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Reversible Dynamics and the Macroscopic Rate Law for a Solvable Kolmogorov System: The Three Bakers' Reaction

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We investigate a piecewise linear (area-preserving) map T describing two coupled baker transformations on two squares, with coupling parameter $0 \leqslant c \leqslant 1$. The resulting dynamical system is Kolmogorov for any $c \neq 0$. For rational values of c, we construct a generating partition on which T induces a Markov chain. This Markov structure is used to discuss the decay of correlation functions: exponential decay is found for a class of functions related to the partition. Explicit results are given for $c = 2^{-n}$. The macroscopic analog of our model is a leaking process between two (badly) stirred containers: according to the Markov analysis, the corresponding progress variable decays exponentially, but the rate coefficients characterizing this decay are not those determined from the one-way flux across the cell boundary. The validity of the macroscopic rate law is discussed.

KEY WORDS: Kolmogorov system; Markov chain; rate laws; correlation function decay; relaxation process.

1. INTRODUCTION

The modern theory of dynamical systems is concerned with the attempt to understand the global behavior of systems with a known local structure.[1-4] One of the most fundamental problems in this respect, namely, the connection between macroscopic irreversible behavior and microscopic reversible evolution laws, is at the center of ergodic theory.

Traditionally irreversible phenomena are described at a finer level by stochastic processes such as random walks in some configuration space.

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The main problem then becomes the relation of these random walks to the underlying deterministic, reversible evolution in phase space: such a connection can be explicitly established for certain classes of system. The most striking results along these lines have been obtained for Bernoulli systems: an appropriate definition of "configuration space" as a partition of phase space maps the deterministic motion onto a sequence of independent states visited by the system.[5,6], Although Bernoulli systems are quite exceptional, similar results may be obtained for Kolmogorov (K) systems, which are characterized by a strong instability of phase point trajectories.[4]

A number of models have been constructed with the aim of analyzing the main features of simple relaxation processes. Some of the more physical models are billiards[2,7] and the Lorentz and Rayleigh gases,[2,8] while the more abstract ones are one- or two-dimensional maps.[3,9] Discrete-time mappings (cascades) may prove a much more flexible tool for investigating this field than gas models; in fact, the analysis of continuous-time dynamical systems is often carried out in terms of such maps constructed from the Poincaré section of the flow.

In this paper we propose a model, discrete-time dynamical system with one arbitrary parameter, c, characterizing the coupling between two strongly mixing systems. The resulting composite system is still sufficiently simple to admit a detailed dynamical and ergodic analysis. More specifically, our model consists of two phase space cells: within the cells phase points evolve by baker transformations[1,6] and may pass from one cell to the other through the action of a third overlapping baker transformation. This triple baker model exhibits many of the features of more complex coupled dynamical systems, in particular those related to the resulting structure of the macroscopic law. Continuous-time models of coupled systems intended for similar uses have been discussed recently by other authors.[10,11]

In Section 2 we describe our model and briefly suggest a phenomenological analog in terms of a simple relaxation process of the diffusion or reaction type. The dynamical analysis in Section 3 investigates the ergodic properties of the model and its underlying mathematical structure.

For rational values of the coupling parameter c, we construct in Section 4 a partition of the phase space on which the triple baker transformation induces a Markov chain with a doubly stochastic transition matrix. We discuss the equivalence between the deterministic system and the stochastic process in terms of symbolic dynamics and its implications for the decay of correlation functions. Section 5 is devoted to special cases: for $c = 1/2$, another partition is found to generate an isomorphic Bernoulli stochastic process; for the case $c = 2^{-k}$, the Markov process associated

with the triple baker model is further analyzed with the focus on the decay constants characterizing the Markov process.

The classical macroscopic analysis of our model is presented in Section 6. The chemical analogy is developed in more detail by associating phase points in the individual cells with distinct chemical species; the triple baker model crudely mimics some features of the dynamics of isomerization kinetics. The rate law for the progress variable $\xi(t)$ of the chemical reaction is derived exactly from the dynamical evolution laws by projection operator techniques. As a consequence of the (metric) Markov structure for rational c the characteristics of the memory kernel appearing in this generalized rate law may be described in detail.

The triple baker model is a very simple coupled dynamical system: it can only be regarded as a prototype of the more complex physical systems it is intended to model. Nonetheless, it displays a rich dynamical structure and our exact results permit a discussion of the validity of the macroscopic rate law and a study of the microscopic structure of the rate coefficients appearing in this law.

2. TRIPLE BAKER MODEL

The triple baker model possesses a phase space Ω composed of two cells A and B; the time evolution of phase points within Ω for each discrete time step is accomplished through the successive action of three baker transformations: two baker transformations acting solely in the A and B cells followed by a third baker transformation acting on a rectangle overlapping the cells (Fig. 1). This third transformation couples the dynamics of the individual cells and allows phase points to "leak" from one cell to the other. The description and characterization of this leaking process are some of the main objectives of this study.

The model may be defined mathematically as follows. Let I and J be semiclosed intervals $I=[0, 1[$ and $J=[-1, 1[$. The triple baker model is the discrete-time dynamical system $(\Omega, \mathscr{B}_\Omega, \mu, T)$ where the phase space $\Omega = I \times J$ is endowed with the Lebesgue measure $d\mu = \frac{1}{2}dx\,dy = d\mu_x\,d\mu_y$ and the Borel σ-algebra of measurable sets $\mathscr{B}_\Omega$. The automorphism T is a sequence of three baker transformations defined on the rectangles $A = I \times I$, $B = I \times I'$ and $C = I \times H$, where $I' = [-1, 0[$ and $H = [-c, c[$:

$$T = B_C B_B B_A \tag{2.1}$$

Letting $\omega = (x, y)$ denote a phase point of Ω we have

$$B_A\omega = \begin{cases} (2x, y/2), & 0 \leqslant x < 1/2 \\ (2x-1, (y+1)/2), & 1/2 \leqslant x < 1 \end{cases} \tag{2.2}$$

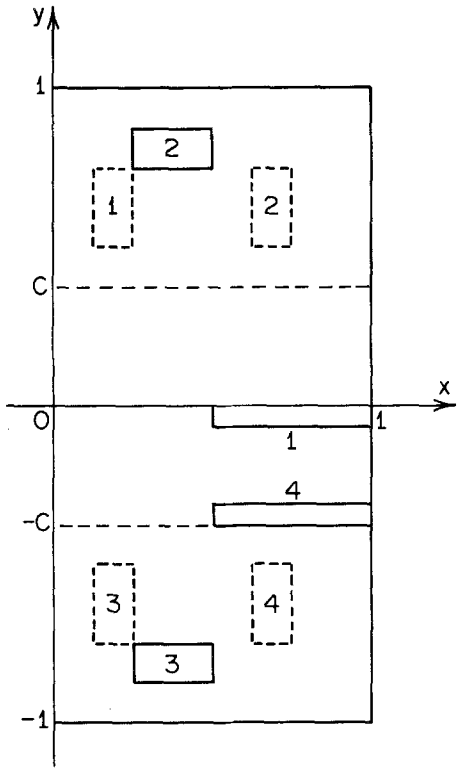

Fig. 1. Diagram of the phase space for the triple baker model showing the upper-A and lower-B cells. The overlapping baker transformation acts on the rectangle between c and $-c$. The figure also shows how four rectangles (labeled 1 to 4 and indicated by dashed borders) evolve under one application of T to produce the rectangles with solid borders.

if $\omega \in A$ and $B_A\omega = \omega$ if $\omega \in B$;

$$B_B\omega = \begin{cases} (2x, (y-1)/2), & 0 \leqslant x < 1/2 \\ (2x-1, y/2), & 1/2 \leqslant x < 1 \end{cases} \tag{2.3}$$

if $\omega \in B$ and $B_B\omega = \omega$ if $\omega \in A$;

$$B_C\omega = \begin{cases} (2x, (y-c)/2), & 0 \leqslant x < 1/2 \\ (2x-1, (y+c)/2), & 1/2 \leqslant x < 1 \end{cases} \tag{2.4}$$

if $\omega \in C$ and $B_C\omega = \omega$ if $\omega \in \Omega \backslash C$.

Thus, the baker transformations B_A and B_B act on the disjoint cells A and B while B_C effects a coupling between them.

The evolution of functions $f(\omega)$ (square integrable with respect to μ) defined on Ω is determined by the unitary operator U induced by T:

$$Uf(\omega) = f(T\omega) \tag{2.5}$$

while the evolution of distribution functions $\rho(\omega)$ on Ω is given by

$$\rho_t(\omega) = U^{*t} \qquad \rho_0(\omega) = \rho_0(T^{-t}\omega) \tag{2.6}$$

This simple dynamical system mimics many features of the more complex, deterministic systems composed of coupled phase space regions mentioned in the Introduction. When c is small, the two cells are weakly coupled and one expects that the long-time decay of this system will be governed by the slow leaking process. In this context B_A and B_B may be considered as a (rough) stirring or a diffusion within the cells while one could call B_C a "reaction" converting A-type phase points to B-type phase points. This in turn suggests that a phenomenological description in terms of a classical rate law may be applicable in some circumstances. Let $N_\alpha(t)$ be the "number of phase points" in $\alpha = A, B$ at time t. The discrete-time chemical rate law then reads

$$N_A(t+1) = (1-k_f)\, N_A(t) + k_r N_B(t) \tag{2.7}$$

with a similar expression for $N_B(t+1)$. The model's symmetry dictates that $k_f = k_r$. Since $N_A + N_B = \text{const}$ we may alternatively write the rate law in terms of the progress variable $\xi(t) = \delta N_A(t) = -\delta N_B(t)$, where $\delta N_\alpha(t) = N_\alpha(t) - N_\alpha^{eq}$ with N_α^{eq} the number of phase points in α at equilibrium:

$$\xi(t) = (1-\tau_c^{-1})\, \xi(t-1) = (1-\tau_c^{-1})^t \xi(0) \tag{2.8}$$

The relaxation time τ_c is defined in terms of the rate constants as $\tau_c^{-1} = k = k_f + k_r$. Since $N_A^{eq} = N_B^{eq}$ it also follows that $\xi(t) = [N_A(t) - N_B(t)]/2$.

We may now ask the following questions: For the dynamical system (Ω, μ, T), under what circumstances does the phenomenological rate law (2.7) or (2.8) apply, and what is the microscopic structure of the rate coefficients characterizing the decay of the system to equilibrium? We return to these questions in Section 6 after characterizing the system and presenting exact solutions for rational values of c.

3. DYNAMICAL ANALYSIS

Like the baker transformations $B_\alpha (\alpha \in \{A, B, C\})$, the triple baker T is piecewise affine and linearizes to

$$\begin{pmatrix} \delta x_{n+1} \\ \delta y_{n+1} \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 1/2 \end{pmatrix}^m \begin{pmatrix} \delta x_n \\ \delta y_n \end{pmatrix} \tag{3.1}$$

with $m = 1$ if $B_A B_B \omega_n \notin C$ and $m = 2$ if $B_A B_B \omega_n \in C$. Thus, T is expanding along the x axis and contracting along the y axis. The stable W_s (unstable W_u) manifolds of a point $\omega = (x, y)$ are composed of vertical (horizontal) lines in Ω; the discontinuities prevent W_s and W_u from extending across the whole phase space. The Lebesgue measure μ is invariant for T (as for each B_α); we show below that μ is ergodic for T on Ω. This result allows direct computation of many time-averaged quantities. For instance, the Liapunov exponents are

$$\lambda_+ = -\lambda_- = \lim_{n \to \infty} \frac{1}{n} \ln \frac{\delta x_n}{\delta x_0} = (1 + c) \ln 2 \tag{3.2}$$

for almost all $x \in \Omega$.

The ergodic properties of the model are conveniently proved by first considering a one-dimensional map related to the inverse map. Indeed, the y component of $T^{-1}(x, y)$ is independent of x, while the x component depends on y:

$$T^{-1}(x, y) = [(x + k)/m, \tau(y)] \tag{3.3}$$

Here $\tau(y)$ is the one-dimensional map on J sketched in Fig. 2 while $m = \tau'(y) \in \{2, 4\}$ and k takes integer values from 0 to 3 depending on y. This construction shows the *skew-product* form of (Ω, T^{-1}) with base (J, τ). It is also easily seen that, as T is dilating by a factor of 2 (at least) in the x direction (Ω, T^{-1}) is isomorphic to the natural extension[4] of (J, τ).

We first discuss the case $c \leqslant 1/2$. Consider the monotonic function $\theta: [0, 4[\to [0, 1[$ such that $\tau(2u - 1) = 2\theta^{-1}(u) - 1 \pmod 2$ for any $u \in [0, 1[$, and its unique, continuous, monotonic extension $\bar{\theta}: [0, 4] \to [0, 1]$. Since $\theta(u_2) - \theta(u_1) < u_2 - u_1$ for any $0 \leqslant u_1 < u_2 \leqslant 4$, a classical result of ergodic theory[12] implies that θ defines a *valid f expansion*. Then the partition $\{\Delta_i^{(1)}\}$, $0 \leqslant i \leqslant 3$, of J determined by the points $\{-1, -1/2, 0, 1/2, 1\}$ (i.e., by the continuous pieces of τ) generates the Borel σ algebra $\mathscr{B}_J$ through successive refinements by τ. Letting $\Delta^{(0)} = J$

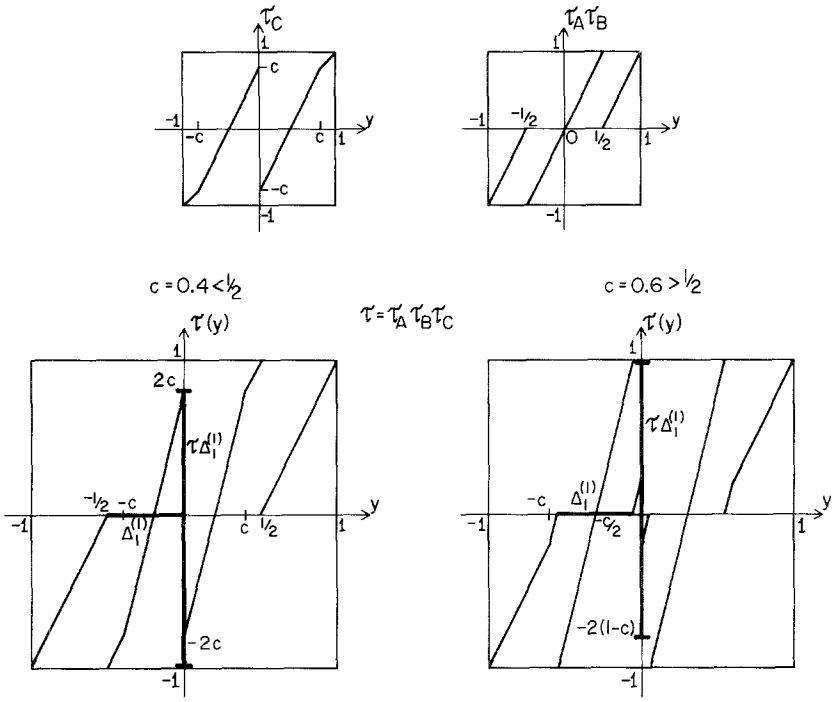

Fig. 2. Sketch of the one-dimensional map $\tau(y)$ versus y used in the construction of the skew-product form for (Ω, μ, T). The upper two panels show τ_C and $\tau_A\tau_B$ used to construct $\tau = \tau_A\tau_B\tau_C$, while the lower panels show τ for $c = 0.4$ ($< 1/2$) (left) and $c = 0.6$ ($> 1/2$) (right). Also shown is the evolution of the partition element $\Delta_1^{(1)}$ under τ.

and $\Delta_{\mathbf{i}}^{(n)} = \bigcap_{k=1}^{n} \tau^{1-k}\Delta_{i_k}^{(1)}$ for any sequence $\mathbf{i} = (i_1, \ldots, i_n)$, $0 \leqslant i_k \leqslant 3$, one sees that for any $n \geqslant 1$ and $\mathbf{i}$

$$\begin{aligned} &\text{(i)} \quad \{\Delta_{\mathbf{i}}^{(n)}\} \text{ is a partition of } J \\ &\text{(ii)} \quad \tau\Delta_{i_1\cdots i_n}^{(n)} \subset \Delta_{i_2\cdots i_n}^{(n-1)} \\ &\text{(iii)} \quad \mu_y(\Delta_{i_1\cdots i_n}^{(n)}) < \tfrac{1}{2}\mu_y(\Delta_{i_2\cdots i_n}^{(n-1)}) \\ &\text{(iv)} \quad \Delta_{\mathbf{i}}^{(n)} \text{ is an interval (maybe empty)} \end{aligned} \tag{3.4}$$

Moreover, for any $c > 0$, the endomorphism τ of J is *exact*,[4] viz. there is no measurable subset $V \subset J$, $0 < \mu_y(V) < 1$, such that for any $m > 0$ there is a measurable set W_m satisfying $V = \tau^{-m}W_m$. For this, it suffices to show that $\forall W \subset J$ with $\mu_y(W) > 0$, $\exists m \geqslant 0$ with $\mu_y(\tau^m W) = 1$; as the intervals $\Delta_{\mathbf{i}}^{(n)}$ generate a basis of $\mathscr{B}_J$ for $n \to \infty$, we only need to prove it for $W \supset \Delta_{\mathbf{i}}^{(n)}$ (mod 0) for some $n > 0$ and $\mathbf{i}$. Now, if $W = \Delta_1^{(1)}$, then $\tau W = [-1, 2c[$ and $\tau^m W = [-1, 2^m c[\cap J$: take $m \geqslant |\log 2c|$; if $W = \Delta_0^{(1)}$, then $\tau W \supset \Delta_1^{(1)}$. The

cases $\Delta_2^{(1)}$ and $\Delta_3^{(1)}$ are symmetrical. If $W \supset \Delta_i^{(n)}$ with $\mu_y(\Delta_i^{(n)}) > 0$ taking $m \geqslant n + 1 + |\log 2c|$ is also sufficient by (iii) in (3.4).

When $c > 1/2$, similar arguments hold starting from the monotonic function θ: $[0, 6[\to [0, 1[$ such that $\tau(2u-1) = 2\theta^{-1}(u) - 1 \pmod 2$ for $0 \leqslant u < 1$, and using the generating partition determined by the points $\{-1, -(1+2c)/4, (1-2c)/4, 0, (2c-1)/4, (1+2c)/4, 1\}$. Properties (3.4) also hold in this case.

It is well known [4] that an exact endomorphism is ergodic and that its natural extension is a K system; the entropy of any generating partition is equal to the Kolmogorov entropy of the system. This entropy is directly given by a theorem on f expansions:

$$h_K(T) = h_K(\tau) = \int_J \ln \frac{d\tau}{dy}\, dy = (1+c) \ln 2 \tag{3.5}$$

The triple baker model is thus a K system, a property that signals strongly random behavior of nearby trajectories.

4. THE EQUIVALENT MARKOV SHIFT

The above dynamical analysis established certain general properties of the model, which hold for any value of c. In the sequel we focus on the case of rational c and use the fact that for such c values this system is isomorphic to a Markov shift. This isomorphism allows one to easily establish the properties of the functions of interest here and has implications for the existence of a phenomenological rate law. We construct this isomorphism below and discuss some of its features.

4.1. The Markovian Partition $\mathcal{Q}$

A Markov shift isomorphic to the triple baker system (Ω, μ, T) for $c = p/q (p, q \in \mathbb{N}_0)$ can be constructed from the partition of Ω into $2q$ horizontal bands:

$$\mathcal{Q} = \{Q_{.k} = I \times [(k-1)/q, k/q[\mid 1 - q \leqslant k \leqslant q\} \tag{4.1}$$

Without loss of generality, q may be taken to be even. The iterates of this partition are defined as

$$T\mathcal{Q} = \{Q_{.-k}\}, \qquad T^2\mathcal{Q} = \{Q_{.--k}\}, \cdots \tag{4.2}$$

with $Q_{.-k} = TQ_{.k}$, $Q_{.--k} = T^2 Q_{.k}$. The corresponding products are $Q_{.kl} = Q_{.k} \cap TQ_{.l}$ and

$$\mathcal{Q}_n^m = \bigvee_{t=n}^{m} T^t \mathcal{Q} = \left\{ \bigcap_{t=n}^{m} T^t Q_{.k} \mid 1-q \leqslant k \leqslant q \right\} \tag{4.3}$$

We write $p_k = \mu(Q_{.k})$ and $p_{kl} = \mu(Q_{.kl})$. Since some $Q_{.kh}$ may have null measure, we remove the corresponding atoms from $\mathcal{Q}_n^m$.

The invariant measure μ is Markovian for the partition $\mathcal{Q}$: the image of any band is a family of horizontal strips; since baker transformations cut the bands vertically before stretching them, the later evolution of a strip $Q_{.kh}$ is determined by the fragmentation of $Q_{.k}$ in more strips (Fig. 3) regardless of h. It is now obvious that, for any product like $Q_{.jkhm}$,

$$\mu(Q_{.jkhm}) = p_{jk} p_k^{-1} p_{kh} p_h^{-1} p_{hm} \tag{4.4}$$

which is just the Markov property with the transition probabilities

$$m_{jk} = P(T\omega \in Q_{.k} \mid \omega \in Q_{.j}) = 2qp_{kj} \tag{4.5}$$

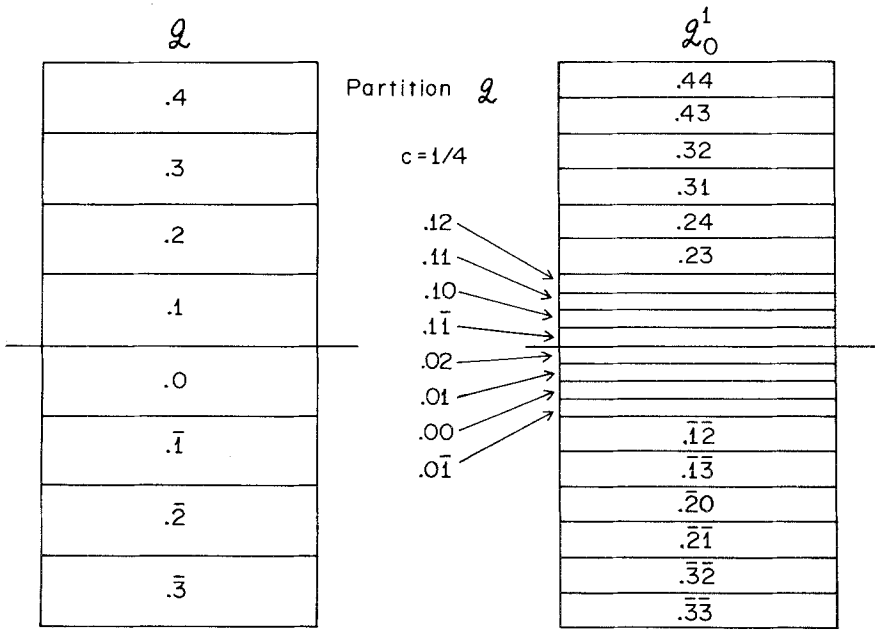

Fig. 3. The Markovian partition $\mathcal{Q}$ for $c = 1/4$. In this figure we have used an overbar for partition elements with negative labels. The intersection set is shown in the right panel of the figure.

So far all of our statements apply to B_A, B_B, and B_C equally, and the Markov matrix for T can be written as $\mathcal{M} = \mathcal{M}_C \mathcal{M}_B \mathcal{M}_A$. Since the elements of a matrix $\mathcal{M}_\alpha$ are simply 1, 0, or 1/2, the elements of $\mathcal{M}$ are 0, 1/2, or 1/4. For instance, we have for $c = 1/4$:

$$\mathcal{M} = \begin{pmatrix} 1/2 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 1/4 & 1/4 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 1/4 & 1/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 1/4 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 1/4 & 1/4 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 0 & 0 & 0 & 1/2 & 0 & 1/2 \end{pmatrix} \tag{4.6}$$

As all the atoms of $\mathcal{Q}$ have the same measure, the transition matrix $\mathcal{M}$ is doubly stochastic.[13] Now, since T is bijective in Ω the time-reversed process on the partitions $T^t\mathcal{Q}$ is another Markov chain, with transition probabilities given by the transpose of $\mathcal{M}$, $\mathcal{M}^T$.

4.2. $\mathcal{Q}$ Is Generating

Since all bands $Q_{\cdot k}$ are fragmented by T in at least two strips of maximal height $1/4q$, each action of T on $Q_{\cdot k}$ reduces the height of the bands by a factor of two (at least). Therefore $\mathcal{Q}_0^n$ contains bands of heights $\delta y_n \leqslant 1/q2^{n+1}$. Similarly T^{-1} fragments the bands vertically with same factor so that $\mathcal{Q}_{-n}^0$ contains rectangles of width $\delta x_n \leqslant 2^{-n}$. Thus, $\mathcal{Q}_{-n}^0$ generates a partition of Q in rectangles of arbitrary smallness: as $n \to \infty$, it generates the Borel algebra on Ω.

Since $\mathcal{Q}$ is a generating, Markovian partition for the K system $(\Omega, \mathcal{B}_\Omega, \mu, T)$, the transition matrix $\mathcal{M}$ is *irreducible* and *aperiodic* (thus mixing). The matrix elements also determine its entropy:

$$h_k = -\sum_{k,j} p_{jk} \ln m_{jk} = (1 + c) \ln 2 \tag{4.7}$$

Because the partition $\mathcal{Q}$ is Markov with matrix $\mathcal{M}$, its powers $\mathcal{Q}_0^{n-1}$ are Markov with an expanded matrix $\mathcal{M}^{(n)}$ whose elements, eigenvalues and eigenvectors are simply related to those of $\mathcal{M}$. For instance, if $n = 2$:

$$m_{ij,kh}^{(2)} = P(T\omega \in Q_{\cdot hk} \mid \omega \in Q_{\cdot ji}) = \delta_{jk} m_{kh} \tag{4.8}$$

In general the expanded matrix $\mathcal{M}^{(n)}$ will have the same eigenvalues as $\mathcal{M}$ and a highly degenerate and defective zero eigenvalue. The backward

process generates another hierarchy $\mathscr{M}^{T(n)}$ for $\mathscr{Q}_{1-n}^{0}$; $\mathscr{M}^{T(n)}$ has the same eigenvalues and similar characteristic spaces to that of $\mathscr{M}^{(n)}$. These expanded matrices are not doubly stochastic.

4.3. Symbolic Dynamics

For any partition $\mathscr{Q}$ it is possible to introduce a symbolic representation of the dynamics in which the action of T amounts to a shift on a set of symbols. The alphabet Σ corresponds to the labels of the elements of partition $\mathscr{Q}$: $\Sigma = \{k \mid 1-q \leqslant k \leqslant q\}$. Any phase point ω is represented by its *symbolic name* (kneading sequence) [3] in Σ: if the decimal dot is used to mark the initial time, the point $\omega = (\cdots k_{-1} \cdot k_0 k_1 \cdots)$ is in the atom $Q_{.k_t}$ at time $-t$. The evolution operator is then a *shift* on the space of sequences $\Sigma^{\mathbf{Z}}$ isomorphic to $\mathscr{Q}_{-\infty}^{\infty}$, which may be described a doubly infinite matrix composed of Kronecker symbols describing transitions between points:

$$m^{(-\infty,\infty)}(\omega_0, \omega_1) = \delta(\omega_1 - T\omega_0) \tag{4.9}$$

For the generating partition $\mathscr{Q}$, distinct phase points have distinct symbolic names, though some names may be meaningless. The Markov property of $\mathscr{Q}$, that only (and all) sequences (k_t) with valid transitions $(m_{k_{t-1},k} \neq 0)$ are meaningful; the ergodic invariant measure μ on Ω is represented in $\Sigma^{\mathbf{Z}}$ by the Markov measure with transition probabilities m_{ij}.

The refinements $\mathscr{Q}_{-k}^{\infty}$ and $\mathscr{Q}_{-\infty}^{k}$ deserve special attention. When $\mathscr{Q}$ is generating, they form *imprimitivity families*,[14] which are the "largest" extension of our Markov chain, and correspond to describing a point by the right (or left) part of its name indicating all its past (or future) locations. The evolution operator is a Markov shift on one-sided sequences $\Sigma^{\mathbf{N}}$; for $\mathscr{Q}_0^{\infty}$ the transition matrix $\mathscr{M}^{+}$ has the form

$$m^{+}(.h, .k) = m_{h_0 k_0} \prod_{t=0}^{\infty} \delta(k_{t+1} - h_t) \tag{4.10}$$

Conversely, T^{-1} corresponds to moving the decimal dot to the right and induces a deterministic evolution on $\mathscr{Q}_0^{\infty}$ described by the same Kronecker products. Such one-sided Markov chains are singular (since their atoms have zero measure) and have been proposed as the basis of a microscopic theory of irreversibility [15].

4.4. Decay of Correlation Functions

The Markov representation $(\mathscr{Q}, \mathscr{M})$ of the system also allows one to discuss the decay of correlation functions

$$\langle f(\omega)\, U^t g(\omega)\rangle = \int_\Omega f(\omega)\, g(T^t\omega)\, d\mu(\omega)$$

$$= \langle g(\omega)\, U^{-t} f(\omega)\rangle \tag{4.11}$$

for integrable functions $g(\omega)$ and $f(\omega)$ defined on Ω.

If g and f are constant over the atoms of $\mathcal{Q}$ (i.e., step functions with respect to $\mathcal{Q}$), one may decompose them in terms of the characteristic functions $\{\chi_{.k}\}$ of $\{Q_{.k}\}$ as

$$f(\omega) = \sum_k a_k \chi_{.k}, \qquad g(\omega) = \sum_k b_k p_k^{-1} \chi_{.k} \tag{4.12}$$

and obtain

$$\langle gU^{-t} f\rangle = \sum_{h,k} a_k b_h (\mathcal{M}^t)_{hk} = \sum_i \tilde{g}_i s_i^t \tilde{f}_i \tag{4.13}$$

where the s_is are the eigenvalues of $\mathcal{M}$ and $\hat{f}_i$ and $\tilde{g}_i$ are the coefficients of the decomposition of f and g in the corresponding (right and left) eigenvectors. These simple correlation functions exhibit exponential decay toward the asymptotic value $(s=1)\langle f\rangle\langle g\rangle$.

Similarly, if f and g are constant over the atoms of $\mathcal{Q}_r^{r+n}$, they can be expressed in the corresponding expanded characteristic bases, so that

$$\langle gU^{-t} f\rangle = \sum_i \tilde{g}_i s_i^t \tilde{f}_i + \mathsf{M}_r^{r+n}(f, g; t) \tag{4.14}$$

where the second term vanishes for $t > n$.

However, this argument does not imply that all correlation functions between square-integrable functions (approximated by such expressions) decay asymptotically as a sum of exponentials fixed by the spectrum of $\mathcal{M}$ (see the comment on "ghost" eigenvalues in Section 5).

5. SPECIAL RESULTS

5.1. The Case $c = 1/2$

When $c = 1/2$ some further results can be established. In particular, we construct an independent finite partition $\mathcal{R}$ and directly compute the time evolution of a cell characteristic function in terms of this partition. Since the partition is also generating we show explicitly the isomorphism of (Ω, T) to a Bernoulli shift.

Consider the partition $\mathscr{R} = \{R_0, R_1, R_2\}$, whose atoms are $R_0 = I \times [-1/2, 0[$ and $R_1 = I \times [0, 1/2[$ with measures $p_0 = p_1 = 1/4$, and $R_2 = I \times [-1, -1/2[\cup I \times [1/2, 1[$ with $p_2 = 1/2$.

We first show that $\mathscr{R}$ is independent for T, i.e.,

$$\mu\left(\bigcap_{t \in I} T^t R_{k_t}\right) = \prod_{t \in I} \mu(R_k) \tag{5.1}$$

with any finite $I \subset \mathbb{Z}$ and any $(k_t) \in \{0, 1, 2\}^I$. A sketch makes it clear that $T^n \mathscr{R} (n \geqslant 0)$ is composed of horizontal bands while $T^{-1}\mathscr{R}$ is composed of vertical bands: (5.1) follows immediately.

Next we introduce a symbolic representation for the partition sets, which facilitates the calculation. Let

$$R_{.k_0 k_1 \cdots k_n} = R_{k_0} \cap T R_{k_1} \cap \cdots \cap T^n R_{k_n}, \qquad k_i \in \{0, 1, 2\} \tag{5.2}$$

As in Section 4.3, the notation can be made compact by writing $\mathbf{k} = k_0 k_1 \cdots k_n$. The A and B cells have the simple representation

$$A = \bigcup_{m=0}^{\infty} R_{.2^m 1} \qquad \text{and} \qquad B = \bigcup_{m=0}^{\infty} R_{.2^m 0} \tag{5.3}$$

where 2^m symbolizes m successive indices 2. Since the Markov partition for $c = 1/2$ is $\mathscr{Q} = \{A \cap R_{.2}, R_{.1}, R_{.0}, B \cap R_{.2}\}$ and since A and B are generated by $\mathscr{R}_0^\infty$, $\mathscr{Q}$ is obtained as a coarse graining of $\mathscr{R}_0^\infty$. Therefore $\mathscr{R}_{-\infty}^{\infty} = \mathscr{Q}_{-\infty}^{\infty} = \mathscr{B}_\Omega$. $\mathscr{R}$ is independent and generating: it is thus *Bernoulli*.[4] The transition probabilities for $\mathscr{R}$ are simply its atoms' measures $\{p_i\}$. As $\mathscr{R}$ is a coarse graining of $\mathscr{Q}$, the kneading sequences of any phase point ω for $\mathscr{Q}$ and $\mathscr{R}$ can be related.

In general any measurable function $f(\omega)$ can be decomposed as

$$f(\omega) = \lim_{n \to \infty} \sum_{k_{-n}=0}^{2} \cdots \sum_{k_n=0}^{2} F_{\mathbf{k}} \chi_{\mathbf{k}}(\omega) \tag{5.4}$$

where $\chi_{\mathbf{k}}$ is the characteristic function of $R_{\mathbf{k}}$ for $k_i \in \{0, 1, 2\}$, $-n \leqslant i \leqslant n$ and $F_{\mathbf{k}}$ is the cell average

$$F_{\mathbf{k}} = \mu(R_{\mathbf{k}})^{-1} \int_{R_{\mathbf{k}}} f(\omega)\, d\mu(\omega) \tag{5.5}$$

In view of (5.3) the characteristic function of cell A may be expressed as

$$\chi_A = \sum_{m=0}^{\infty} \chi_{.2^m 1} = \sum_{\mathbf{k}}{}' \chi_{.\mathbf{k}} \tag{5.6}$$

where the prime on the summation signifies that only (right-infinite) sequences $\mathbf{k}$ beginning with $.2^m1$ are admissible.

It is now straightforward to compute the evolution of the autocorrelation function of $\chi_A(\omega)$,

$$S_A(t) = \int_\Omega \chi_A(\omega)\, \chi_A(T^t\omega)\, d\mu(\omega)$$

$$= \sum_{\mathbf{k}}' \sum_{\mathbf{h}}' \int_\Omega \chi(Q_{.\mathbf{h}} \cap T^t Q_{.\mathbf{k}})\, d\mu \tag{5.7}$$

Since the partition $\mathscr{R}$ is independent, the integrals are readily computed and

$$S_A(t) = 1/2 \sum_{\mathbf{l}}' \mu(.\mathbf{l}) = (1 + 2^{-t})/4 \tag{5.8}$$

Hence, $S_A(t)$ has a simple exponential decay to its equilibrium value when $c = 1/2$. Noting that the spectrum of a Bernoulli transition matrix is $\{0, 1\}$, we observe that the exponential factor $1/2$ here comes from the consideration of sequences $\mathbf{l}$ of increasing length. The same decay could be found directly from the Markov representation where $A = Q_{.1} \cup Q_{.2}$ and Spec $\mathscr{M} = \{0, 1/2, 1\}$. In Section 6 we show that this correlation function also determines the evolution of the progress variable for a particular class of initial states.

5.2. The Case $c = 2^{-K}$

The partition $\mathscr{Q}$ for the triple baker model discussed in Section 4 was instrumental in establishing a number of general results for this model. However, the eigenvalue spectrum was not determined for arbitrary rational c values. On the other hand the results of the previous section showed that coarse graining $\mathscr{Q}$ for the case $c = 1/2$ produced an independent and generating partition in terms of which explicit calculations were possible. Here we consider the case $c = 2^{-K}$ $(K \geqslant 2)$ for which explicit results may also be obtained. Coarse-graining $\mathscr{Q}$ does not generally yield a Bernoulli partition as it did for $c = 1/2$, but another partition with Markov measure, which facilitates the calculations, may be constructed.

Consider the following partition $\mathscr{R} = \{R_k\}(-K \leqslant k \leqslant K, k \neq 0)$ obtained by coarse-graining $\mathscr{Q}$:

$$R_1 = I \times [0, 2^{1-K}[\text{ and } R_k = I \times [2^{k-K-1}, 2^{k-K}[\quad \text{for} \quad K \geqslant k \geqslant 2$$

$$R_{-1} = I \times [-2^{1-k}, 0[\text{ and } R_{-k} = I \times [-2^{k-K}, -2^{k-K-1}[$$

$$\text{for} \quad -K \leqslant -k \leqslant -2 \tag{5.9}$$

The Markov property of $\mathscr{R}$ is proved by the same argument as for $\mathscr{Q}$; each baker transformation fragments a band into strips with half its size. Moreover, the strips produced by the fragmentation of each band belong to different bands, so that $\mathscr{R}_0^\infty$ generates the "fiber algebra" $I \times \mathscr{B}_J$. Backward refinements of $\mathscr{R}_0^\infty$ are also seen to generate $\mathscr{B}_\Omega$.

The coarse-grained Markov chain has the (singly) stochastic matrix:

$$\mathscr{M}^R = \left[\begin{array}{cccccc|ccccc} 1/2 & 1/2 & & & & & & & & & \\ 1/2 & 0 & 1/2 & & & & & & & & \\ \cdot & \cdot & \cdot & \cdot & & & & & & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & & & & & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & & & & & \\ 1/2 & 0 & \cdot & \cdot & \cdot & 1/4 & 1/4 & & & & \\ \hline & & & & & 1/4 & 1/4 & & & & 1/2 \\ & & & & & & 1/2 & & & & 1/2 \\ & & & & & & & \cdot & & & \cdot \\ & & & & & & & & \cdot & & \cdot \\ & & & & & & & & & \cdot & \cdot \\ & & & & & & & & & 1/2 & 1/2 \end{array}\right] \tag{5.10}$$

whose characteristic polynomial is readily derived by recursion.

Since $\mathscr{R}$ is obtained by coarse-graining $\mathscr{Q}$, all its characteristic functions are sums of characteristic functions of $\mathscr{Q}$ and the spectrum of $\mathscr{M}^R$ must be part of the spectrum of $\mathscr{M}$. On the other hand, $\mathscr{Q}$ is also coarser than $\mathscr{R}_0^{K-1}$: the spectrum of $\mathscr{M}$ is included in that of $\mathscr{M}^{R(K)}$. Thus, Spec $\mathscr{M} = \{0\} \cup$ Spec $\mathscr{M}^R$.[3]

The characteristic polynomial of $\mathscr{M}$ is

$$M(s, c) = s^N(s-1)\,\psi_K(s) \tag{5.11}$$

With $N = 2^{K+1} - K - 1$. The simple eigenvalue 1 corresponds to the unique stationary (uniform) state. The K nontrivial eigenvalues are the roots of the polynomial

$$\psi_K(s) = 2s^K - (s^{K+1} - 2^{-K-1})/(s - 1/2) \tag{5.12}$$

[3] No "ghost" eigenvalue (like 1/2 for $c = 1/2$ in Section 5.1) can appear here as $\mathscr{Q}$ is coarser than a *finite* power of $\mathscr{R}$.

These special eigenvalues can be computed perturbatively as $K \to \infty$:

(i) The largest eigenvalue lies close to 1:

$$s_0 \simeq 1 - c/2 + O(c^2) \tag{5.13}$$

and its eigenvector is close to the A–B odd uniform vector:

$$(11\cdots11-1\cdots-1-1)\,\mathscr{M} = (11\cdots100-1\cdots-1-1) \tag{5.14}$$

For small c, the slowest process is thus the leakage between A and B, so that asymptotically the correlation function $C_f(t)$ of $f(\omega)$ will satisfy: $C_f(t+1) \sim s_0 C_f(t)$ as $t \to \infty$.

(ii) The other eigenvalues lie close to $\frac{1}{2}\rho_n = \frac{1}{2}\exp(2\pi i n/K)$ $(n \neq 0)$:

$$s_n = \rho_n \left\{ \frac{1}{2} - \frac{1}{K}(\rho_n - 2)/(\rho_n - 1) \right\} + O(K^{-2}) \tag{5.15}$$

These eigenvalues describe the mixing in A and B induced by the stirring B_A and B_B, as their moduli and regularly spaced phases suggest.

6. MICROSCOPIC BASIS OF THE RATE LAW

The characterization and solutions of the triple baker model presented above enable one to investigate the microscopic basis of the rate law determining the decay of the progress variable to equilibrium. In particular, the fact that the dynamics for rational c can be mapped onto a Markov shift immediately implies that the progress variable decays as a sum of exponential terms since the A and B cells are unions of the $\mathscr{Q}$-partition elements; hence a macroscopic law does apply for large times. In this section we examine the structure of the rate coefficient characterizing this decay in some detail.

A formally exact expression for the decay of $\xi(t)$ is easily derived from the evolution equation (2.6) of the distribution function with the aid of projection operator techniques.[16] It is convenient to assume here that the distribution function $\rho_t(\omega)$ is normalized to the conserved number N of phase points in the system, $\int \rho_t \, d\mu = N$. To reinforce our chemical analogy we shall henceforth refer to phase points in cell α as species α.

Consider the deviation of the distribution function from its equilibrium value $\rho_{eq}(\omega) = N$: $\delta\rho_t(\omega) = \rho_t(\omega) - N$. The progress variable takes the form

$$\xi(t) = \delta N_A(t) = \int \chi_A(\omega)\, \delta\rho_t(\omega)\, d\mu = -\delta N_B(t) \tag{6.1}$$

Given some initial distribution of phase points $\delta\rho_0(\omega)$, the equation determining the decay of $\xi(t)$ can be derived by employing the orthogonal projection operators

$$\mathscr{P}_\alpha h(\omega) = \frac{\chi_\alpha(\omega)}{\mu_\alpha} \langle \chi_\alpha(\omega)\, h(\omega) \rangle \tag{6.2}$$

where $h(\omega)$ is an arbitrary integrable function defined in Ω and $\mu_\alpha = 1/2$ is the measure of cell α. Note that $\mathscr{P}_\alpha \mathscr{P}_\beta = \delta_{\alpha\beta}\mathscr{P}_\alpha$. Applying $\mathscr{P} = \mathscr{P}_A + \mathscr{P}_B$ and its complement $\mathscr{P}_\perp = \mathbb{1} - \mathscr{P}$ to (2.6) yields

$$\xi(t) = C(t)\, \xi(0) + I(\rho_0, t) \tag{6.3}$$

where

$$I(\rho_0, t) = \langle \chi_A(\omega)\, U^t \mathscr{P}_\perp\, \delta\rho_0(\omega) \rangle \tag{6.4}$$

and

$$C(t) = 4S_A(t) - 1 \tag{6.5}$$

$S_A(t)$ is defined by (5.7) for any value of c. Since we are primarily concerned with the intrinsic evolution of $\xi(t)$ characterized by the correlation function $C(t)$ rather than with the decay arising from an arbitrary initial condition $\delta\rho_0(t)$, we consider the particular class of initial states where $I(\rho_0, t)$ vanishes. As an example of such states suppose that the initial density is uniform over each cell of phase space, with a disequilibrium between the species

$$\rho_0(\omega) = N + \gamma N \chi_A(\omega) - \gamma N \chi_B(\omega) \tag{6.6}$$

where γ is the fractional excess of species A. Clearly $\mathscr{P}_\perp\, \delta\rho_0(\omega) = 0$ and the calculation of $\xi(t)$ for this class of initial states is equivalent to that of the autocorrelation function $C(t)$.

In the phenomenological description (2.8) of the rate processes, the decay of $\xi(t)$ is determined by the rate coefficient $k = k_f + k_r$. A generalization of this phenomenological description can be obtained by casting the equation of motion for $\xi(t)$ in a memory kernel form. Starting from the evolution equation (2.5) applied to $\phi(\omega) = \chi_A(\omega) - \chi_B(\omega)$ and using the projection operators $\mathscr{P}$ and $\mathscr{P}_\perp$ we find[17]:

$$\xi(t+1) = (1+c)\, \xi(t) + \sum_{l=0}^{t-1} \mathscr{K}(l)\, \xi(t-l-1) \tag{6.7}$$

where the memory kernel $\mathscr{K}(l)$ is defined by

$$\mathscr{K}(l) = \langle (\mathscr{P}_\perp U^{-1} \phi(\omega)(\mathscr{P}_\perp U)^{l+1} \phi(\omega) \rangle \tag{6.8}$$

and the coefficient of $\xi(t)$ is $C(1) = 1 - c$. An effective rate coefficient for the decay process can be deduced using the z transform

$$\hat{g}(z) = \sum_{t=0}^{\infty} g(t)\, z^{-t} \tag{6.9}$$

of (6.7):

$$\hat{\xi}(z) = [1 - (1-c)\, z^{-1} - \hat{\mathscr{K}}(z)\, z^{-2}]^{-1}\, \xi(0) \tag{6.10}$$

Comparison with the transform of the phenomenological rate law suggests the definition of a generalized rate coefficient as

$$\hat{k}(z) = c - z^{-1} \hat{\mathscr{K}}(z) \tag{6.11}$$

The projection operator formalism produces a decomposition of the rate coefficient into two parts with simple physical interpretations: the first contribution is due to the "one-way-flux" $C(1)$ of the species across the cell boundary while the second arising from the memory kernel takes into account recrossings of this boundary and is a "nonequilibrium" contribution to the reaction rate.

The results of the previous section and the above formulation of the rate law provide a framework for discussing the dynamics of the cell-boundary crossing. The exact short-time decay of the progress variable is easily found from considering the action of U on the characteristic function χ_A:

$$\xi(t) = (1 - (|t| + 1)\, c/2)\, \xi(0), \qquad 0 < |t| < t^* \tag{6.12}$$

where t^* is given by $2^{t^*-1} c = 1$. Hence, $\xi(t)$ possesses two linear portions in a short-time region whose duration is determined by the magnitude of c: the initial time step with slope $-c$ determined by the one-way flux across the cell boundary and t^* time steps with slope $-c/2$. The restriction of the linear region to times $|t| < t^*$ can be understood from the following observation: Iteration of an initially uniform A density under U produces fragmentation; when the "holes" introduced in the A cell reenter the "reaction" C region the linear decay breaks down. Thus t^* is related to the time or number of iterations it takes a parcel of probability fluid with height c to traverse a cell and reenter C.

All the behavior apart from the initial one-way-flux contribution is contained in the rate kernel $\mathscr{K}(t)$, whose structure we now examine in

more detail. Since the decay of $\xi(t)$ is a sum of exponential terms one may represent $\hat{\mathscr{K}}(z)$ as a finite continued fraction, which is equivalent to a representation in terms of a sequence of equations in memory kernel form like (6.7):

$$\mathscr{K}_n(t+1) = \alpha_n \mathscr{K}_n(t) + \sum_{l=0}^{t-1} \mathscr{K}_{n+1}(l)\, \mathscr{K}_n(t-l-1) \tag{6.13}$$

where $\alpha_n = \mathscr{K}_n(1)/\mathscr{K}_n(0)$ and $\mathscr{K}_1(t) = \mathscr{K}(t)$. When $c = 2^{-K}$, this representation yields especially simple results since the memory kernel $\mathscr{K}_K(t)$ vanishes.

As an illustration, plots of $\xi(t)$ for $c = 1/2$, $1/4$, and $1/8$ are shown in Fig. 4. For $c = 1/2$ the Bernoulli and Markov representations yield $\xi(t)/\xi(0) = 2^{-t}$ and linear combinations of exponentials in the other cases. The linear and exponential regions of the $\xi(t)$ decay are evident in the figure.

We may further extend the analogy between the dynamics of this model and real rate processes. The one-way-flux contribution c in (6.11) may be written in the form

$$c = \langle \phi(\omega)(1 - U)\, \phi(\omega) \rangle \tag{6.14}$$

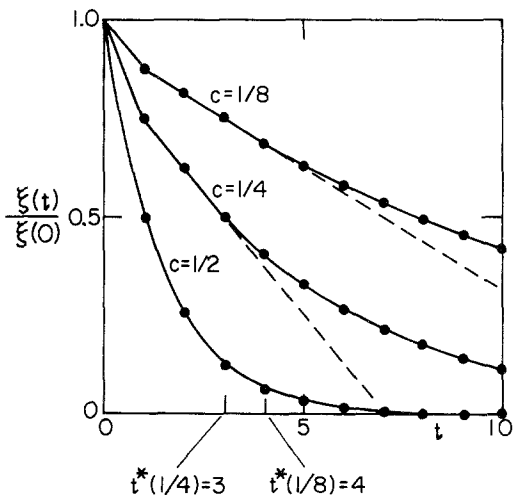

Fig. 4. Decay of the progress variable $c = 1/2$, $1/4$, and $1/8$. In this figure we have also indicated the initial linear decay regions of t^* time steps. The dashed lines are extensions of these linear regions. The solid lines connecting the points are only guides to the eye. Similar results for $c = 2^{-K}$ can be deduced from the discussion in Section 5.2.

which is an exact analog of the RRKM rate coefficient formula.[18] The kernel $\mathscr{K}(t)$ provides corrections to this formula.

Our exact solutions have the following implications for the description in terms of a phenomenological rate law:

(i) Since the decay of $\xi(t)$ is a sum of exponentials for rational c, the system admits a description in terms of a macroscopic rate law provided t is large enough.

(ii) The phenomenological rate law is valid for *all* t only for the special value $c = 1/2$ (and for 0 and 1).

(iii) For $c = 2^{-K}$ (K large) the eigenvalue closest to unity can be determined from perturbation theory and one finds $\xi(t+1) = (1 - c/2)\,\xi(t)$ for t large. Hence, the rate coefficient after (2.8) is $k = c/2$, which differs from the one-way-flux value of c. We also remark that the decay constants of the model are not the Liapunov exponents or K entropy.

Some of the implications of the results (i)–(iii) are rather interesting. In general one might expect that the phenomenological rate law with k given by the one-way-flux value will apply when the cell leaking rate is small. In fact this is only true for the large value of $c = 1/2$; for $c = 2^{-K}$ the nonequilibrium corrections lead to a lowering of the rate coefficient by a factor of two. Thus, the mixing within the A and B cells is generally insufficient to destroy the correlations set up by the "reaction." It is not difficult to construct a class of models where the mixing within the cells can be varied for a fixed c. Consider replacing the automorphism T by the following form:

$$T^{(n)} = B_C B_B^n B_A^n \tag{6.15}$$

i.e., for each time step in the evolution one carries out n applications of the baker transformation within the A and B cells. In the limit $n \to \infty$ one has perfect mixing within the cells prior to the application of the "reactive" B_C transformation. In this situation the K property of (α, B_α) suggests an approximation of the dynamics by a two-state Markov chain on $\{A, B\}$ with transition probabilities computed from the one-way fluxes across the cell boundary. This leads to

$$\xi(t+1) = (1 - c)\,\xi(t) \tag{6.16}$$

as $n \to \infty$. Clearly $n = 1$ even with small c is insufficient to achieve complete mixing within the cells and (6.16) does not hold.

7. CONCLUSIONS

We have shown by this example that coupling two K systems could result in a new K system with an interesting structure.

An important aspect of our analysis is the construction of a partition on which the invariant measure is Markov for any rational value of c: the corresponding symbolic representation provides the proper setting for the discussion of various ergodic properties. For instance, the decay of (measurable) correlation functions should be envisaged in this context rather than in terms of the unitary evolution operator: it is only in the Markov representation that one obtains nontrivial eigenvalues hinting at the irreversible evolution of the macroscopic model.

For the special case $c = 1/2$, we succeeded in constructing a finite, measurable Bernoulli partition, leading to a much simpler analysis of correlation functions. It is well known[4,19] that any finite Markov shift (as ours) is isomorphic to a Bernoulli shift $(\mathscr{S}, S)$ but the canonical Bernoulli partition $\mathscr{S}$ is infinite and S is obtained as some power of $\mathscr{M}$. We also succeeded in coarse-graining our partition for $c = 2^{-K}$ (while preserving the Markov property), but the general case of irrational c may admit no finite partition with a Markov property. However, we have not investigated this case in any detail and successive rational approximations of c may describe it well enough.

The model, although extremely idealized, displays a number of features characteristic of more complex, coupled, conservative, dynamical systems. The exponential decay of the progress variable (implying the existence of a macroscopic law) follows directly from the expression of the cell characteristic functions as $\mathscr{Q}$-partition step functions; if the phase space regions corresponding to a given species (cells) cannot be simply expressed in terms of partition elements, more complex decays are possible. In addition, the breakdown of simple one-way-flux models for the rate coefficient in our K system is a feature already noted by Berne and de Leon[10] in their study of the Siamese stadium billiard, a K flow. Other analogies may be drawn between their system and the triple baker model.

All the results presented in this paper are based on measure-theoretic properties: Liapunov exponents, isomorphic Markov shifts, correlation functions, etc. A simple examination of the case $c = 1/2$ suggests that our model has peculiar topological dynamics: the partitions $\mathscr{Q}$ and $\mathscr{R}$ have different topological entropies (as defined in Ref. 19). The measure-theoretic properties, especially the Markov shift representation, are also the starting point for a deeper discussion on the manner in which irreversibility can arise in a microscopically reversible system.

A number of extensions of the model are possible. In Section 6 we

proposed a model in which an arbitrary number of stirrings in the individual cells could be carried out for each discrete time step. Such a model could provide a means for studying the progressive passage to a simple rate law. Another variant of the triple baker system is a ladder model where the phase space is a pile of N squares and by an obvious extension the dynamics proceeds through baker transformations acting in the individual cells followed by baker transformations in the overlapping regions. The system models a diffusion process. The study of such extended models may provide some insight into the nature of the dynamical behavior of complex coupled systems.

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REFERENCES

1. V. I. Arnold and A. Avez, *Problemes Ergodiques de la Mechanique Classique* (Gauthier-Villars, Paris, 1967).
2. L. A. Bunimovich and Ya. G. Sinai, *Commun. Math. Phys.* **78**:479 (1981).
3. P. Collet and J.-P. Eckmann, *Iterated Maps on the Interval as Dynamical Systems* (Birkhauser, Basel, 1980).
4. I. P. Cornfeld, S. V. Formin, and Ya. G. Sinai, *Ergodic Theory* (Springer, Berlin, 1982).
5. D. Ornstein, *Ergodic Theory, Randomness and Dynamical Systems* (Yale University Press, New Haven, 1974).
6. P. Shields, *The Theory of Bernoulli Shifts* (University of Chicago Press, Chicago, 1973).
7. Ya. G. Sinai, *Introduction to Ergodic Theory* (Princeton University Press, Princeton, 1977).
8. H. Spohn, *Rev. Mod. Phys.* **53**:569 (1980).
9. I. Gumowski and C. Mira, *Dynamique Chaotique* (Cepadues, Toulouse, 1980).
10. N. de Leon and B. J. Berne, *Chem. Phys. Letts.* **93**:162, 169 (1982).
11. R. Zwanzig, *J. Stat. Phys.* **30**:255 (1983).
12. W. Parry, *Acta Math. Acad. Sci. Hung.* **15**:95, 107 (1964).
13. W. Feller, *An Introduction to Probability Theory and Its Applications* (Wiley, Nex York, 1970), Vol. 1.
14. S. Goldstein, B. Misra, and M. Courbage, *J. Stat. Phys.* **25**:111 (1981).
15. B. Misra and I. Prigogine, *Suppl. Prog. Theor. Phys.* **69**:101 (1980).

16. P. Résibois and M. De Leener, *Classical Kinetic Theory of Fluids* (Wiley, New York, 1977).
17. H. Fujisaka and T. Yamada, *Z. Naturforsch.* **33A**:1455 (1978).
18. W. Forst, *Theory of Unimolecular Reactions* (Academic Press, New York, 1973).
19. N. F. G. Martin and J. W. England, *Mathematical Theory of Entropy* (Addison-Wesley, Reading, Massachusetts 1981).