Chapter 7

Transporting densities

O what is my destination? (I fear it is henceforth chaos;)
Walt Whitman,
Leaves of Grass: Out of the Cradle Endlessly Rocking

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

In chapters 2, 3 and 5 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, 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 evolution operators.

7.1 Measures

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

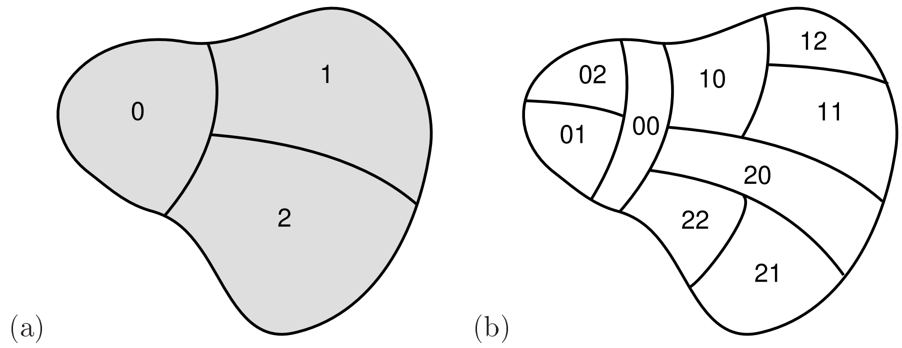

Figure 7.1: (a) First level of partitioning: A coarse partition of $\mathcal{M}$ into regions $\mathcal{M}_0$, $\mathcal{M}_1$, and $\mathcal{M}_2$. (b) $n = 2$ level of partitioning: A refinement of the above partition, with each region $\mathcal{M}_i$ subdivided into $\mathcal{M}_{i0}$, $\mathcal{M}_{i1}$, and $\mathcal{M}_{i2}$.

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 more and more refined partitions of the phase space, fig. 7.1, into regions $\mathcal{M}_i$ defined by the characteristic function

$$\chi_i(x) = \begin{cases} 1 & \text{if } x \in \text{ region } \mathcal{M}_i \\ 0 & \text{otherwise} \end{cases} \,. \tag{7.1}$$

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 phase space:

$$\Delta\mu_i = \int_{\mathcal{M}} d\mu(x)\chi_i(x) = \int_{\mathcal{M}_i} d\mu(x) = \int_{\mathcal{M}_i} dx\, \rho(x) \,. \tag{7.2}$$

$\rho(x) = \rho(x,t)$ is the *density* of representative points in the phase 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. As our intent is to sprinkle the phase space with a finite number of initial points, we shall assume that the measure can be normalized

$$\sum_i^{(n)} \Delta\mu_i = 1 \,, \tag{7.3}$$

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

$$\int_{\mathcal{M}} dx\, \rho(x) = 1\,. \tag{7.4}$$

So far, any arbitrary sequence of partitions will do. What are intelligent ways of partitioning the phase space? We postpone the answer to chapter 9, after we have developed some intuition about how the dynamics transports densities.

☞ chapter 9

7.2 Perron-Frobenius operator

> 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*

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 $t = 0$. As the flow evolves, this region is carried into $f^t(\mathcal{M}_i)$, as in fig. 2.1(b). No trajectory is created or destroyed, so the conservation of representative points requires that

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

If the flow is invertible and the transformation $x_0 = f^{-t}(x)$ is single valued, we can transform the integration variable in the expression on the left to

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

We conclude that the density changes with time as the inverse of the Jacobian (4.46)

$$\rho(x,t) = \frac{\rho(x_0, 0)}{|\det \mathbf{J}^t(x_0)|}\,, \qquad x = f^t(x_0)\,, \tag{7.5}$$

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

The manner in which a flow transports densities may be recast into language of operators, by writing

$$\rho(x,t) = \mathcal{L}^t \rho(x) = \int_{\mathcal{M}} dx_0 \, \delta\big(x - f^t(x_0)\big)\, \rho(x_0, 0)\,. \tag{7.6}$$

Let us check this formula. Integrating Dirac delta functions is easy: $\int_{\mathcal{M}} dx\, \delta(x) = 1$ if $0 \in \mathcal{M}$, zero otherwise. Integral over a one-dimensional Dirac delta function picks up the Jacobian of its argument evaluated at all of its zeros:

$$\int dx\, \delta(h(x)) = \sum_{x \in \mathrm{Zero}\,[h]} \frac{1}{|h(x)'|}\,, \tag{7.7}$$

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and in d dimensions the denominator is replaced by

$$\int dx\, \delta(h(x)) = \sum_{x \in \mathrm{Zero}\,[h]} \frac{1}{\left|\det \frac{\partial h(x)}{\partial x}\right|}\,. \tag{7.8}$$

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Now you can check that (7.6) is just a rewrite of (7.5):

$$\begin{aligned} \mathcal{L}^t \rho(x) &= \sum_{x_0 = f^{-t}(x)} \frac{\rho(x_0)}{|f^t(x_0)'|} && \text{(1-dimensional)} \\ &= \sum_{x_0 = f^{-t}(x)} \frac{\rho(x_0)}{|\det \mathbf{J}^t(x_0)|} && \text{(d-dimensional)}\,. \end{aligned} \tag{7.9}$$

For a deterministic, invertible flow there is only one x_0 preimage of x; allowing for multiple preimages also takes account of noninvertible mappings such as the "stretch&fold" maps of the interval, to be discussed in the next example, or more generally in sect. 9.4.

We shall refer to the kernel of (7.6) as the *Perron-Frobenius operator*:

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$$\mathcal{L}^t(x,y) = \delta\big(x - f^t(y)\big)\,. \tag{7.10}$$

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remark 12.4

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. 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 $t = 0$.

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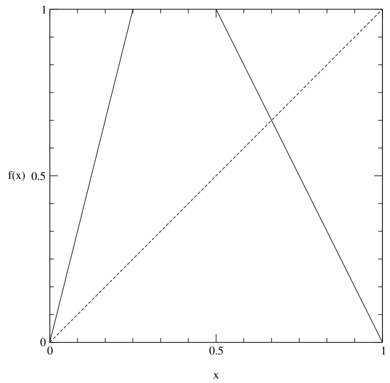

Figure 7.2: A piecewise-linear repeller (7.11): All trajectories that land in the gap between the f_0 and f_1 branches escape ($\Lambda_0 = 4$, $\Lambda_1 = -2$).

Example 7.1 A piecewise-linear example

What is gained by reformulation of dynamics in terms of "operators"? We start by considering a simple example where the operator is a $[2 \times 2]$ *matrix. Assume the expanding 1-*d *map* $f(x)$ *of fig. 7.2, a piecewise-linear 2–branch repeller with slopes* $\Lambda_0 > 1$ *and* $\Lambda_1 < -1$ *:*

$$f(x) = \begin{cases} f_0 = \Lambda_0 x & \text{if} \quad x \in \mathcal{M}_0 = [0, 1/\Lambda_0] \\ f_1 = \Lambda_1(x-1) & \text{if} \quad x \in \mathcal{M}_1 = [1 + 1/\Lambda_1, 1] \end{cases} . \tag{7.11}$$

Both $f(\mathcal{M}_0)$ *and* $f(\mathcal{M}_1)$ *map onto the entire unit interval* $\mathcal{M} = [0,1]$*. Assume a piecewise constant density*

$$\rho(x) = \begin{cases} \rho_0 & \text{if } x \in \mathcal{M}_0 \\ \rho_1 & \text{if } x \in \mathcal{M}_1 \end{cases} . \tag{7.12}$$

There is no need to define $\rho(x)$ *in the gap between* $\mathcal{M}_0$ *and* $\mathcal{M}_1$*, as any point that lands in the gap escapes. The physical motivation for studying this kind of mapping is the pinball game:* f *is the simplest model for the pinball escape, fig. 1.7, with* f_0 *and* f_1 *modelling its two strips of survivors.*

As can be easily checked by using (7.9), the Perron-Frobenius operator acts on this piecewise constant function as a [2×2] "transfer" matrix with matrix elements

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$$\begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} \to \mathcal{L}\rho = \begin{pmatrix} \frac{1}{|\Lambda_0|} & \frac{1}{|\Lambda_1|} \\ \frac{1}{|\Lambda_0|} & \frac{1}{|\Lambda_1|} \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} , \tag{7.13}$$

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stretching both ρ_0 *and* ρ_1 *over the whole unit interval* Λ*, and decreasing the density at every iteration. As in this example the density is constant after one iteration,* $\mathcal{L}$ *has only one non-zero eigenvalue* $e^{s_0} = 1/|\Lambda_0| + 1/|\Lambda_1|$*, with the constant density eigenvector* $\rho_0 = \rho_1$. $1/|\Lambda_0|$, $1/|\Lambda_1|$ *are respectively the sizes of* $|\mathcal{M}_0|$, $|\mathcal{M}_1|$ *intervals, so the* exact *escape rate (1.3) – the log of the fraction of survivors at each iteration for this linear repeller – is given by the sole eigenvalue of* $\mathcal{L}$*:*

$$\gamma = -s_0 = -\ln(1/|\Lambda_0| + 1/|\Lambda_1|) . \tag{7.14}$$

Voila! Here is the rationale for introducing operators – in one time step we have solved the problem of evaluating escape rate at infinite time. This simple explicit matrix *representation of the Perron-Frobenius operator is a consequence of piecewise linearity of f, and the restriction of the densities ρ to the space of piecewise constant functions. The example gives a foretaste of the enterprise upon which we are to embark in this book, but the full story is much subtler: in general case there will exist no such finite-dimensional representation for the Perron-Frobenius operator.*

To a student with practical bend the example does suggest a strategy for constructing evolution operators for smooth maps, as limits of partitions of phase space into regions $\mathcal{M}_i$, with a piecewise-linear approximation f_i to 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 13

7.3 Invariant measures

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

$$\rho(x,t) = \rho(x,0) = \rho(x)\,. \tag{7.15}$$

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 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 (7.10), with the unit eigenvalue:

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$$\mathcal{L}^t\rho(x) = \int_{\mathcal{M}} dy\, \delta(x - f^t(y))\rho(y) = \rho(x). \tag{7.16}$$

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 (7.16). For instance, a singular measure $d\mu(x) = \delta(x - x^*)dx$ concentrated on an equilibrium point $x^* = f^t(x^*)$, or any linear combination of such measures, each concentrated on a different equilibrium point, is stationary. So there are infinitely many stationary measures you can construct, almost all of them unnatural in the sense that a slightest perturbation will destroy them.

From a physical point of view, there is no way to prepare initial densities which are singular, so it makes sense to concentrate on measures which are limits of transformations which an initial smooth distribution $\rho(x)$ experiences under the action of f, rather than as a limit computed from a single trajectory,

$$\rho_0(x) = \lim_{t\to\infty} \int_{\mathcal{M}} dy\, \delta(x - f^t(y))\rho(y,0)\,, \qquad \int_{\mathcal{M}} dy\, \rho(y,0) = 1\,. \quad (7.17)$$

Intuitively, the "natural" measure should also be the one least sensitive to inevitable facts of life, such as noise, not matter how weak.

7.3.1 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*

The *natural* or *equilibrium measure* can be defined as the limit

$$\overline{\rho}_{x_0}(y) = \begin{cases} \lim_{t\to\infty} \frac{1}{t}\int_0^t d\tau\, \delta(y - f^\tau(x_0)) & \text{flows} \\ \lim_{n\to\infty} \frac{1}{n}\sum_{k=0}^{n-1} \delta\big(y - f^k(x_0)\big) & \text{maps} \end{cases}, \quad (7.18)$$

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where x_0 is a generic inital point. Staring at an average over ∞ many Dirac deltas is not a prospect we cherish. Generated by the action of f, the natural measure satisfies the stationarity condition (7.16) and is thus invariant by construction. From the computational point of view, the natural measure is the visitation frequency defined by coarse-graining, integrating (7.18) over the $\mathcal{M}_i$ region

$$\Delta\overline{\mu}_i = \lim_{t\to\infty} \frac{t_i}{t}\,, \quad (7.19)$$

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 $\rho(x)$.

Let $a = a(x)$ be any *observable*. In 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 phase space a number or a set of numbers. In physical application the observable $a(x)$ is of necessity a smooth function. The observable reports on some property of the dynamical system (several examples will be given in sect. 8.1).

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

$$\langle a \rangle_\rho = \frac{1}{|\rho_\mathcal{M}|}\int_\mathcal{M} dx\, \rho(x)a(x)\,, \quad |\rho_\mathcal{M}| = \int_\mathcal{M} dx\, \rho(x) = \text{mass in } \mathcal{M}\,. \tag{7.20}$$

For the time being we assume that the phase space $\mathcal{M}$ has a finite dimension and a finite volume. By its definition $\langle a \rangle_\rho$ is a function(al) of ρ.

Inserting the right hand side of (7.18) into (7.20) we see that the natural measure corresponds to *time average* of the observable a along a trajectory of the initial point x_0,

$$\overline{a(x_0)} = \lim_{t\to\infty} \frac{1}{t}\int_0^t d\tau\, a(f^\tau(x_0))\,. \tag{7.21}$$

☞ appendix A

Analysis of the above asymptotic time limit is the central problem of ergodic theory. More precisely, the Birkhoff ergodic theorem asserts that if a natural measure ρ exists, the limit $\overline{a(x_0)}$ for the time average (7.21) 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 over almost any trajectory tends to the space average

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t d\tau\, a(f^\tau(x_0)) = \langle a \rangle \tag{7.22}$$

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, stronger than ergodicity: if you can establish the space average of a product of any two variables decorrelates with time,

$$\lim_{t\to\infty} \left\langle a(x)b(f^t(x))\right\rangle = \langle a \rangle \langle b \rangle\,, \tag{7.23}$$

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the dynamical system is said to be *mixing*.

An example of a numerical calculation of the natural measure (7.19) for the Hénon attractor (3.10) is given by the histogram of fig. 7.3. The phase space is partitioned into many equal size areas $\mathcal{M}_i$, and the coarse grained measure (7.19) computed by a long time iteration of the Hénon map, and represented by the height of the column over area $\mathcal{M}_i$. What you see is a typical invariant measure - a complicated, singular function concentrated

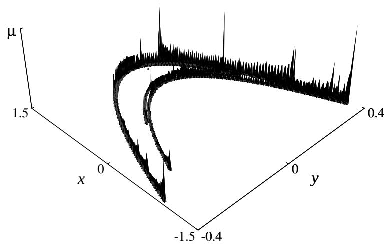

Figure 7.3: Natural measure (7.19) for the Hénon map (3.10) strange attractor at parameter values $(a, b) = (1.4, 0.3)$. See fig. 3.4 for a sketch of the attractor without the natural measure binning. (Courtesy of J.-P. Eckmann)

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 limited physical import. No smooth inital density will converge to this measure if the dynamics is unstable. In practice the average (7.18) 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, is a strange attractor or merely a long stable cycle.

8.1
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While dynamics can lead to very singular ρ's, in any physical setting we cannot do better than to measure it 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 on: for deterministic flows our trace and determinant formulas will be *exact*, while for quantum and stochastic flows they will only be the leading saddlepoint approximations. Clearly, while deceptively easy to define, measures spell trouble. The good news is that if you hang on, you will never ever need to compute them, not in this book. How so? The evolution operators that we turn to next, and the trace and determinant formulas that they will lead us to will assign the correct natural measure weights to desired averages without recourse to any explicit computation of the coarse-grained measure $\Delta\rho_i$.

chapter 12

7.4 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 $\delta\tau$:

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

$$\rho(x, \delta\tau) \;=\; \rho(x,0) - \delta\tau \sum_{i=1}^{d} \frac{\partial}{\partial x_i}(v_i(x)\rho(x,0))\,. \tag{7.24}$$

Here we have used the infinitesimal form of the flow (2.5), Dirac delta jacobian (7.9), and the $\ln \det = \operatorname{tr} \ln$ relation. 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:

$$\partial_t \rho + \partial \cdot (\rho v) \;=\; 0\,. \tag{7.25}$$

The family of Perron-Frobenius operators operators $\left\{\mathcal{L}^t\right\}_{t\in\mathbb{R}_+}$ forms a semi-group parametrized 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) .

The *generator* of the semigroup, the generator of infinitesimal time translation by an infinitesimal step $\delta\tau$ is determined by (7.24)

$$\mathcal{A}\rho(x) \;=\; + \lim_{\delta\tau\to 0^+} \frac{1}{\delta\tau}\left(\mathcal{L}^{\delta\tau} - I\right)\rho(x)\,.\;=\; -\partial_i(v_i(x)\rho(x))\,. \tag{7.26}$$

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

$$\left(\frac{\partial}{\partial t} - \mathcal{A}\right)\rho(x) \;=\; 0\,. \tag{7.27}$$

☞ appendix D.3

The above statements apply to any deterministic flow. If the density itself is a material invariant, combining (D.1) and (7.25) we conclude that $\partial_i v_i = 0$ and $\mathbf{J}^t(x_0) = 1$. An example of such incompressible flow is the Hamiltonian flow of sect. 5.1.1. For incompressible flows the continuity equation (7.25) becomes a statement of conservation of the phase space volume (see sect. 5.1.1), or the *Liouville theorem*

$$\partial_t \rho + v_i \partial_i \rho = 0\,. \tag{7.28}$$

The finite time Perron-Frobenius operator (7.10) can be formally expressed by exponentiating the time evolution generator $\mathcal{A}$ as

$$\mathcal{L}^t = e^{t\mathcal{A}} . \tag{7.29}$$

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

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$$e^{-tv\frac{\partial}{\partial x}} a(x) = a(x - tv) . \tag{7.30}$$

As we will not need to implement a computational formula for general $e^{t\mathcal{A}}$ in what follows, we relegate making sense of such operators to appendix D.3. Here we limit ourselves to a brief remark about the notion of "spectrum" of a linear operator.

appendix D.3

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 we defined the matrix norms in sect. K.2: 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 (7.14). 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

$$\int_0^\infty dt\, e^{-st}\mathcal{L}^t = \frac{1}{s - \mathcal{A}} , \qquad \mathrm{Re}\, s > \beta , \tag{7.31}$$

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

sect. K.2

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

If one is interested in the spectrum of $\mathcal{L}$, as we will be, the resolvent operator is a natural object to study. The main lesson of this brief aside is that for the continuous time flows the Laplace transform is the tool that brings down the generator in (7.29) into the resolvent form (7.31) and enables us to study its spectrum.

in depth:
appendix D.3, p. 631

7.4.1 Liouville operator

A case of special interest is the Hamiltonian or symplectic flow defined by the time-independent Hamilton's equations of motion (5.1). 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, (7.27) looks rather much 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.

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

$$\dot{q}_i = \frac{p_i}{m}, \qquad \dot{p}_i = -\frac{\partial V(q)}{\partial q_i}. \tag{7.32}$$

The evolution equations for any p, q dependent quantity $Q = Q(p, q)$ are given by

$$\frac{dQ}{dt} = \frac{\partial Q}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial Q}{\partial p_i}\frac{dp_i}{dt} = \frac{\partial H}{\partial p_i}\frac{\partial Q}{\partial q_i} - \frac{\partial Q}{\partial p_i}\frac{\partial H}{\partial q_i}. \tag{7.33}$$

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

$$[A, B] = \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} - \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i}. \tag{7.34}$$

In terms of Poisson brackets the time evolution equation (7.33) takes the compact form

$$\frac{dQ}{dt} = [H, Q]. \tag{7.35}$$

The phase space flow velocity is $\mathbf{v} = (\dot{q}, \dot{p})$, where the dot signifies time derivative for fixed initial point. Hamilton's equations (5.1) 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 density:

appendix D

$$\partial_t \rho + \partial_i (\rho v_i) = 0 \,. \tag{7.36}$$

Consider evolution of the phase space density ρ of an ensemble of noninteracting particles subject to the potential $V(q)$; 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 (5.1) we obtain the *Liouville equation*, a special case of (7.27):

$$\frac{\partial}{\partial t}\rho(q,p,t) = -\mathcal{A}\rho(q,p,t) = [H, \rho(q,p,t)] \,, \tag{7.37}$$

where [,] is the Poisson bracket (7.34). The generator of the flow (7.26) is now the generator of infinitesimal symplectic transformations,

$$\mathcal{A} = \dot{q}_i \frac{\partial}{\partial q_i} + \dot{p}_i \frac{\partial}{\partial p_i} = \frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i} \,. \tag{7.38}$$

or, by the Hamilton's equations for separable Hamiltonians

$$\mathcal{A} = -\frac{p_i}{m}\frac{\partial}{\partial q_i} + \partial_i V(q) \frac{\partial}{\partial p_i} \,. \tag{7.39}$$

7.12
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This special case of the time evolution generator (7.26) 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, or along a road from Liouville to Boltzmann. Here its action will be very tangible; we shall apply the evolution operator to systems as small as 1 or 2 hard balls and to our surprise learn that that suffices to get a grip on the foundations of the classical nonequilibrium statistical mechanics.

in depth:
sect. D.3, p. 631

Commentary

Remark 7.1 Ergodic theory. An overview of ergodic theory is outside the scope of this book: the interested reader may find it useful to consult [7.1]. The existence of time average (7.21) is the basic result of ergodic theory, known as the Birkhoff theorem, see for example refs. [7.1, 1.11], or the statement of the theorem 7.3.1 in ref. [D.1]. The natural measure (7.19) (more carefully defined than in the above sketch) is often referred to as the SBR or Sinai-Bowen-Ruelle measure [1.14, 1.13, 1.16].

Remark 7.2 Bounded semigroup. For a discussion of bounded semigroups of page 115 see, for example, Marsden and Hughes [7.2].

Résumé

In physically realistic setting initial state of a system can be specified only to a finite precision. Depending on the desired precision, and given a deterministic law of evolution, h, the system can then be tracked for some finite time, however, if dynamics is chaotic, it is not possible to calculate accurately the long time trajectory of a given initial point. Hence, the study of long time dynamics requires going into a trading in evolution of a single phase space point for the evolution of the *measure*, or the *density* of representative points in phase space, acted upon by an *evolution operator*. Essentially this means trading in nonlinear dynamical equations on finite low-dimensional spaces $x = (x_1, x_2 \cdots x_d)$ for linear equations on infinite dimensional vector spaces of density functions $\rho(x)$.

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 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 accessible to measure is the energy spectrum.

For long times the dynamics is described in terms of stationary measures, that is, fixed points of certain evolution operators. The most physical of stationary measures is the natural measure, a measure robust under perturbations by weak noise.

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 the 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 this altogether.

References

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

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

[7.3] 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); `chao-dyn/9807034`.

[7.4] We thank Laurette Tuckerman for providing us with the pseudospectral code.

[7.5] We have used the NAG library integration routine D02BHF. Our code and numerical results are available on `www.nbi.dk/ChaosBook/extras`.