Chapter 14

Transporting densities

Paulina: I'll draw the curtain:
My lord's almost so far transported that
He'll think anon it lives.
—W. Shakespeare: *The Winter's Tale*

(P. Cvitanović, R. Artuso, L. Rondoni, and E.A. Spiegel)

In chapters 2, 3, 7 and 8 we learned how to track an individual trajectory, and saw that such a trajectory can be very complicated. In chapter 4 we studied a small neighborhood of a trajectory and learned that such neighborhood can grow exponentially with time, making the concept of tracking an individual trajectory for long times a purely mathematical idealization.

While the trajectory of an individual representative point may be highly convoluted, as we shall see, the density of these points might evolve in a manner that is relatively smooth. The evolution of the density of representative points is for this reason (and other that will emerge in due course) of great interest. So are the behaviors of other properties carried by the evolving swarm of representative points.

We shall now show that the global evolution of the density of representative points is conveniently formulated in terms of linear action of evolution operators. We shall also show that the important, long-time "natural" invariant densities are unspeakably unfriendly and essentially uncomputable everywhere singular functions with support on fractal sets. Hence, in chapter 15 we rethink what is it that the theory needs to predict ("expectation values" of "observables"), relate these to the eigenvalues of evolution operators, and in chapters 16 to 18 show how to compute these without ever having to compute a natural" invariant densities ρ_0.

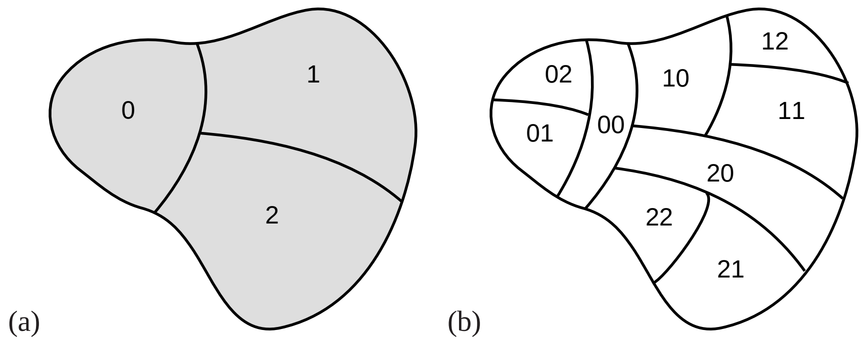


Figure 14.1: (a) First level of partitioning: A coarse partition of $\mathcal{M}$ into regions $\mathcal{M}_0$, $\mathcal{M}_1$, and $\mathcal{M}_2$. (b) $n = 2$ level of partitioning: A refinement of the above partition, with each region $\mathcal{M}_i$ subdivided into $\mathcal{M}_{i0}$, $\mathcal{M}_{i1}$, and $\mathcal{M}_{i2}$.

14.1 Measures

> Do I then measure, O my God, and know not what I measure?
>
> —St. Augustine, *The confessions of Saint Augustine*

A fundamental concept in the description of dynamics of a chaotic system is that of *measure*, which we denote by $d\mu(x) = \rho(x)dx$. An intuitive way to define and construct a physically meaningful measure is by a process of *coarse-graining*. Consider a sequence 1, 2, ..., n, ... of increasingly refined partitions of state space, figure 14.1, into regions $\mathcal{M}_i$ defined by the characteristic function

$$\chi_i(x) = \begin{cases} 1 & \text{if } x \in \mathcal{M}_i\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{14.1}$$

A coarse-grained measure is obtained by assigning the “mass,” or the fraction of trajectories contained in the ith region $\mathcal{M}_i \subset \mathcal{M}$ at the nth level of partitioning of the state space:

$$\Delta\mu_i = \int_{\mathcal{M}} d\mu(x)\chi_i(x) = \int_{\mathcal{M}_i} d\mu(x) = \int_{\mathcal{M}_i} dx\,\rho(x)\,. \tag{14.2}$$

The function $\rho(x) = \rho(x,t)$ denotes the *density* of representative points in state space at time t. This density can be (and in chaotic dynamics, often is) an arbitrarily ugly function, and it may display remarkable singularities; for instance, there may exist directions along which the measure is singular with respect to the Lebesgue measure. We shall assume that the measure is normalized

$$\sum_i^{(n)} \Delta\mu_i = 1\,, \tag{14.3}$$

where the sum is over subregions i at the nth level of partitioning. The infinitesimal measure $\rho(x)\,dx$ can be thought of as an infinitely refined partition limit of $\Delta\mu_i = |\mathcal{M}_i|\rho(x_i)\,,\ x_i \in \mathcal{M}_i$, with normalization

$$\int_{\mathcal{M}} dx\,\rho(x) = 1\,. \tag{14.4}$$

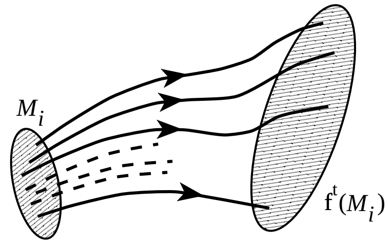


Figure 14.2: The evolution rule f^t can be used to map a region $\mathcal{M}_i$ of the state space into the region $f^t(\mathcal{M}_i)$.

Here $|\mathcal{M}_i|$ is the volume of region $\mathcal{M}_i$, and all $|\mathcal{M}_i| \to 0$ as $n \to \infty$.

So far, any arbitrary sequence of partitions will do. What are intelligent ways of partitioning state space? We already know the answer from chapter 10, but let us anyway develope some intuition about how the dynamics transports densities.

[chapter 10]

14.2 Perron-Frobenius operator

Given a density, the question arises as to what it might evolve into with time. Consider a swarm of representative points making up the measure contained in a region $\mathcal{M}_i$ at time $t = 0$. As the flow evolves, this region is carried into $f^t(\mathcal{M}_i)$, as in figure 14.2. No trajectory is created or destroyed, so the conservation of representative points requires that

$$\int_{f^t(\mathcal{M}_i)} dx\, \rho(x,t) = \int_{\mathcal{M}_i} dx_0\, \rho(x_0, 0)\,.$$

Transform the integration variable in the expression on the left hand side to the initial points $x_0 = f^{-t}(x)$,

$$\int_{\mathcal{M}_i} dx_0\, \rho(f^t(x_0), t) \left|\det J^t(x_0)\right| = \int_{\mathcal{M}_i} dx_0\, \rho(x_0, 0)\,.$$

The density changes with time as the inverse of the Jacobian (4.46)

$$\rho(x,t) = \frac{\rho(x_0, 0)}{|\det J^t(x_0)|}\,, \qquad x = f^t(x_0)\,, \tag{14.5}$$

which makes sense: the density varies inversely with the infinitesimal volume occupied by the trajectories of the flow.

The relation (14.5) is linear in ρ, so the manner in which a flow transports densities may be recast into the language of operators, by writing

[exercise 14.1]

$$\rho(x,t) = \left(\mathcal{L}^t \circ \rho\right)(x) = \int_{\mathcal{M}} dx_0\, \delta\!\left(x - f^t(x_0)\right) \rho(x_0, 0)\,. \tag{14.6}$$

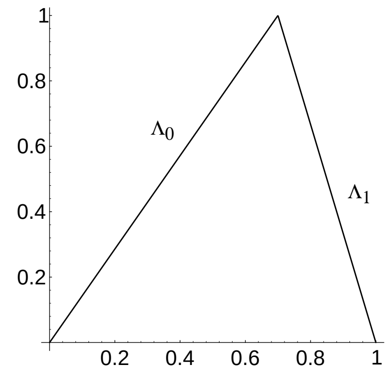


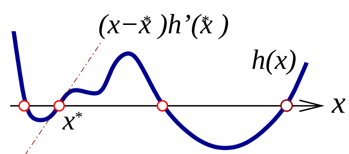
Figure 14.3: A piecewise-linear skew "Ulam tent" map (14.11) ($\Lambda_0 = 4/3$, $\Lambda_1 = -4$).

Let us check this formula. As long as the zero is not smack on the border of $\partial\mathcal{M}$, integrating Dirac delta functions is easy: $\int_{\mathcal{M}} dx\,\delta(x) = 1$ if $0 \in \mathcal{M}$, zero otherwise. The integral over a 1-dimensional Dirac delta function picks up the Jacobian of its argument evaluated at all of its zeros:

$$\int dx\,\delta(h(x)) = \sum_{\{x:h(x)=0\}} \frac{1}{|h'(x)|}\,, \tag{14.7}$$

and in d dimensions the denominator is replaced by

$$\int dx\,\delta(h(x)) \quad = \tag{14.8}$$



$$= \sum_j \int_{\mathcal{M}_j} dx\,\delta(h(x)) \;=\; \sum_{\{x:h(x)=0\}} \frac{1}{\left|\det \frac{\partial h(x)}{\partial x}\right|}\,.$$

Now you can check that (14.6) is just a rewrite of (14.5):

[exercise 14.2]

$$\begin{aligned}\left(\mathcal{L}^t \circ \rho\right)(x) &= \sum_{x_0 = f^{-t}(x)} \frac{\rho(x_0)}{|f^{t\,\prime}(x_0)|} && \text{(1-dimensional)} \\ &= \sum_{x_0 = f^{-t}(x)} \frac{\rho(x_0)}{|\det J^t(x_0)|} && (d\text{-dimensional})\,.\end{aligned} \tag{14.9}$$

For a deterministic, invertible flow x has only one preimage x_0; allowing for multiple preimages also takes account of noninvertible mappings such as the "stretch & fold" maps of the interval, to be discussed briefly in the next example, and in more detail in sect. 10.2.1.

We shall refer to the kernel of (14.6) as the *Perron-Frobenius operator*:

[exercise 14.3]
[example 21.7]

$$\mathcal{L}^t(x,y) = \delta\left(x - f^t(y)\right)\,. \tag{14.10}$$

If you do not like the word "kernel" you might prefer to think of $\mathcal{L}^t(x,y)$ as a matrix with indices x, y, and index summation in matrix multiplication replaced by an integral over y, $(\mathcal{L}^t \circ \rho)(x) = \int dy\, \mathcal{L}^t(x,y)\rho(y)$. The Perron-Frobenius operator assembles the density $\rho(x,t)$ at time t by going back in time to the density $\rho(x_0, 0)$ at time $t = 0$. [remark 17.4]

Example 14.1 ***Perron-Frobenius operator for a piecewise-linear map:*** *Assume the expanding 1-d map $f(x)$ of figure 14.3, a piecewise-linear 2–branch map with slopes $\Lambda_0 > 1$ and $\Lambda_1 = -\Lambda_0/(\Lambda_0 - 1) < -1$:* [exercise 14.7]

$$f(x) = \begin{cases} f_0(x) = \Lambda_0 x\,, & x \in \mathcal{M}_0 = [0, 1/\Lambda_0) \\ f_1(x) = \Lambda_1(1-x)\,, & x \in \mathcal{M}_1 = (1/\Lambda_0, 1]\,. \end{cases} \tag{14.11}$$

Both $f(\mathcal{M}_0)$ and $f(\mathcal{M}_1)$ map onto the entire unit interval $\mathcal{M} = [0, 1]$. We shall refer to any unimodal map whose critical point maps onto the "left" unstable fixed point x_0 as the "Ulam" map. Assume a piecewise constant density

$$\rho(x) = \begin{cases} \rho_0 & \text{if } x \in \mathcal{M}_0 \\ \rho_1 & \text{if } x \in \mathcal{M}_1 \end{cases}\,. \tag{14.12}$$

As can be easily checked using (14.9), the Perron-Frobenius operator acts on this piecewise constant function as a [2×2] Markov matrix $\mathbf{L}$ with matrix elements [exercise 14.1] [exercise 14.5]

$$\begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} \to \mathbf{L}\rho = \begin{pmatrix} \frac{1}{|\Lambda_0|} & \frac{1}{|\Lambda_1|} \\ \frac{1}{|\Lambda_0|} & \frac{1}{|\Lambda_1|} \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix}, \tag{14.13}$$

stretching both ρ_0 and ρ_1 over the whole unit interval Λ. In this example the density is constant after one iteration, so $\mathbf{L}$ has only a unit eigenvalue $e^{s_0} = 1/|\Lambda_0| + 1/|\Lambda_1| = 1$, with constant density eigenvector $\rho_0 = \rho_1$. The quantities $1/|\Lambda_0|$, $1/|\Lambda_1|$ are, respectively, the fractions of state space taken up by the $|\mathcal{M}_0|$, $|\mathcal{M}_1|$ intervals. This simple explicit matrix representation of the Perron-Frobenius operator is a consequence of the piecewise linearity of f, and the restriction of the densities ρ to the space of piecewise constant functions. The example gives a flavor of the enterprize upon which we are about to embark in this book, but the full story is much subtler: in general, there will exist no such finite-dimensional representation for the Perron-Frobenius operator. (Continued in example 15.2.)

14.3 Why not just leave it to a computer?

(R. Artuso and P. Cvitanović)

To a student with a practical bent the above Example 14.1 suggests a strategy for constructing evolution operators for smooth maps, as limits of partitions of state space into regions $\mathcal{M}_i$, with a piecewise-linear approximations f_i to the dynamics in each region, but that would be too naive; much of the physically interesting spectrum would be missed. As we shall see, the choice of function space for ρ is crucial, and the physically motivated choice is a space of smooth functions, rather than the space of piecewise constant functions. [chapter 21]

All of the insight gained in this chapter and in what is to follow is nothing but an elegant way of thinking of the evolution operator, $\mathcal{L}$, as a matrix (this point of view will be further elaborated in chapter 21). There are many textbook methods of approximating an operator $\mathcal{L}$ by sequences of finite matrix approximations $\mathcal{L}$, but in what follows the great achievement will be that we shall avoid constructing any matrix approximation to $\mathcal{L}$ altogether. Why a new method? Why not just run it on a computer, as many do with such relish in diagonalizing quantum Hamiltonians?

The simplest possible way of introducing a state space discretization, figure 14.4, is to partition the state space $\mathcal{M}$ with a non-overlapping collection of sets $\mathcal{M}_i$, $i = 1, \ldots, N$, and to consider piecewise constant densities (14.2), constant on each $\mathcal{M}_i$:

$$\rho(x) = \sum_{i=1}^{N} \rho_i \frac{\chi_i(x)}{|\mathcal{M}_i|}$$

where $\chi_i(x)$ is the characteristic function (14.1) of the set $\mathcal{M}_i$. The density ρ_i at a given instant is related to the densities at the previous step in time by the action of the Perron-Frobenius operator, as in (14.6):

$$\begin{aligned}\rho'_j &= \int_{\mathcal{M}} dy\, \chi_j(y)\rho'(y) = \int_{\mathcal{M}} dx\, dy\, \chi_j(y)\, \delta(y - f(x))\, \rho(x) \\ &= \sum_{i=1}^{N} \rho_i \frac{|\mathcal{M}_i \cap f^{-1}(\mathcal{M}_j)|}{|\mathcal{M}_i|} .\end{aligned}$$

In this way

$$\mathbf{L}_{ij} = \frac{|\mathcal{M}_i \cap f^{-1}(\mathcal{M}_j)|}{|\mathcal{M}_i|}, \quad \rho' = \rho\mathbf{L} \tag{14.14}$$

is a matrix approximation to the Perron-Frobenius operator, and its leading left eigenvector is a piecewise constant approximation to the invariant measure. It is an old idea of Ulam that such an approximation for the Perron-Frobenius operator is a meaningful one.

[remark 14.3]

The problem with such state space discretization approaches is that they are blind, the grid knows not what parts of the state space are more or less important. This observation motivated the development of the invariant partitions of chaotic systems undertaken in chapter 10, we exploited the intrinsic topology of a flow to give us both an invariant partition of the state space and a measure of the partition volumes, in the spirit of figure 1.11.

Furthermore, a piecewise constant ρ belongs to an unphysical function space, and with such approximations one is plagued by numerical artifacts such as spurious eigenvalues. In chapter 21 we shall employ a more refined approach to extracting

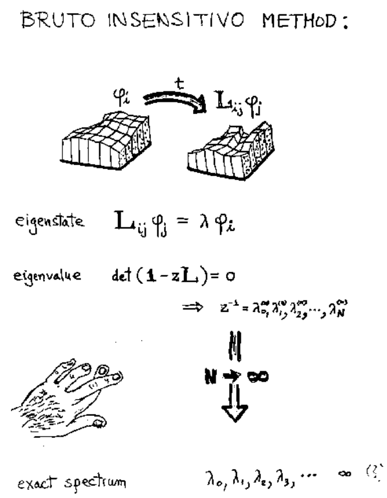


Figure 14.4: State space discretization approach to computing averages.

spectra, by expanding the initial and final densities ρ, ρ' in some basis φ_0, φ_1, $\varphi_2, \cdots$ (orthogonal polynomials, let us say), and replacing $\mathcal{L}(y, x)$ by its φ_α basis representation $\mathbf{L}_{\alpha\beta} = \langle\varphi_\alpha|\mathcal{L}|\varphi_\beta\rangle$. The art is then the subtle art of finding a "good" basis for which finite truncations of $\mathbf{L}_{\alpha\beta}$ give accurate estimates of the eigenvalues of $\mathcal{L}$.

[chapter 21]

Regardless of how sophisticated the choice of basis might be, the basic problem cannot be avoided - as illustrated by the natural measure for the Hénon map (3.18) sketched in figure 14.5, eigenfunctions of $\mathcal{L}$ are complicated, singular functions concentrated on fractal sets, and in general cannot be represented by a nice basis set of smooth functions. We shall resort to matrix representations of $\mathcal{L}$ and the φ_α basis approach only insofar this helps us prove that the spectrum that we compute is indeed the correct one, and that finite periodic orbit truncations do converge.


in depth:
chapter 1, p. 1

14.4 Invariant measures

A *stationary* or *invariant density* is a density left unchanged by the flow

$$\rho(x, t) = \rho(x, 0) = \rho(x)\,. \tag{14.15}$$

Conversely, if such a density exists, the transformation $f^t(x)$ is said to be *measure-preserving*. As we are given deterministic dynamics and our goal is the computation of asymptotic averages of observables, our task is to identify interesting invariant measures for a given $f^t(x)$. Invariant measures remain unaffected by dynamics, so they are fixed points (in the infinite-dimensional function space of ρ densities) of the Perron-Frobenius operator (14.10), with the unit eigenvalue:

[exercise 14.3]

$$\mathcal{L}^t\rho(x) = \int_{\mathcal{M}} dy\, \delta(x - f^t(y))\rho(y) = \rho(x). \tag{14.16}$$

In general, depending on the choice of $f^t(x)$ and the function space for $\rho(x)$, there may be no, one, or many solutions of the eigenfunction condition (14.16). For instance, a singular measure $d\mu(x) = \delta(x - x_q)dx$ concentrated on an equilibrium point $x_q = f^t(x_q)$, or any linear combination of such measures, each concentrated on a different equilibrium point, is stationary. There are thus infinitely many stationary measures that can be constructed. Almost all of them are unnatural in the sense that the slightest perturbation will destroy them.

From a physical point of view, there is no way to prepare initial densities which are singular, so we shall focus on measures which are limits of transformations experienced by an initial smooth distribution $\rho(x)$ under the action of f,

$$\rho_0(x) = \lim_{t\to\infty} \int_{\mathcal{M}} dy\, \delta(x - f^t(y))\rho(y, 0)\,, \qquad \int_{\mathcal{M}} dy\, \rho(y, 0) = 1\,. \tag{14.17}$$

Intuitively, the "natural" measure should be the measure that is the least sensitive to the (in practice unavoidable) external noise, no matter how weak.

14.4.1 Natural measure

> **Huang:** Chen-Ning, do you think ergodic theory gives us useful insight into the foundation of statistical mechanics?
> **Yang:** I don't think so.
> —Kerson Huang, *C.N. Yang interview*

In computer experiments, as the Hénon example of figure 14.5, the long time evolution of many "typical" initial conditions leads to the same asymptotic distribution. Hence the *natural* (also called equilibrium measure, SRB measure, Sinai-Bowen-Ruelle measure, physical measure, invariant density, natural density, or even "natural invariant") is defined as the limit

[exercise 14.8]
[exercise 14.9]

$$\overline{\rho}_{x_0}(y) = \begin{cases} \lim_{t\to\infty} \frac{1}{t}\int_0^t d\tau\, \delta(y - f^\tau(x_0)) & \text{flows} \\ \lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} \delta\big(y - f^k(x_0)\big) & \text{maps}\,, \end{cases} \tag{14.18}$$

where x_0 is a generic initial point. Generated by the action of f, the natural measure satisfies the stationarity condition (14.16) and is thus invariant by construction.

Staring at an average over infinitely many Dirac deltas is not a prospect we cherish. From a computational point of view, the natural measure is the visitation frequency defined by coarse-graining, integrating (14.18) over the $\mathcal{M}_i$ region

$$\Delta\overline{\mu}_i = \lim_{t\to\infty} \frac{t_i}{t}\,, \tag{14.19}$$

where t_i is the accumulated time that a trajectory of total duration t spends in the $\mathcal{M}_i$ region, with the initial point x_0 picked from some smooth density $\rho(x)$.

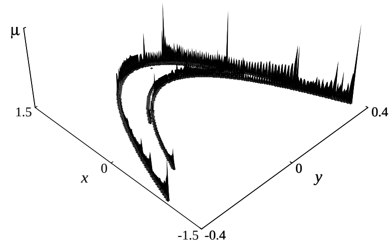


Figure 14.5: Natural measure (14.19) for the Hénon map (3.18) strange attractor at parameter values $(a, b) = (1.4, 0.3)$. See figure 3.9 for a sketch of the attractor without the natural measure binning. (Courtesy of J.-P. Eckmann)

Let $a = a(x)$ be any *observable*. In the mathematical literature $a(x)$ is a function belonging to some function space, for instance the space of integrable functions L^1, that associates to each point in state space a number or a set of numbers. In physical applications the observable $a(x)$ is necessarily a smooth function. The observable reports on some property of the dynamical system. Several examples will be given in sect. 15.1.

The *space average* of the observable a with respect to a measure ρ is given by the d-dimensional integral over the state space $\mathcal{M}$:

$$\begin{aligned} \langle a \rangle_\rho &= \frac{1}{|\rho_\mathcal{M}|} \int_\mathcal{M} dx\, \rho(x) a(x) \\ |\rho_\mathcal{M}| &= \int_\mathcal{M} dx\, \rho(x) = \text{mass in } \mathcal{M}\,. \end{aligned} \tag{14.20}$$

For now we assume that the state space $\mathcal{M}$ has a finite dimension and a finite volume. By definition, $\langle a \rangle_\rho$ is a function(al) of ρ. For $\rho = \rho_0$ natural measure we shall drop the subscript in the definition of the space average; $\langle a \rangle_\rho = \langle a \rangle$.

Inserting the right-hand-side of (14.18) into (14.20), we see that the natural measure corresponds to a *time average* of the observable a along a trajectory of the initial point x_0,

$$\overline{a_{x_0}} = \lim_{t\to\infty} \frac{1}{t} \int_0^t d\tau\, a(f^\tau(x_0))\,. \tag{14.21}$$

Analysis of the above asymptotic time limit is the central problem of ergodic theory. The *Birkhoff ergodic theorem* asserts that if a natural measure ρ exists, the limit $\overline{a(x_0)}$ for the time average (14.21) exists for all initial x_0. As we shall not rely on this result in what follows we forgo a proof here. Furthermore, if the dynamical system is *ergodic*, the time average tends to the space average [remark 14.1] [appendix A]

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t d\tau\, a(f^\tau(x_0)) = \langle a \rangle \tag{14.22}$$

for "almost all" initial x_0. By "almost all" we mean that the time average is independent of the initial point apart from a set of ρ-measure zero.

For future reference, we note a further property that is stronger than ergodicity: if the space average of a product of any two variables decorrelates with time,

$$\lim_{t\to\infty} \left\langle a(x) b(f^t(x)) \right\rangle = \langle a \rangle \langle b \rangle\,, \tag{14.23}$$

[section 20.4]

the dynamical system is said to be *mixing*.

Example 14.2 ***The Hénon attractor natural measure:*** *A numerical calculation of the natural measure (14.19) for the Hénon attractor (3.18) is given by the histogram in figure 14.5. The state space is partitioned into many equal-size areas $\mathcal{M}_i$, and the coarse grained measure (14.19) is computed by a long-time iteration of the Hénon map, and represented by the height of the column over area $\mathcal{M}_i$. What we see is a typical invariant measure - a complicated, singular function concentrated on a fractal set.*

If an invariant measure is quite singular (for instance a Dirac δ concentrated on a fixed point or a cycle), its existence is most likely of no physical import; no smooth initial density will converge to this measure if its neighborhood is repelling. In practice the average (14.18) is problematic and often hard to control, as generic dynamical systems are neither uniformly hyperbolic nor structurally stable: it is not known whether even the simplest model of a strange attractor, the Hénon attractor of figure 14.5, is "strange," or merely a transient to a very long stable cycle.

[exercise 15.1]

14.4.2 Determinism vs. stochasticity

While dynamics can lead to very singular ρ's, in any physical setting we cannot do better than to measure ρ averaged over some region $\mathcal{M}_i$; the coarse-graining is not an approximation but a physical necessity. One is free to think of a measure as a probability density, as long as one keeps in mind the distinction between deterministic and stochastic flows. In deterministic evolution the evolution kernels are not probabilistic; the density of trajectories is transported *deterministically*. What this distinction means will became apparent later: for deterministic flows our trace and determinant formulas will be *exact*, while for quantum and stochastic flows they will only be the leading saddle point (stationary phase, steepest descent) approximations.

[chapter 17]

Clearly, while deceptively easy to define, measures spell trouble. The good news is that if you hang on, you will *never need to compute them*, at least not in this book. How so? The evolution operators to which we next turn, and the trace and determinant formulas to which they will lead us, will assign the correct weights to desired averages without recourse to any explicit computation of the coarse-grained measure $\Delta\rho_i$.

14.5 Density evolution for infinitesimal times

Consider the evolution of a smooth density $\rho(x) = \rho(x, 0)$ under an infinitesimal step $\delta\tau$, by expanding the action of $\mathcal{L}^{\delta\tau}$ to linear order in $\delta\tau$:

$$\mathcal{L}^{\delta\tau}\rho(y) = \int_{\mathcal{M}} dx\, \delta\big(y - f^{\delta\tau}(x)\big)\rho(x)$$

$$
\begin{aligned}
&= \int_{\mathcal{M}} dx\, \delta(y - x - \delta\tau v(x))\, \rho(x) \\
&= \frac{\rho(y - \delta\tau v(y))}{\left|\det\left(1 + \delta\tau \frac{\partial v(y)}{\partial x}\right)\right|} = \frac{\rho(y) - \delta\tau v_i(y)\partial_i \rho(y)}{1 + \delta\tau \sum_{i=1}^{d} \partial_i v_i(y)} \\
\rho(x, \delta\tau) &= \rho(x, 0) - \delta\tau\,.
\end{aligned} \tag{14.24}
$$

Here we have used the infinitesimal form of the flow (2.6), the Dirac delta Jacobian (14.9), and the $\ln\det = \mathrm{tr}\,\ln$ relation. By the Einstein summation convention, repeated indices imply summation, $v_i(y)\partial_i = \sum_{i=1}^{d} v_i(y)\partial_i$. Moving $\rho(y, 0)$ to the left hand side and dividing by $\delta\tau$, we discover that the rate of the deformation of ρ under the infinitesimal action of the Perron-Frobenius operator is nothing but the *continuity equation* for the density: [exercise 4.1]

$$
\partial_t \rho + \partial \cdot (\rho v) = 0\,. \tag{14.25}
$$

The family of Perron-Frobenius operators operators $\{\mathcal{L}^t\}_{t \in \mathbb{R}_+}$ forms a semigroup parameterize by time

(a) $\mathcal{L}^0 = I$

(b) $\mathcal{L}^t \mathcal{L}^{t'} = \mathcal{L}^{t+t'} \qquad t, t' \geq 0 \qquad$ (semigroup property) .

From (14.24), time evolution by an infinitesimal step $\delta\tau$ forward in time is generated by

$$
\mathcal{A}\rho(x) = +\lim_{\delta\tau \to 0^+} \frac{1}{\delta\tau}\left(\mathcal{L}^{\delta\tau} - I\right)\rho(x) = -\partial_i(v_i(x)\rho(x))\,. \tag{14.26}
$$

We shall refer to

$$
\mathcal{A} = -\partial \cdot v + \sum_{i}^{d} v_i(x)\partial_i \tag{14.27}
$$

as the time evolution *generator*. If the flow is finite-dimensional and invertible, $\mathcal{A}$ is a generator of a full-fledged group. The left hand side of (14.26) is the definition of time derivative, so the evolution equation for $\rho(x)$ is

$$
\left(\frac{\partial}{\partial t} - \mathcal{A}\right)\rho(x) = 0\,. \tag{14.28}
$$

The finite time Perron-Frobenius operator (14.10) can be formally expressed by exponentiating the time evolution generator $\mathcal{A}$ as

$$
\mathcal{L}^t = e^{t\mathcal{A}}\,. \tag{14.29}
$$

The generator $\mathcal{A}$ is reminiscent of the generator of translations. Indeed, for a constant velocity field dynamical evolution is nothing but a translation by (time $\times$ velocity):

[exercise 14.10]

$$e^{-tv\frac{\partial}{\partial x}}a(x) = a(x - tv)\,. \tag{14.30}$$

14.5.1 Resolvent of $\mathcal{L}$

Here we limit ourselves to a brief remark about the notion of the "spectrum" of a linear operator.

The Perron-Frobenius operator $\mathcal{L}$ acts multiplicatively in time, so it is reasonable to suppose that there exist constants $M > 0$, $\beta \geq 0$ such that $||\mathcal{L}^t|| \leq Me^{t\beta}$ for all $t \geq 0$. What does that mean? The operator norm is defined in the same spirit in which one defines matrix norms:We are assuming that no value of $\mathcal{L}^t\rho(x)$ grows faster than exponentially for any choice of function $\rho(x)$, so that the fastest possible growth can be bounded by $e^{t\beta}$, a reasonable expectation in the light of the simplest example studied so far, the exact escape rate (15.20). If that is so, multiplying $\mathcal{L}^t$ by $e^{-t\beta}$ we construct a new operator $e^{-t\beta}\mathcal{L}^t = e^{t(\mathcal{A}-\beta)}$ which decays exponentially for large t, $||e^{t(\mathcal{A}-\beta)}|| \leq M$. We say that $e^{-t\beta}\mathcal{L}^t$ is an element of a *bounded* semigroup with generator $\mathcal{A} - \beta I$. Given this bound, it follows by the Laplace transform

$$\int_0^\infty dt\, e^{-st}\mathcal{L}^t = \frac{1}{s - \mathcal{A}}\,, \qquad \mathrm{Re}\, s > \beta\,, \tag{14.31}$$

that the *resolvent* operator $(s - \mathcal{A})^{-1}$ is bounded ("resolvent" = able to cause separation into constituents)

$$\left\|\frac{1}{s - \mathcal{A}}\right\| \leq \int_0^\infty dt\, e^{-st}Me^{t\beta} = \frac{M}{s - \beta}\,.$$

If one is interested in the spectrum of $\mathcal{L}$, as we will be, the resolvent operator is a natural object to study; it has no time dependence, and it is bounded. The main lesson of this brief aside is that for continuous time flows, the Laplace transform is the tool that brings down the generator in (14.29) into the resolvent form (14.31) and enables us to study its spectrum.

14.6 Liouville operator

A case of special interest is the Hamiltonian or symplectic flow defined by Hamilton's equations of motion (7.1). A reader versed in quantum mechanics will have observed by now that with replacement $\mathcal{A} \to -\frac{i}{\hbar}\hat{H}$, where $\hat{H}$ is the quantum

Hamiltonian operator, (14.28) looks rather like the time dependent Schrödinger equation, so this is probably the right moment to figure out what all this means in the case of Hamiltonian flows.

The Hamilton's evolution equations (7.1) for any time-independent quantity $Q = Q(q, p)$ are given by

$$\frac{dQ}{dt} = \frac{\partial Q}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial Q}{\partial p_i}\frac{dp_i}{dt} = \frac{\partial H}{\partial p_i}\frac{\partial Q}{\partial q_i} - \frac{\partial Q}{\partial p_i}\frac{\partial H}{\partial q_i}. \tag{14.32}$$

As equations with this structure arise frequently for symplectic flows, it is convenient to introduce a notation for them, the *Poisson bracket*

[remark 14.4]

$$\{A, B\} = \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} - \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i}. \tag{14.33}$$

In terms of Poisson brackets the time evolution equation (14.32) takes the compact form

$$\frac{dQ}{dt} = \{H, Q\}. \tag{14.34}$$

The full state space flow velocity is $\dot{x} = v = (\dot{q}, \dot{p})$, where the dot signifies time derivative.

The discussion of sect. 14.5 applies to any deterministic flow. If the density itself is a material invariant, combining

$$\partial_t I + v \cdot \partial I = 0.$$

and (14.25) we conclude that $\partial_i v_i = 0$ and $\det J^t(x_0) = 1$. An example of such incompressible flow is the Hamiltonian flow of sect. 7.2. For incompressible flows the continuity equation (14.25) becomes a statement of conservation of the state space volume (see sect. 7.2), or the *Liouville theorem*

$$\partial_t \rho + v_i \partial_i \rho = 0. \tag{14.35}$$

Hamilton's equations (7.1) imply that the flow is incompressible, $\partial_i v_i = 0$, so for Hamiltonian flows the equation for ρ reduces to the *continuity equation* for the phase space density:

$$\partial_t \rho + \partial_i(\rho v_i) = 0, \qquad i = 1, 2 \ldots, D. \tag{14.36}$$

Consider the evolution of the phase space density ρ of an ensemble of noninteracting particles; the particles are conserved, so

$$\frac{d}{dt}\rho(q, p, t) = \left(\frac{\partial}{\partial t} + \dot{q}_i \frac{\partial}{\partial q_i} + \dot{p}_i \frac{\partial}{\partial p_i}\right)\rho(q, p, t) = 0.$$

Inserting Hamilton's equations (7.1) we obtain the *Liouville equation*, a special case of (14.28):

$$\frac{\partial}{\partial t}\rho(q,p,t) = -\mathcal{A}\rho(q,p,t) = \{H,\rho(q,p,t)\}\,, \tag{14.37}$$

where { , } is the Poisson bracket (14.33). The generator of the flow (14.27) is in this case a generator of infinitesimal symplectic transformations,

$$\mathcal{A} = \dot{q}_i\frac{\partial}{\partial q_i} + \dot{p}_i\frac{\partial}{\partial p_i} = \frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i}\,. \tag{14.38}$$

For example, for separable Hamiltonians of form $H = p^2/2m+V(q)$, the equations of motion are

$$\dot{q}_i = \frac{p_i}{m}\,, \qquad \dot{p}_i = -\frac{\partial V(q)}{\partial q_i}\,. \tag{14.39}$$

and the action of the generator

[exercise 14.11]

$$\mathcal{A} = -\frac{p_i}{m}\frac{\partial}{\partial q_i} + \partial_i V(q)\frac{\partial}{\partial p_i}\,. \tag{14.40}$$

can be interpreted as a translation (14.30) in configuration space, followed by acceleration by force $\partial V(q)$ in the momentum space.

The time evolution generator (14.27) for the case of symplectic flows is called the *Liouville operator*. You might have encountered it in statistical mechanics, while discussing what ergodicity means for 10^{23} hard balls. Here its action will be very tangible; we shall apply the Liouville operator to systems as small as 1 or 2 hard balls and to our surprise learn that this suffices to already get a bit of a grip on foundations of the nonequilibrium statistical mechanics.

Résumé

In physically realistic settings the initial state of a system can be specified only to a finite precision. If the dynamics is chaotic, it is not possible to calculate accurately the long time trajectory of a given initial point. Depending on the desired precision, and given a deterministic law of evolution, the state of the system can then be tracked for a finite time.

The study of long-time dynamics thus requires trading in the evolution of a single state space point for the evolution of a *measure*, or the *density* of representative points in state space, acted upon by an *evolution operator*. Essentially this means trading in *nonlinear* dynamical equations on a finite dimensional space $x = (x_1, x_2 \cdots x_d)$

for a *linear* equation on an infinite dimensional vector space of density functions $\rho(x)$. For finite times and for maps such densities are evolved by the *Perron-Frobenius operator*,

$$\rho(x,t) = \left(\mathcal{L}^t \circ \rho\right)(x)\,,$$

and in a differential formulation they satisfy the the *continuity equation*:

$$\partial_t \rho + \partial \cdot (\rho v) \;=\; 0\,.$$

The most physical of stationary measures is the natural measure, a measure robust under perturbations by weak noise.

Reformulated this way, classical dynamics takes on a distinctly quantum-mechanical flavor. If the Lyapunov time (1.1), the time after which the notion of an individual deterministic trajectory loses meaning, is much shorter than the observation time, the "sharp" observables are those dual to time, the eigenvalues of evolution operators. This is very much the same situation as in quantum mechanics; as atomic time scales are so short, what is measured is the energy, the quantum-mechanical observable dual to the time. For long times the dynamics is described in terms of stationary measures, i.e., fixed points of the appropriate evolution operators. Both in classical and quantum mechanics one has a choice of implementing dynamical evolution on densities ("Schrödinger picture," sect. 14.5) or on observables ("Heisenberg picture," sect. 15.2 and chapter 16).

In what follows we shall find the second formulation more convenient, but the alternative is worth keeping in mind when posing and solving invariant density problems. However, as classical evolution operators are not unitary, their eigenstates can be quite singular and difficult to work with. In what follows we shall learn how to avoid dealing with these eigenstates altogether. As a matter of fact, what follows will be a labor of radical deconstruction; after having argued so strenuously here that only smooth measures are "natural," we shall merrily proceed to erect the whole edifice of our theory on periodic orbits, i.e., objects that are δ-functions in state space. The trick is that each comes with an interval, its neighborhood – cycle points only serve to pin these intervals, just as the millimeter marks on a measuring rod partition continuum into intervals.

Commentary

Remark 14.1 Ergodic theory: An overview of ergodic theory is outside the scope of this book: the interested reader may find it useful to consult ref. [1]. The existence of time average (14.21) is the basic result of ergodic theory, known as the Birkhoff theorem, see for example refs. [1, 22], or the statement of theorem 7.3.1 in ref. [8]. The natural measure (14.19) of sect. 14.4.1 is often referred to as the SRB or Sinai-Ruelle-Bowen measure [26, 24, 28].

Remark 14.2 Time evolution as a Lie group: Time evolution of sect. 14.5 is an example of a 1-parameter Lie group. Consult, for example, chapter 2. of ref. [9] for a clear and pedagogical introduction to Lie groups of transformations. For a discussion of the bounded semigroups of page 246 see, for example, Marsden and Hughes [2].

Remark 14.3 Discretization of the Perron-Frobenius operator operator It is an old idea of Ulam [12] that such an approximation for the Perron-Frobenius operator is a meaningful one. The piecewise-linear approximation of the Perron-Frobenius operator (14.14) has been shown to reproduce the spectrum for expanding maps, once finer and finer Markov partitions are used [13, 17, 14]. The subtle point of choosing a state space partitioning for a "generic case" is discussed in ref. [15, 22].

Remark 14.4 The sign convention of the Poisson bracket: The Poisson bracket is antisymmetric in its arguments and there is a freedom to define it with either sign convention. When such freedom exists, it is certain that both conventions are in use and this is no exception. In some texts [9, 3] you will see the right hand side of (14.33) defined as $\{B, A\}$ so that (14.34) is $\frac{dQ}{dt} = \{Q, H\}$. Other equally reputable texts [18] employ the convention used here. Landau and Lifshitz [4] denote a Poisson bracket by $[A, B]$, notation that we reserve here for the quantum-mechanical commutator. As long as one is consistent, there should be no problem.

Remark 14.5 "Anon it lives"? "Anon it lives" refers to a statue of King Leontes's wife, Hermione, who died in a fit of grief after he unjustly accused her of infidelity. Twenty years later, the servant Paulina shows Leontes this statue of Hermione. When he repents, the statue comes to life. Or perhaps Hermione actually lived and Paulina has kept her hidden all these years. The text of the play seems deliberately ambiguous. It is probably a parable for the resurrection of Christ. (John F. Gibson)

Exercises

14.1. **Integrating over Dirac delta functions.** Let us verify a few of the properties of the delta function and check (14.9), as well as the formulas (14.7) and (14.8) to be used later.

(a) If $f : \mathbb{R}^d \to \mathbb{R}^d$, show that

$$\int_{\mathbb{R}^d} dx\, \delta\,(f(x)) = \sum_{x\in f^{-1}(0)} \frac{1}{|\det \partial_x f|}\,.$$

(b) The delta function can be approximated by a sequence of Gaussians

$$\int dx\, \delta(x) f(x) = \lim_{\sigma\to 0} \int dx\, \frac{e^{-\frac{x^2}{2\sigma}}}{\sqrt{2\pi\sigma}} f(x)\,.$$

Use this approximation to see whether the formal expression

$$\int_{\mathbb{R}} dx\, \delta(x^2)$$

makes sense.

14.2. **Derivatives of Dirac delta functions.** Consider $\delta^{(k)}(x) = \frac{\partial^k}{\partial x^k}\delta(x)$.

Using integration by parts, determine the value of

$$\int_{\mathbb{R}} dx\, \delta'(y) \quad , \qquad \text{where } y = f(x) - x \quad (14.41)$$

$$\int dx\, \delta^{(2)}(y) = \sum_{\{x:y(x)=0\}} \frac{1}{|y'|}\left\{3\frac{(y'')^2}{(y')^4} - \frac{y'''}{(y')^3}\right\} \quad (14.42)$$

$$\int dx\, b(x)\delta^{(2)}(y) = \sum_{\{x:y(x)=0\}} \frac{1}{|y'|}\left\{\frac{b''}{(y')^2} - \frac{b'y''}{(y')^3} + b\left(3\frac{(y'')^2}{(y')^4} - \frac{y'''}{(y')^3}\right)\right\} \quad (14.43)$$

These formulas are useful for computing effects of weak noise on deterministic dynamics [5].

14.3. **$\mathcal{L}^t$ generates a semigroup.** Check that the Perron-Frobenius operator has the semigroup property,

$$\int_M dz \mathcal{L}^{t_2}(y,z)\, \mathcal{L}^{t_1}(z,x) = \mathcal{L}^{t_2+t_1}(y,x)\,, \qquad t_1, t_2 \geq 0\,. \quad (14.44)$$

As the flows in which we tend to be interested are invertible, the $\mathcal{L}$'s that we will use often do form a group, with $t_1, t_2 \in \mathbb{R}$.

14.4. **Escape rate of the tent map.**

(a) Calculate by numerical experimentation the log of the fraction of trajectories remaining trapped in the interval $[0, 1]$ for the tent map

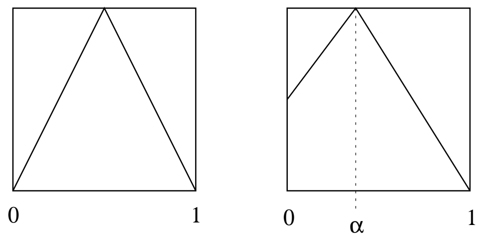
$$f(x) = a(1 - 2|x - 0.5|)$$

for several values of a.

(b) Determine analytically the a dependence of the escape rate $\gamma(a)$.

(c) Compare your results for (a) and (b).

14.5. **Invariant measure.** We will compute the invariant measure for two different piecewise linear maps.



(a) Verify the matrix $\mathcal{L}$ representation (15.19).

(b) The maximum value of the first map is 1. Compute an invariant measure for this map.

(c) Compute the leading eigenvalue of $\mathcal{L}$ for this map.

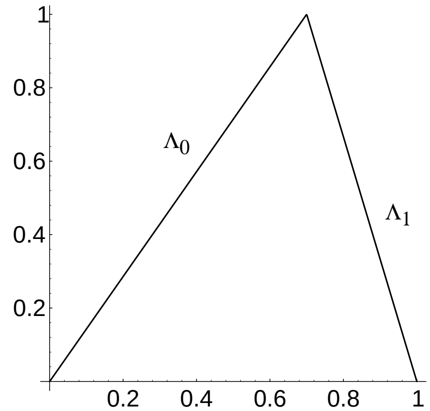
(d) For this map there is an infinite number of invariant measures, but only one of them will be found when one carries out a numerical simulation. Determine that measure, and explain why your choice is the natural measure for this map.

(e) In the second map the maximum occurs at $\alpha = (3 - \sqrt{5})/2$ and the slopes are $\pm(\sqrt{5} + 1)/2$. Find the natural measure for this map. Show that it is piecewise linear and that the ratio of its two values is $(\sqrt{5} + 1)/2$.

(medium difficulty)

14.6. **Escape rate for a flow conserving map.** Adjust Λ_0, Λ_1 in (15.17) so that the gap between the intervals $\mathcal{M}_0$, $\mathcal{M}_1$ vanishes. Show that the escape rate equals zero in this situation.

14.7. **Eigenvalues of the Perron-Frobenius operator for the skew Ulam tent map.** Show that for the skew Ulam tent map



$$f(x) = \begin{cases} f_0(x) = \Lambda_0 x\,, & x \in \mathcal{M}_0 = [0, 1/\Lambda_0) \\ f_1(x) = \frac{\Lambda_0}{\Lambda_0 - 1}(1 - x)\,, & x \in \mathcal{M}_1 = (1/\Lambda_0, 1 \end{cases}$$

the eigenvalues are available analytically, compute the first few.

14.8. **"Kissing disks"*** (continuation of exercises 8.1 and 8.2). Close off the escape by setting $R = 2$, and look in real time at the density of the Poincaré section iterates for a trajectory with a randomly chosen initial condition. Does it look uniform? Should it be uniform? (Hint - phase space volumes are preserved for Hamiltonian flows by the Liouville theorem). Do you notice the trajectories that loiter near special regions of phase space for long times? These exemplify "intermittency," a bit of unpleasantness to which we shall return in chapter 23.

14.9. **Invariant measure for the Gauss map.** Consider the Gauss map:

$$f(x) = \begin{cases} \frac{1}{x} - \left[\frac{1}{x}\right] & x \neq 0 \\ 0 & x = 0 \end{cases} \quad (14.46)$$

where [ ] denotes the integer part.

(a) Verify that the density

$$\rho(x) = \frac{1}{\log 2} \frac{1}{1+x}$$

is an invariant measure for the map.

(b) Is it the natural measure?

14.10. **$\mathcal{A}$ as a generator of translations.** Verify that for a constant velocity field the evolution generator $\mathcal{A}$ in (14.30) is the generator of translations,

$$e^{tv\frac{\partial}{\partial x}} a(x) = a(x + tv).$$

14.11. **Incompressible flows.** Show that (14.9) implies that $\rho_0(x) = 1$ is an eigenfunction of a volume-preserving flow with eigenvalue $s_0 = 0$. In particular, this implies that the natural measure of hyperbolic and mixing Hamiltonian flows is uniform. Compare this results with the numerical experiment of exercise 14.8.

References

[14.1] Ya.G. Sinai, *Topics in Ergodic Theory* (Princeton Univ. Press, Princeton, New Jersey 1994).

[14.2] J.E. Marsden and T.J.R. Hughes, *Mathematical Foundations of Elasticity* (Prentice-Hall, Englewood Cliffs, New Jersey 1983)

[14.3] H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, 1980).

[14.4] L.D. Landau and E.M. Lifshitz, *Mechanics* (Pergamon, London, 1959).

[14.5] P. Cvitanović, C.P. Dettmann, R. Mainieri and G. Vattay, *Trace formulas for stochastic evolution operators: Weak noise perturbation theory*, *J. Stat. Phys.* **93**, 981 (1998); arXiv:chao-dyn/9807034.

[14.6] P. Cvitanović, C.P. Dettmann, R. Mainieri and G. Vattay, *Trace formulas for stochastic evolution operators: Smooth conjugation method*, *Nonlinearity* **12**, 939 (1999); arXiv:chao-dyn/9811003.

[14.7] P. Cvitanović, C.P. Dettmann, G. Palla, N. Søndergård and G. Vattay, *Spectrum of stochastic evolution operators: Local matrix representation approach*, *Phys. Rev.* **E 60**, 3936 (1999); arXiv:chao-dyn/9904027.

[14.8] A. Lasota and M.C. Mackey, *Chaos, Fractals and Noise* (Springer, New York 1994).

[14.9] G. W. Bluman and S. Kumei, *Symmetries and Differential Equations* (Springer, New York 1989).

[14.10] L. Billings and E.M. Bolt, "Invariant densities for skew tent maps," *Chaos Solitons and Fractals* **12**, 365 (2001);
see also www.mathstat.concordia.ca/pg/bilbollt.html.

[14.11] G.D. Birkhoff, *Collected Math. Papers*, Vol. **II** (Amer. Math. Soc., Providence R.I., 1950).

[14.12] S. M. Ulam, *A Collection of Mathematical Problems* (Interscience Publishers, New York, 1960).

[14.13] G. Froyland, *Commun. Math. Phys.* **189**, 237 (1997).