure preserving transformations that have the property of strong, or Hopf, mixing. Systems with reversible mixing dynamics have entropies that are forever fixed by their mode of preparation. However, it is important to discuss mixing for two reasons. First there is a general misconception that mixing is sufficient to allow the evolution of entropy to a maximum. This is most certainly not the case in spite of the fact that mixing is necessary for the evolution of system entropy to a maximum. Secondly, as we will show in Section 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.

### 6.1. Mixing.

Gibbs<sup>[11]</sup> realized that ergodicity was inadequate to guarantee the approach of system entropy to equilibrium. As a consequence he qualitatively discussed a property stronger than ergodicity which is now called **(strong) mixing**. This was subsequently developed mathematically by Hopf<sup>[14]</sup>, Koopman<sup>[20]</sup>, and von Neumann<sup>[33]</sup>.

Let  $S_t$  be an  $f_*$  measure preserving transformation operating on a finite normalized space. Then  $S_t$  is called  **$f_*$  mixing** if  $\lim_{t \rightarrow \infty} \mu_*(A \cap S_t^{-1}(B)) = \mu_*(A)\mu_*(B)$  for all sets  $A$  and  $B$ . If  $f_*$  is the uniform density of the microcanonical ensemble, then we say that  $S_t$  is **uniformly mixing**. The defining relation for  $f_*$  mixing could equally well be written  $\lim_{t \rightarrow \infty} \mu_*(A \cap S_t(B)) = \mu_*(A)\mu_*(B)$ , whenever  $S_t$  is reversible (invertible).

It is a straightforward consequence of the definition that  $f_*$  mixing implies ergodicity. Furthermore, an  $f_*$  measure preserving transformation  $S_t$ , with associated Frobenius-Perron operator  $P^t$  and stationary density  $f_*$ , is  $f_*$  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 6.1.** *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  $f_*$ , i.e.,  $\lim_{t \rightarrow \infty} \langle P^t f, g \rangle = \langle f_*, g \rangle$ .*

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

Gibbs<sup>[11]</sup>, Krylov<sup>[21]</sup>, and many others have emphasized the importance of mixing for the understanding of thermodynamic behaviour. Indeed, at first one might think that this 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 not sufficient as we show in Section 7.

## 6.2. Kolmogorov Automorphisms.

In this section, a concept that will be used later is briefly introduced, namely that of Kolmogorov automorphisms, or K automorphisms. We use the notation  $S_t(\mathcal{A}) = \{S_t(A) : A \in \mathcal{A}\}$ ,  $t = 0, \pm 1, \pm 2, \dots$ , where  $\mathcal{A}$  is a sigma algebra. Then if  $S_t$  is an invertible transformation operating on a normalized space, and both  $S_t$  and  $S_{-t}$  are  $f_*$  measure preserving,  $S_t$  is said to be a **K-automorphism** 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  $\cap_{t=0}^{\infty} S_{-t}(\mathcal{A}_0)$  is trivial in the sense that it only contains sets of  $f_*$  measure 0 or 1; and (3) The smallest sigma algebra containing  $\cup_{t=0}^{\infty} S_t(\mathcal{A}_0)$  is identical to  $\mathcal{A}$ .

Kolmogorov automorphisms have behaviors stronger than mixing in that if a transformation is a K-automorphism then this also implies that it is  $f_*$  mixing<sup>[4,34]</sup>. The other property of K-automorphisms 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-automorphism is identically equal to the initial entropy determined by the initial density with which the system is prepared.

## 7. ENTROPY EVOLUTION TO ITS MAXIMUM.

The results of the previous sections indicate that attention should be focused on extensions of the concepts of ergodicity, asymptotic periodicity, and mixing that may only occur in irreversible systems. Since we also know that increases in entropy need not culminate in the maximum value of the entropy (*e.g.* asymptotically periodic systems, Section 5), the essential question we must now face is:

**Under what circumstances will the entropy of an irreversible system approach its maximum value of zero?** This section provides a complete answer to this question.

### 7.1. Exactness.

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  $\lim_{t \rightarrow \infty} \mu_*(S_t(A)) = 1$  for all sets  $A$  of nonzero measure. If  $f_*$  is the uniform density,  $f_* = 1$ , then we say that  $S_t$  is **uniformly exact**. The  $f_*$  exactness of a transformation implies that it is  $f_*$  mixing.

To understand the nature of exactness, it is first important to realize that *reversible systems can never be exact*. To see this, note that for a reversible  $f_*$  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.

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. Specifically,

**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, then  $S_t$  is  $f_*$  exact if and only if  $\lim_{t \rightarrow \infty} \|P^t f - f_*\| = 0$ , 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 and mixing conditions.

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  **$f_*$  exact** if  $\{P^t f\}$  is strongly convergent to  $f_*$  for all initial densities  $f$ .<sup>1</sup> For Markov operators,  $f_*$  exactness implies  $f_*$  mixing implies  $f_*$  ergodicity. We close with a simple sufficient condition for the  $f_*$  exactness of asymptotically periodic Markov operators.

**Theorem 7.2.** *Let  $P$  be a smoothing, and therefore asymptotically periodic, Markov operator. If  $r = 1$  in the spectral decomposition (7) of  $P^t f$ , then  $P$  is  $f_*$  exact.*

### 7.2. The Second Law of Thermodynamics.

The main result of this section is a condition for the Second Law of thermodynamics to operate in its strongest possible ( $3^{rd}$  order) 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. Namely we have:

<sup>1</sup>Operators  $P^t$  that are  $f_*$  exact have been called strong Markov operators<sup>[27]</sup> and monotonic Markov operators<sup>[13]</sup>.



**Theorem 7.3.** *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  $t \rightarrow \infty$ ,*

$$\lim_{t \rightarrow \infty} H_c(P^t f | f_*) = 0,$$

*if and only if  $P^t$  is  $f_*$  exact.*

Theorem 7.3 is remarkable in that it sets forth *necessary and sufficient criteria for the operation of the strongest 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

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*. Hence, in general

$$P^t \text{ is } f_* \text{ exact} \Leftrightarrow \lim_{t \rightarrow \infty} H_c(P^t f | f_*) = 0.$$

These results point out a very interesting property of the entropy *vis à 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” by 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 ( $f_* = 1$ ) 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 do preserve the Lebesgue measure and for which the attendant density  $f_* = 1$  is a stationary density.

With the results of this section 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. However, 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 *irreversible*  $f_*$  exact systems that the entropy will increase to its maximal value (Theorem 7.3). 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 reversible or invertible dynamical (as opposed to irreversible or 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. [Penrose<sup>[28]</sup> has argued quite lucidly and simply for this point of view, basing his thesis on CPT violation in  $K^0$  meson decay. Fer<sup>[8]</sup> makes a similar point, basing his argument on the neglect of time delays in the usual formulations of physical laws. Gal-Or<sup>[9,10]</sup> and Davies<sup>[5]</sup> have extensively 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 observed behaviour.

The following sections 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.

## 8. COARSE GRAINING.

To this point, in calculating the entropy from the defining equations it has been assumed that the dynamical variables were 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. Several consequences may ensue from this. The first and perhaps most obvious is that due to errors (arising, for example, from measurement impreciseness or numerical roundoff in computer experiments),  $f$  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 section we examine the consequences of imprecision in the measurement of dynamical variables by studying the properties of the coarse grained entropy.

### 8.1. Coarse Grained Entropy.

To examine the effect of imprecision in the measurement of dynamical variables on entropy calculations, we introduce the concept of 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<sup>[11]</sup>, and quantified by Ehrenfest and Ehrenfest<sup>[7]</sup>. Denbigh and Denbigh<sup>[6]</sup> 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  $\cup_i A_i = X$  and  $A_i \cap_{i \neq j} A_j = \emptyset$ . 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  $\mu_L$  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  $\langle f \rangle_i$ ,

$$\langle f \rangle_i = \frac{1}{\mu(A_i)} \int_{A_i} f(x) dx, \quad (11)$$

so the density  $f$  coarse grained with respect to the partition  $A_i$  is given by

$$f^{cg}(x) = \sum_i \langle f \rangle_i 1_{A_i}(x). \quad (12)$$

[Here,  $1_A(x) = 1$  for  $x \in A$  and  $1_A(x) = 0$  when  $x \notin A$ .] Clearly  $\sum_i \langle f \rangle_i \mu_L(A_i) = 1$ , and it is important to realize that  $f^{cg}$  is constant within each cell  $A_i$ , having the value given by (11).

Therefore, given a nontrivial partition  $A_i$ , a density  $f$ , and a coarse grained density  $f^{cg}$  defined by (11)-(12), then the Boltzmann-Gibbs entropy of the coarse grained density  $f^{cg}$  is given by

$$H(f^{cg}) = - \sum_i \langle f \rangle_i \mu_L(A_i) \log \langle f \rangle_i .$$

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  $X$ ,  $H(f) \leq H(f^{cg})$ .*

Thus, the effect of any imprecision 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  $H_c(f^{cg}|g^{cg}) = -\sum_i \langle f \rangle_i \mu_L(A_i) \log[\langle f \rangle_i / \langle g \rangle_i]$ . It is equally easy to show that  $H(f|g) \leq H_c(f^{cg}|g^{cg})$  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*.

In analogy with (12), the coarse grained  $P^t f$  is given by  $(P^t f(x))^{cg} = \sum_i \langle P^t f \rangle_i 1_{A_i}(x)$  where  $\langle P^t f \rangle_i = [\mu_L(A_i)]^{-1} \int_{A_i} P^t f(x) dx$ . 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 Sections 10 and 11 where we consider system interactions with a heat bath.

Simple examples show that, for reversible systems, coarse graining: (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; (3) The approach is not necessarily symmetric with respect to a reversal of time; and (4) The approach may be dependent on the partition chosen.

## 8.2. Coarse Graining of Mixing Systems.

Coarse graining has interested numerous authors since the concept was first introduced by Gibbs<sup>[11]</sup> with the observation that coarse graining of a mixing system should lead to an increase in the entropy to its maximal value. More specifically,

**Theorem 8.2.** *If  $P^t$  is a reversible  $f_*$  mixing Markov operator with a unique stationary density  $f_*$ , and  $\{A_i\}$  is a nontrivial partition of the phase space  $X$ , then  $\lim_{t \rightarrow \pm\infty} (P^t f)^{cg} = f_*^{cg}$  for all initial densities  $f$ .*

As a consequence of this result and Theorem 7.3, we have

**Theorem 8.3.** *If  $P^t$  is a reversible  $f_*$  mixing Markov operator with a unique stationary density  $f_*$  and  $\{A_i\}$  is a nontrivial partition of the phase space  $X$ , then  $\lim_{t \rightarrow \pm\infty} H_c((P^t f)^{cg}|f_*^{cg}) = 0$  for all initial densities  $f$ . [Notice that the entropy approach to zero is independent of the direction of time!]*

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 density of the microcanonical ensemble, and that the Boltzmann-Gibbs entropy will approach its maximum value of zero.

### 8.3. Summary.

Even setting aside the lack of irreversibility in 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 reversible 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.

## 9. TRACES AND FACTORS.

As an alternative to the coarse graining of the previous section, we now explore the consequences of a reversible 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.

### 9.1. Traces.

Let  $X$  and  $Y$  be two (topological Hausdorff) phase spaces,  $F : Y \rightarrow X$  a given continuous function, and  $S_t : Y \rightarrow Y$  a dynamical system operating in the phase space  $Y$ . A function  $h : R \rightarrow X$  is the **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 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.

**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  $F : Y \rightarrow X$  such that every continuous trajectory  $h : R \rightarrow X$  is the trace of  $S_t$ .*

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 a reversible system to change (Theorem 3.2.). However, this may not be the case for the entropy of the density of a trace of a dynamical system, since the simple act of 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 certainly approach a limit considerably less than its maximal value if, for example, the trace is asymptotically periodic.

## 9.2. 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.

$$\begin{array}{ccc} Y & \xrightarrow{S_t} & Y \\ F \downarrow & & \downarrow F \\ X & \xrightarrow{T_t} & X \end{array}$$

Let  $X$  and  $Y$  be two different phase spaces with normalized measures  $\mu_f$  and  $\mu_g$ , and associated densities  $f_*$  and  $g_*$  respectively, and  $T_t : X \rightarrow X$  and  $S_t : Y \rightarrow Y$  be two measure preserving transformations. If there is a transformation  $F : Y \rightarrow X$  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 *the trajectory of the factor  $T_t$  is a trace of the system  $S_t$ .*

The formal connection between these concepts and the behaviour of the entropy is furnished by the following theorem due to Rochlin<sup>[30]</sup>.

**Theorem 9.2.** *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.*<sup>[27]</sup> and Prigogine<sup>[29]</sup> refer to as a projection operator in their work on the generation of irreversible behaviour from reversible dynamics. Theorem 9.2 serves as the analytic link in their work between reversible K-automorphisms and  $f_*$  exact transformations (or strong or monotonic Markov operators).

As noted in Section 6, since K-automorphisms are invertible their entropy is forever fixed at its initial value by Theorem 3.2. On the other hand, by Theorem 7.3 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.

### 9.3. Coarse Graining and Traces.

There is a connection between the effects of coarse graining the phase space and taking the trace of a dynamical system. In nontrivial 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, *i.e.* the partition is trivial.

Viewed from this perspective, it is surprising that there is such a difference between the results of a nontrivial coarse graining of the phase space (no induction of irreversible thermodynamic behaviour), and examining only the trace of a dynamical system operating in a higher dimensional space than our observations permit. However, it is precisely trivial coarse graining of a phase space in which the evolution of densities is governed by the Liouville equation 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.

### 9.4. Summary.

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. This and the previous section have presented two possible ways out of the clear problems associated with the necessity of an irreversible system for entropy to increase, and the fact that all of the laws of physics are formulated as reversible dynamical systems.

## 10. OPEN DISCRETE TIME SYSTEMS.

This section examines the consequences of having a discrete time deterministic transformation experience a perturbation from an outside source. Thus we are starting to consider open systems, the mathematical analogue of the interaction between a system and a “heat bath”. Stochastically perturbed continuous time systems with dynamics described by ordinary differential equations are considered in the Section 11.

### 10.1. An Operator Equation.

Assume that, in general, a system evolves according to a given transformation  $S(x_t)$ . The qualifying phrase ‘in general’ means that the transition  $x_t \rightarrow x_{t+1} = S(x_t)$  occurs with probability  $(1 - \epsilon)$ . In addition, with probability  $\epsilon$ , 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  $y$ .

One interpretation of this process is that  $\epsilon$  corresponds to the degree of coupling between the system under study and the heat bath. If this is the case, then the parameter  $\epsilon$  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', while for  $\epsilon = 1$ , in which the influence of the external system is always experienced, we will speak of strong (or continuous) coupling. However, as will become clear in Section 10.3, precisely the same formulation may be interpreted in a totally different fashion.

Assume that the dynamics of our system 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 and have an associated Frobenius Perron operator  $P_S$ . Then the operator  $P$  describing the evolution of densities in this mixed system operating with both deterministic and perturbed elements is

$$Pf(x) = (1 - \epsilon)P_S f(x) + \epsilon \int_X K(x, y)f(y) dy. \quad (13)$$

It is straightforward to show that (13) is a Markov operator.

Since for fixed  $y$ ,  $K(x, y)$  is a density it clearly satisfies  $K(x, y) \geq 0$  and  $\int_X K(x, y) dx = 1$ . This condition, 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  $\int_E K(x, y) dx \leq \eta$ , for every  $y$  in  $X$  and subset  $E$  of  $X$  with  $\mu_L(E) \leq \delta$ .

## 10.2. Loosely Coupled Systems.

We are now in a position to state our main 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 (13), 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

$$|S(x)| \leq a_0|x| + a_1 \quad (14)$$

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,

$$\int_X |x|K(x, y) dx \leq b_0|y| + b_1. \quad (15)$$



This condition is automatically satisfied if the phase space  $X$  is finite, but if it is unbounded then (15) 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 this following result is equivalent to the 2<sup>nd</sup> order formulation of the Second Law of thermodynamics.

**Theorem 10.1.** *If  $S$  is a nonsingular transformation that satisfies (14) and  $K$  is a uniformly integrable stochastic kernel satisfying (15), then for  $0 < \epsilon \leq 1$  the operator  $P$  given by (13) is smoothing, and thus asymptotically periodic.*

Therefore, for any closed system whose dynamics evolve through the action of a nonsingular transformation  $S$  satisfying (14), placing it in contact with a second system whose effect on the first is a perturbation characterized by a kernel  $K$  satisfying (15) 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 that the conditional entropy  $H(P^t f | f_*)$  is an increasing function with a limiting value given by  $H_{max}(f, f_*)$  as defined in (10).

Under certain circumstances involving loose coupling to a heat bath, there are even stronger results concerning the behaviour of the entropy, corresponding to the 3<sup>rd</sup> order formulation 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  $\xi_t$ . In this case, with the external perturbations independent of the state of the system  $S$ , the perturbations  $\xi_t$  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 Section 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 (13) takes the simple form

$$Pf(x) = (1 - \epsilon)P_S f(x) + \epsilon g(x). \quad (16)$$

There are some surprising consequences of making the loose coupling independent of the state of the system  $S$ . Namely

**Theorem 10.2.** *If  $P$  is the operator defined by (16), then  $\{P^t f\}$  is  $f_*$  exact.*

Thus, by the simple expedient of 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  $S$ !

### 10.3. 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 between a deterministic system and an external source of noise. When  $\epsilon = 1$  and  $X = R^d$ , then equation (13) takes the form

$$Pf(x) = \int_{R^d} K(x, y)f(y) dy. \quad (17)$$

In thinking about the interpretation of (17), consider the following. Take the quantities  $\xi_0, \xi_1, \dots$  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,  $W : R^d \times R^d \rightarrow R$ , 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 (17) describes the evolution of the densities corresponding to  $x_{t+1} = W(x_t, \xi_t)$ . We can make this more formal through the following unpublished theorem initially formulated and proved by A. Lasota, J. Traple, and J. Tyrcha.

**Theorem 10.3.** *Let  $g : R^d \rightarrow R^d$  be a density and  $K : R^d \times R^d \rightarrow R^d$  be a stochastic kernel. Then the (generally nonunique) function  $W : R^d \times R^d \rightarrow R^d$  defined implicitly by  $\int_0^{W(y,z)} K(r, y) dr = \int_0^z g(u) du$  defines a dynamical system  $x_{t+1} = W(x_t, \xi_t)$  where the  $\xi_t$  are independent random variables with density  $g$ . This system has an evolution of densities described by  $f_{t+1} = Pf_t$  where the operator  $P$  is given by  $Pf(x) = \int_{R^d} K(x, y)f(y) dy$ .*

### 10.4. Asymptotic Periodicity and Additive Perturbations.

Often the perturbations are additive,  $W(y, z) = S(y) + z$ , so we have  $x_{t+1} = S(x_t) + \xi_t$ . It is rather surprising that a dynamics of this form may also appear as the consequence of taking a factor or trace<sup>[25,25a]</sup>.

If the sequence  $\{\xi_t\}$  of random variables has a common density  $g$ , then it follows that  $K(x, y) = g(x - S(y))$ , and equation (17) becomes

$$Pf(x) = \int_{R^d} f(y)g(x - S(y)) dy. \quad (18)$$

For the special case of additive noise, (18) can be derived independent of any assumption concerning the nonsingularity of  $S$ . Furthermore, in this case the condition given by equation (15) reduces to  $m = \int_{R^d} |x|g(x) dx < \infty$ . Thus we have an immediate corollary to Theorem 10.1 for systems with added noise<sup>[23]</sup>.

**Corollary 10.4.** *If  $S$  (nonsingular or not) is a transformation operating in the phase space  $R^d$ , satisfies inequality (14), and experiences an additive perturbation whose density has a finite first moment, then the sequence  $\{P^t f\}$ , where  $P$  is the Markov operator defined by equation (18), is asymptotically periodic.*

Hence 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 (9), and *guarantee the approach of the conditional entropy to a maximum* (Theorem 5.3).

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. The surprising content of Theorem 10.1 (and Corollary 10.4) is that even in a transformation that has aperiodic limiting behavior, additive perturbations will result in asymptotic periodicity.

### 10.5. $f_*$ Exactness and Additive Perturbations.

Under certain circumstances there are even stronger results concerning the effects of additive perturbations. Namely, additive perturbations may induce  $f_*$  exactness with a consequent increase in the conditional entropy to its maximal value of zero corresponding to the strongest ( $3^{rd}$  order) form of the Second Law of thermodynamics.

### 10.6. Parametric Perturbations.

As another specific example, consider the case when  $W(y, z) = zS(y)$  and  $S > 0$ , so  $x_{t+1} = \xi_t S(x_t)$ . Using Theorem 10.3, it is straightforward to show that the operator (17) takes the explicit form

$$Pf(x) = \int_{R^d} f(y)g\left(\frac{x}{S(y)}\right) \frac{dy}{S(y)}. \quad (19)$$

Horbachz<sup>[15,16]</sup> has considered the behaviour of this system when  $S : R^+ \rightarrow R^+$ . The flavor of her results are summarized in the following two theorems.

**Theorem 10.5.** *Let the Markov operator  $P$  be defined by (19). Assume that  $g$  is a density,  $0 < S(x) \leq \alpha x + \beta$ , and  $\alpha m < 1$  with  $m = \int_0^\infty xg(x) dx$ , where  $\alpha$  and  $\beta$  are nonnegative constants. Then the sequence  $\{P^t f\}$  is asymptotically periodic.*

We close with a second theorem concerning  $f_*$  exactness induced by multiplicative perturbations.

**Theorem 10.6.** *If the Markov operator  $P$  defined by (19) satisfies the conditions of Theorem 10.5 and, in addition,  $g(x) > 0$  then  $\{P^t f\}$  is  $f_*$  exact.*

Theorems 10.5 and 10.6 illustrate the behaviors that may be induced by multiplicative perturbations in discrete time systems. A number of other results concerning asymptotic periodicity and  $f_*$  exactness induced by multiplicative perturbations may be proved, but rather than giving these the reader is referred to Horbacz<sup>[15,16]</sup>.

### 10.7. Markov Operators and Deterministic Processes.

On several occasions we have emphasized that the interpretation of a given dynamics is not necessarily clear cut. 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<sup>[2]</sup> and Kim<sup>[18]</sup>, but we state this in the spirit of an unpublished result of Lasota.

**Theorem 10.7.** *Let  $P$  be a given Markov operator operating in a finite normalized space  $X = [0, 1)$ . Then there is a sequence of transformations  $S_n : X \rightarrow X$  with Frobenius-Perron operators  $P_{S_n}$  such that  $\lim_{n \rightarrow \infty} \|P_{S_n} f - P f\| = 0$ .*

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.*

### 10.8. Summary.

In this section 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 may be to either induce asymptotic periodicity or  $f_*$  exactness. It is interesting that asymptotic periodicity or  $f_*$  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 5.3). If, on the other hand,  $f_*$  exactness is induced, then the entropy will increase to its absolute maximal value of zero (Theorem 7.3).

## 11. OPEN CONTINUOUS TIME SYSTEMS.

Given the results for discrete time dynamics, it is natural to wonder if the perturbation of systems with continuous time dynamics (that is, placing them in contact with a heat bath) will yield analogous results concerning the entropy. The effects of perturbation on the entropy of systems with dynamics described by sets of ordinary differential equations is briefly considered in this section.

### 11.1. Stochastic Differential Equations.

Often, the dynamics of physical processes are formulated by a system of ordinary differential equations  $dx_i/dt = F_i(x)$ ,  $i = 1, \dots, d$  operating in some region of  $R^d$  with initial conditions  $x_i(0) = x_{i,0}$ . Here we examine the behaviour of the stochastically perturbed analog

$$\frac{dx_i}{dt} = F_i(x) + \sum_{j=1}^d \sigma_{ij}(x)\xi_j, \quad i = 1, \dots, d \quad (20)$$

with the same initial conditions, where  $\sigma_{ij}(x)$  is the amplitude of the stochastic perturbation and  $\xi_j = dw_j/dt$  is a “white noise” term that is the derivative of a Wiener process. [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  $t$ ,  $0 \leq s \leq t$  the random variable  $w(t) - w(s)$  has the Gaussian density  $g(t-s, x) = [2\pi(t-s)]^{-1/2} \exp[-x^2/2(t-s)]$ . In a completely natural manner this definition can be extended to say that the  $d$ -dimensional vector  $w(t) = \{w_1(t), \dots, w_d(t)\}_{t>0}$  is a **d-dimensional Wiener process** if its components are one dimensional Wiener processes.]

Equation (20) 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, then (20) has a unique solution<sup>[12]</sup>.

### 11.2. The Fokker Planck Equation.

The density function  $f(t, x)$  of the process  $x(t)$  generated as the solution to the stochastic differential equation (20) is defined by  $\text{prob}(x(t) \in B) = \int_B f(t, s) ds$ . To guarantee the existence and differentiability of  $f(t, x)$ , we will assume the **uniform parabolicity condition**:  $\sum_{i,j=1}^d a_{ij}(x)\lambda_i\lambda_j \geq \rho \sum_{i=1}^d \lambda_i^2$  where  $\rho > 0$ . If the  $a_{ij}(x)$  satisfy the uniform parabolicity condition and if they and the  $F_i(x)$  are continuous and  $C^3$ , then  $f(t, x)$  exists and is differentiable.

Under the assumption that  $\sigma_{ij}$  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, the evolution equation for the density  $f(t, x)$  is given by

$$\frac{\partial f}{\partial t} = - \sum_{i=1}^d \frac{\partial [F_i(x)f]}{\partial x_i} + \frac{1}{2} \sum_{i,j=1}^d \frac{\partial^2 [a_{ij}(x)f]}{\partial x_i \partial x_j} \quad (21)$$

in the Ito interpretation of (20). This evolution equation is known as the **Fokker-Planck equation**. In the absence of the diffusion term ( $a_{ij} \equiv 0$ ) it reduces to the **generalized Liouville equation**.

If the stochastic differential equation (20) has an initial condition  $x(0)$  and an associated initial density  $f_0$ , then the solution  $f(t, x)$  of the Fokker-Planck equation satisfies  $f(0, x) = f_0(x)$ . Further, if the solution of the Fokker-Planck equation can be written in the form  $f(t, x) = \int_{R^d} \Gamma(t, x, s) f_0(s) ds$ , where the kernel  $\Gamma$  is independent of the initial density  $f(0, x) = f_0(x)$  and  $\lim_{t \rightarrow 0} f(t, x) = f(0, x) = f_0(x)$ , 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.

From the expression for the generalized solution, a family  $\{P^t\}_{t \geq 0}$  of integral operators can be defined by  $P^0 f_0(x) = f_0(x)$ ,  $P^t f_0(x) = \int_{R^d} \Gamma(t, x, s) f_0(s) ds$ , where  $f(0, x) = f_0(x)$ . If the generalized solution is unique, then the operator  $P$  is a Markov operator. It is a rather simple demonstration that the unique stationary density  $f_*$  defined by  $\lim_{t \rightarrow \infty} P^t f(x) = f_*(x)$  is given by the (unique) solution of the elliptic equation  $-\sum_{i=1}^d \partial[F_i(x)f]/\partial x_i + \frac{1}{2} \sum_{i,j=1}^d \partial^2[a_{ij}(x)f]/\partial x_i \partial x_j = 0$

For the continuous time closed system without noise, the evolution of the Frobenius-Perron operator  $P^t$  is determined by the the generalized Liouville equation. When the very same 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 (20) which is just the same as the generalized Liouville equation with the addition of the diffusion term.

### 11.3. The Behaviour of Entropy.

A closed continuous time system with dynamics described by ordinary differential equations (reversible) has an entropy that is absolutely constant and equal to the entropy of the initial density with which the system was prepared (Theorem 3.2).

We now examine the effects of perturbations on the entropy of these continuous time reversible systems. For one dimensional systems ( $d = 1$ ), Rudnicki<sup>[31]</sup> (1991) has recently proved a very interesting necessary and sufficient condition for the  $f_*$  exactness, and consequent existence of  $2^{nd}$  Law behaviour in its strongest form. We extend his result to the behaviour of the conditional entropy.

**Theorem 11.3.** *Assume that  $d = 1$  and (21) has a unique generalized solution. Then the Markov operator  $P^t$  whose evolution is governed by equation (21) is  $f_*$  exact and the corresponding conditional entropy  $H_c(P^t f|f_*)$  approaches its maximal value of zero as  $t \rightarrow \infty$  if and only if  $\int_{-\infty}^{+\infty} \exp\left[-\int^x \frac{2F(z)}{\sigma^2(z)} dz\right] dx = \infty$ .*

### 11.4. Phase Transitions and Perturbations.

A variety of studies<sup>[17]</sup> have shown that in systems of differential equations that display a Hopf bifurcation as a parameter is varied, when noise is added as in (20) the stationary density of the Fokker Planck equation has behavior like that encountered in phase transitions. Though general results are not available at this time, it appears that if, in the absence of noise the system has a supercritical Hopf bifurcation, then when noise is added the stationary density has behaviour like that seen in  $2^{nd}$  order phase transitions. Alternately, if the unperturbed system has a subcritical Hopf bifurcation then the density of the perturbed system has  $1^{st}$  order phase transition like behaviour<sup>[26]</sup>.

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