confession!St. Augustine
St. Augustine

Chapter 9

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*

what does "anon it lives" refer to?

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

In chapters 2, 3, 5 and 6 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.

9.1 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

coarse-graining
partition!state space
state space!partition
characteristic!function
measure
density

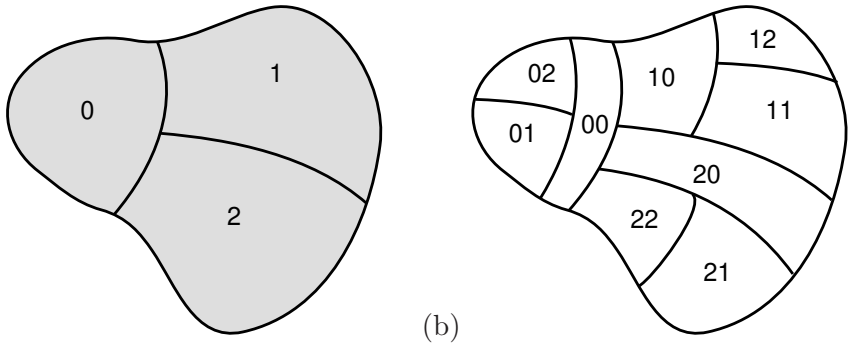

Figure 9.1: (a) First level of partitioning: A coarse partition of $\mathcal{M}$ into regions $\mathcal{M}_0$, $\mathcal{M}_1$, and $\mathcal{M}_2$. (b) $n = 2$ level of partitioning: A refinement of the above partition, with each region $\mathcal{M}_i$ subdivided into $\mathcal{M}_{i0}$, $\mathcal{M}_{i1}$, and $\mathcal{M}_{i2}$.

of *coarse-graining*. Consider a sequence 1, 2, ..., n, ... of increasingly refined partitions of state space, figure 9.1, into regions $\mathcal{M}_i$ defined by the characteristic function

$$\chi_i(x) = \begin{cases} 1 & \text{if } x \in \mathcal{M}_i\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{9.1}$$

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:

$$\Delta\mu_i = \int_{\mathcal{M}} d\mu(x)\chi_i(x) = \int_{\mathcal{M}_i} d\mu(x) = \int_{\mathcal{M}_i} dx\,\rho(x)\,. \tag{9.2}$$

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. As our intent is to sprinkle state space with a finite number of initial points (repeat an experiment a finite number of times), we shall assume that the measure can be normalized

AH, MAP: define Lebesgue measure

$$\sum_i^{(n)} \Delta\mu_i = 1\,, \tag{9.3}$$

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

$$\int_{\mathcal{M}} dx\ \rho(x) = 1\,. \tag{9.4}$$

So far, any arbitrary sequence of partitions will do. What are intelligent ways of partitioning state space? We postpone the answer to chapter 11, after we have developed some intuition about how the dynamics transports densities.

Jacobian
Dirac delta function

☞ chapter 11

9.2 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 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

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

We conclude that the density changes with time as the inverse of the Jacobian (4.36)

$$\rho(x,t) = \frac{\rho(x_0,0)}{|\det M^t(x_0)|}\,, \qquad x = f^t(x_0)\,, \tag{9.5}$$

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 the language of operators, by writing

$$\rho(x,t) = \mathcal{L}^t\rho(x) = \int_{\mathcal{M}} dx_0\, \delta\big(x - f^t(x_0)\big)\, \rho(x_0,0)\,. \tag{9.6}$$

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. The integral over a one-dimensional Dirac delta function picks up the Jacobian of its argument evaluated at all of its zeros:

$$\int dx\, \delta(h(x)) = \sum_{\{x:h(x)=0\}} \frac{1}{|h'(x)|}\,, \tag{9.7}$$

Dirac delta function
delta function!Dirac
Perron-Frobenius!operator
operator!Perron-Frobenius

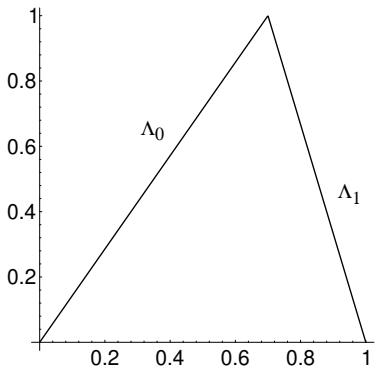

Figure 9.2: A piecewise-linear skew "Ulam tent" map (9.11) ($\Lambda_0 = 4/3$, $\Lambda_1 = -4$).

and in d dimensions the denominator is replaced by

9.1 page 146

$$\int dx\, \delta(h(x)) = \sum_{\{x:h(x)=0\}} \frac{1}{\left|\det \frac{\partial h(x)}{\partial x}\right|} \,. \tag{9.8}$$

use my transparencies here.

9.2 page 146

Now you can check that (9.6) is just a rewrite of (9.5):

$$\begin{aligned} \mathcal{L}^t \rho(x) &= \sum_{x_0=f^{-t}(x)} \frac{\rho(x_0)}{|f^{t\prime}(x_0)|} && \text{(1-dimensional)} \\ &= \sum_{x_0=f^{-t}(x)} \frac{\rho(x_0)}{|\det M^t(x_0)|} && (d\text{-dimensional})\,. \end{aligned} \tag{9.9}$$

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. 11.3.1.

We shall refer to the kernel of (9.6) as the *Perron-Frobenius operator*:

9.3 page 146

$$\mathcal{L}^t(x,y) = \delta\big(x - f^t(y)\big) \,. \tag{9.10}$$

remember to link with (10.24)

example 16.7

remark 15.4

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 $t=0$.

move this remark to ?: (for nomenclature, see remark 15.4).

in depth: appendix E, p. 907

Example 9.1 Perron-Frobenius operator for a piecewise-linear map: *Assume the expanding 1-d map $f(x)$ of figure 9.2, a piecewise-linear 2–branch map with slopes $\Lambda_0 > 1$ and $\Lambda_1 = -\Lambda_0/(\Lambda_0 - 1) < -1$:*

9.7 page 148

$$f(x) = \begin{cases} f_0(x) = \Lambda_0 x\,, & x \in \mathcal{M}_0 = [0, 1/\Lambda_0) \\ f_1(x) = \frac{\Lambda_0}{\Lambda_0 - 1}(1 - x)\,, & x \in \mathcal{M}_1 = (1/\Lambda_0, 1]\,. \end{cases} \tag{9.11}$$

transfer!matrix
stationary!state
measure!invariant
invariant!measure

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

$$\rho(x) = \begin{cases} \rho_0 & \text{if } x \in \mathcal{M}_0 \\ \rho_1 & \text{if } x \in \mathcal{M}_1 \end{cases}\,. \tag{9.12}$$

As can be easily checked using (9.9), the Perron-Frobenius operator acts on this piecewise constant function as a [2×2] "transfer" matrix with matrix elements

9.1 page 146

$$\begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix} \to \mathcal{L}\rho = \begin{pmatrix} \frac{1}{|\Lambda_0|} & \frac{1}{|\Lambda_1|} \\ \frac{1}{|\Lambda_0|} & \frac{1}{|\Lambda_1|} \end{pmatrix} \begin{pmatrix} \rho_0 \\ \rho_1 \end{pmatrix}\,, \tag{9.13}$$

9.5 page 147

introduce, explain "transfer" matrix

stretching both ρ_0 and ρ_1 over the whole unit interval Λ. In this example the density is constant after one iteration, so $\mathcal{L}$ 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 enterprise 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 10.1.)

To a student with a practical bent the example 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 16

9.3 Invariant measures

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

rethink - where did the Jacobian in (9.5) go?

$$\rho(x, t) = \rho(x, 0) = \rho(x)\,. \tag{9.14}$$

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 (9.10), with the unit eigenvalue:

repeller measures?

9.3 page 146

equilibrium!point
confession!C.N. Yang
Yang, C.N.
natural measure
measure!natural

$$\mathcal{L}^t\rho(x) = \int_{\mathcal{M}} dy\, \delta(x - f^t(y))\rho(y) = \rho(x). \tag{9.15}$$

resurect after replacing with the no-escape example the above.

⇑PRELIMINARY

⇓PRELIMINARY

For the piecewise linear map example worked out above, in example 10.1, we have already constructed explicitly such eigenfunction, $\rho(y) = \text{const.}$, with eigenvalue 1. 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 (9.15). 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 it makes sense to concentrate on measures which are limits of transformations experienced by an initial smooth distribution $\rho(x)$ under the action of f, rather than as a limit computed from a single trajectory,

$$\rho_0(x) = \lim_{t\to\infty} \int_{\mathcal{M}} dy\, \delta(x - f^t(y))\rho(y,0)\,, \qquad \int_{\mathcal{M}} dy\, \rho(y,0) = 1\,. \tag{9.16}$$

Intuitively, the "natural" measure (or measures) should be the least sensitive to facts of life, such as noise (no matter how weak).

connect to chapter 35: make the robustness under external noise more convincing here

9.3.1 Natural measure

add to refsMeasure.tex

> **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

$$\overline{\rho}_{x_0}(y) \quad = \quad \begin{cases} \lim_{t\to\infty} \frac{1}{t} \int_0^t d\tau\, \delta(y - f^\tau(x_0)) & \text{flows} \\ \lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} \delta\big(y - f^k(x_0)\big) & \text{maps}\,, \end{cases} \tag{9.17}$$

9.8 page 148
9.9 page 148

where x_0 is a generic inital point. [1] Staring at an average over infinitely many Dirac deltas is not a prospect we cherish. Generated by the action of f, the natural measure satisfies the stationarity condition (9.15) and is thus invariant by construction. From a computational point of view, the natural

[1] Driebe: emphasize generic, not periodic: use normal (Borel definition of irrationals) vs. non-normal. Explained in the green book edited by Series

measure is the visitation frequency defined by coarse-graining, integrating (9.17) over the $\mathcal{M}_i$ region

visitation frequency
observable
average!space
space!average
functional
time!average
average!time
ergodic!theory
ergodic!average
Birkhoff!ergodic theorem

$$\Delta\overline{\mu}_i = \lim_{t\to\infty} \frac{t_i}{t}\,, \tag{9.18}$$

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 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. 10.1.

put pointer, refer to the example there

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

$$\begin{aligned} \langle a\rangle_\rho &= \frac{1}{|\rho_{\mathcal{M}}|}\int_{\mathcal{M}} dx\,\rho(x)a(x) \\ |\rho_{\mathcal{M}}| &= \int_{\mathcal{M}} dx\,\rho(x) = \text{mass in } \mathcal{M}\,. \end{aligned} \tag{9.19}$$

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.

Inserting the right-hand-side of (9.17) into (9.19), we see that the natural measure corresponds to a *time average* of the observable a along a trajectory of the initial point x_0,

$$\overline{a_{x_0}} = \lim_{t\to\infty} \frac{1}{t}\int_0^t d\tau\, a(f^\tau(x_0))\,. \tag{9.20}$$

☞ appendix A

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 (9.20) 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

definition of ergodic (Webster?)

$$\lim_{t\to\infty} \frac{1}{t}\int_0^t d\tau\, a(f^\tau(x_0)) = \langle a\rangle \tag{9.21}$$

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.

explain we drop suffix ρ if ρ is the natural measure

mixing
Henon@Hénon!attractor
deterministic flow
flow!deterministic
stochastic flow
flow!stochastic
evolution!kernel!probabilistic

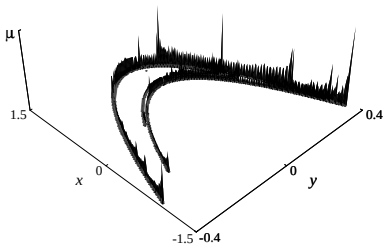

Figure 9.3: Natural measure (9.18) for the Hénon map (3.15) strange attractor at parameter values $(a, b) = (1.4, 0.3)$. See figure 3.5 for a sketch of the attractor without the natural measure binning. (Courtesy of J.-P. Eckmann)

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, explain *mixing*

$$\lim_{t\to\infty} \langle a(x)b(f^t(x))\rangle = \langle a\rangle \langle b\rangle \ , \tag{9.22}$$

☞ sect. 19.4

the dynamical system is said to be *mixing*.

Example 9.2 The Hénon attractor natural measure: *A numerical calculation of the natural measure (9.18) for the Hénon attractor (3.15) is given by the histogram in figure 9.3. The state space is partitioned into many equal-size areas $\mathcal{M}_i$, and the coarse grained measure (9.18) 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 limited physical import. (See however discussion of orbital measures, sect. **??**). No smooth inital density will converge to this measure if the dynamics is unstable. In practice the average (9.17) 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.

⇓PRELIMINARY
⇑PRELIMINARY

10.1
page 169

Genuflect here to refs. [12.34, 12.35, 12.36]

9.3.2 Determinism vs. stochasticity

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: for deterministic flows our trace and determinant formulas will be *exact*, while for quantum and stochastic flows they will only be the leading saddlepoint (stationary phase, steepest descent) approximations.

☞ chapter 15

refer to noise.tex as well

☞ chapter 34

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 $\Delta\rho_i$.

continuity equation
semigroup
group!semi-

9.4 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 $\delta\tau$:

$$\begin{aligned}
\mathcal{L}^{\delta\tau}\rho(y) &= \int_{\mathcal{M}} dx\, \delta\Big(y - f^{\delta\tau}(x)\Big)\, \rho(x) \\
&= \int_{\mathcal{M}} dx\, \delta(y - x - \delta\tau v(x))\, \rho(x) \\
&= \frac{\rho(y - \delta\tau v(y))}{\left|\det\left(1 + \delta\tau \frac{\partial v(y)}{\partial x}\right)\right|} = \frac{\rho(y) - \delta\tau \sum_{i=1}^{d} v_i(y)\partial_i\rho(y)}{1 + \delta\tau \sum_{i=1}^{d} \partial_i v_i(y)} \\
\rho(x,\delta\tau) &= \rho(x,0) - \delta\tau \sum_{i=1}^{d} \frac{\partial}{\partial x_i}(v_i(x)\rho(x,0))\,. \qquad (9.23)
\end{aligned}$$

Here we have used the infinitesimal form of the flow (2.5), the Dirac delta Jacobian (9.9), and the $ln\, det = tr\, ln$ 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:

4.1
page 78

$$\partial_t\rho + \partial\cdot(\rho v) = 0\,. \qquad (9.24)$$

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

From (9.23), time evolution by an infinitesimal step $\delta\tau$ is generated by

$$\mathcal{A}\rho(x) = +\lim_{\delta\tau\to 0^+} \frac{1}{\delta\tau}\left(\mathcal{L}^{\delta\tau} - I\right)\rho(x) = -\partial_i(v_i(x)\rho(x))\,. \qquad (9.25)$$

We shall refer to

$$\mathcal{A} = -\partial\cdot v + \sum_{i}^{d} v_i(x)\partial_i \qquad (9.26)$$

flow!generator of
looks like Hamiltonian
generator of flow but it is not
operator!semigroup!bounded
semigroup!operator
Laplace!transform
resolvent!operator
operator!resolvent

as the time evolution (semigroup) *generator*. If the flow is finite-dimensional and invertible, $\mathcal{A}$ is a generator of a full-fledged group. The left hand side of (9.25) is the definition of time derivative, so the evolution equation for $\rho(x)$ is

$$\left(\frac{\partial}{\partial t} - \mathcal{A}\right)\rho(x) \;=\; 0\,. \tag{9.27}$$

☞ appendix E.2

The finite time Perron-Frobenius operator (9.10) can be formally expressed by exponentiating the time evolution generator $\mathcal{A}$ as

$$\mathcal{L}^t = e^{t\mathcal{A}}\,. \tag{9.28}$$

⇓PRELIMINARY
?? page ??
⇑PRELIMINARY
9.10 page 148

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):

$$e^{-tv\frac{\partial}{\partial x}}a(x) = a(x - tv)\,. \tag{9.29}$$

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 E.2.

☞ appendix E.2

9.4.1 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 (see appendix M.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 (10.20). 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

☞ appendix M.2

EAS: need to define the norm of this operator

$$\int_0^\infty dt\, e^{-st}\mathcal{L}^t = \frac{1}{s - \mathcal{A}}\,, \qquad \mathrm{Re}\, s > \beta\,, \tag{9.30}$$

$\mathcal{A}$ sign wrong here

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

☞ sect. M.2

cause separation into constituents)

Poisson!bracket

be also as Fourier sform of (9.27), a en's" function

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

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 continuous time flows, the Laplace transform is the tool that brings down the generator in (9.28) into the resolvent form (9.30) and enables us to study its spectrum.

in depth:
appendix E.2, p. 909

9.5 Liouville operator

A case of special interest is the Hamiltonian or symplectic flow defined by the 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, (9.27) 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 (5.1) for any time-independent quantity $Q = Q(q,p)$ are given by

$$\frac{dQ}{dt} = \frac{\partial Q}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial Q}{\partial p_i}\frac{dp_i}{dt} = \frac{\partial H}{\partial p_i}\frac{\partial Q}{\partial q_i} - \frac{\partial Q}{\partial p_i}\frac{\partial H}{\partial q_i}\,. \tag{9.31}$$

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

$$\{A,B\} = \frac{\partial A}{\partial p_i}\frac{\partial B}{\partial q_i} - \frac{\partial A}{\partial q_i}\frac{\partial B}{\partial p_i}\,. \tag{9.32}$$

Gaspard has $\{A,B\}$ defined the other way around; use $\{,\}$

In terms of Poisson brackets the time evolution equation (9.31) takes the compact form

$$\frac{dQ}{dt} = \{H,Q\}\,. \tag{9.33}$$

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

flow!incompressible
conservation!phase space volume
Liouville!theorem
density!phase space
phase space!density
continuity!equation
Liouville!equation
Poisson!bracket
symplectic!transformation

The discussion of sect. 9.4 applies to any deterministic flow. If the density itself is a material invariant, combining (??) and (9.24) we conclude that $\partial_i v_i = 0$ and $\det M^t(x_0) = 1$. An example of such incompressible flow is the Hamiltonian flow of sect. 5.2. For incompressible flows the continuity equation (9.24) becomes a statement of conservation of the state space volume (see sect. 5.2), or the *Liouville theorem*

⇓PRIVATE
⇑PRIVATE

$$\partial_t \rho + v_i \partial_i \rho = 0\,. \tag{9.34}$$

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 phase space density:

☞ appendix E

confused - conflicts with (9.24) and (9.34)

$$\partial_t \rho + \partial_i(\rho v_i) = 0\,. \tag{9.35}$$

reference is Goldstein

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

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

recheck sign!

Inserting Hamilton's equations (5.1) we obtain the *Liouville equation*, a special case of (9.27):

$$\frac{\partial}{\partial t}\rho(q,p,t) = -\mathcal{A}\rho(q,p,t) = \{H, \rho(q,p,t)\}\,, \tag{9.36}$$

rescue the Poisson brackets from appendix D

where $\{\ ,\ \}$ is the Poisson bracket (9.32). The generator of the flow (9.26) is now the generator of infinitesimal symplectic transformations,

$$\mathcal{A} = \dot{q}_i\frac{\partial}{\partial q_i} + \dot{p}_i\frac{\partial}{\partial p_i} = \frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i}\,. \tag{9.37}$$

photoshop

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

$$\dot{q}_i = \frac{p_i}{m}\,, \qquad \dot{p}_i = -\frac{\partial V(q)}{\partial q_i}\,. \tag{9.38}$$

move to appendix F

and the action of the generator

$$\mathcal{A} = -\frac{p_i}{m}\frac{\partial}{\partial q_i} + \partial_i V(q)\frac{\partial}{\partial p_i}\,. \tag{9.39}$$

9.11
page 149

man notation is $-\mathcal{A}$

can be interpreted as a translation (9.29) in configuration space, followed by acceleration by force $\partial V(q)$ in the momentum space.

Liouville!operator
operator!Liouville
Poisson!bracket

This special case of the time evolution generator (9.26) 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. 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 alredy get a bit of a grip on foundations of the classical nonequilibrium statistical mechanics.

in depth:
sect. E.2, p. 909

Commentary

Remark 9.1 Ergodic theory: An overview of ergodic theory is outside the scope of this book: the interested reader may find it useful to consult ref. [9.1]. The existence of time average (9.20) is the basic result of ergodic theory, known as the Birkhoff theorem, see for example refs. [9.1, 1.20], or the statement of theorem 7.3.1 in ref. [9.8]. The natural measure (9.18) (more carefully defined than in the above sketch) is often referred to as the SRB or Sinai-Ruelle-Bowen measure [1.24, 1.22, 1.26].

Remark 9.2 Time evolution as a Lie group: Time evolution of sect. 9.4 is an example of a 1-parameter Lie group. Consult, for example, chapter 2. of ref. [9.9] for a clear and pedagogical introduction to Lie groups of transformations. For a discussion of the bounded semigroups of page 140 see, for example, Marsden and Hughes [9.2].

Remark 9.3 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 [1.8, 9.3] you will see the right hand side of (9.32) defined as $\{B, A\}$ so that (9.33) is $\frac{dQ}{dt} = \{Q, H\}$. Other equally reputable texts [31.2] employ the convention used here. Landau and Lifshitz [9.4] 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.

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 finite dimensional spaces $x = (x_1, x_2 \cdots x_d)$ for linear equations on infinite dimensional vector spaces of density functions $\rho(x)$. 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 certain evolution operators. Both in classical and quantum mechanics one has a choice of implementing dynamical evolution on densities ("Schrödinger picture", sect. 9.4) or on observables ("Heisenberg picture", sect. 10.2 and chapter 14). By "Schrödinger picture" we mean computer eigenvalues...., and then expectation values by extreme sandwiching the observables between the eigen.....

⇓PRELIMINARY

⇑PRELIMINARY

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.

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need more realistic set of refs on ergodic theory

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