Chapter 21

Trace formulas

The trace formula is not a formula, it is an idea.
—Martin Gutzwiller

Dynamics is posed in terms of local equations, but the ergodic averages require global information. How can we use a local description of a flow to learn something about the global behavior? In chapter 20 we have related global averages to the eigenvalues of appropriate evolution operators. Here we show that the traces of evolution operators can be evaluated as integrals over Dirac delta functions, and in this way the spectra of evolution operators become related to periodic orbits. If there is one idea that one should learn about chaotic dynamics, it happens in this chapter, and it is this: there is a fundamental local ↔ global duality which says that

the spectrum of eigenvalues is dual to the spectrum of periodic orbits

For dynamics on the circle, this is called Fourier analysis; for dynamics on well-tiled manifolds, Selberg traces and zetas; and for generic nonlinear dynamical systems the duality is embodied in the trace formulas that we will now derive. These objects are to dynamics what partition functions are to statistical mechanics.

The above phrasing is a bit too highfalutin, so it perhaps pays to go again through the quick sketch of sects. 1.5 and 1.6. We have a state space that we would like to tessellate by periodic orbits, one short orbit per neighborhood, as in figure 21.1 (a). How big is the neighborhood of a given cycle?

Along stable directions neighbors of the periodic orbit get closer with time, so we only have to keep track of those who are moving away along the unstable directions. The fraction of those who remain in the neighborhood for one recurrence time T_p is given by the overlap ratio along the initial sphere and the returning ellipsoid, figure 21.1 (b), and along the expanding eigen-direction $\mathbf{e}^{(i)}$ of $J_p(x)$ this is given by the expanding Floquet multiplier $1/|\Lambda_{p,i}|$. A bit more

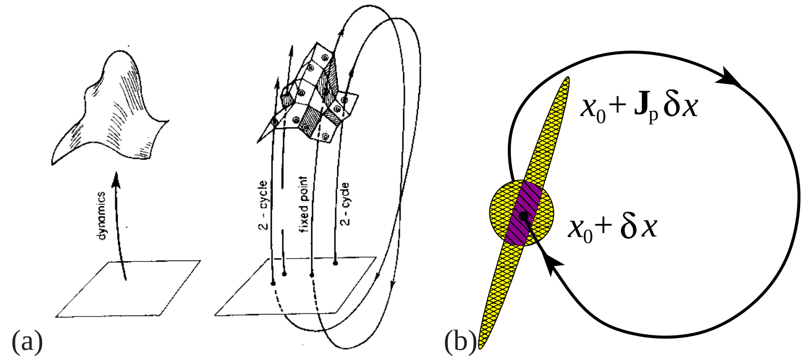

Figure 21.1: (a) Smooth dynamics tesselated by the skeleton of periodic points, together with their linearized neighborhoods. (b) Jacobian matrix J_p maps spherical neighborhood of x_0 $\to$ ellipsoidal neighborhood time T_p later, with the overlap ratio along the expanding eigdirection $\mathbf{e}^{(i)}$ of $J_p(x)$ given by the expanding eigenvalue $1/|\Lambda_{p,i}|$.

thinking leads to the conclusion that one also cares about how long it takes to return (the long returns contributing less to the time averages), so the weight t_p of the p-neighborhood $t_p = e^{-sT_p}/|\Lambda_p|$ decreases exponentially both with the shortest recurrence period and the product (5.6) of expanding Floquet multipliers $\Lambda_p = \prod_e \Lambda_{p,e}$. With emphasis on *expanding* - the flow could be a 60,000-dimensional dissipative flow, and still the neighborhood is defined by the handful of expanding eigen-directions. Now the long-time average of a physical observable -let us say power D dissipated by viscous friction of a fluid flowing through a pipe- can be estimated by its mean value (20.5) D_p/T_p computed on each neighborhood, and weighted by the above estimate

$$\langle D \rangle \approx \sum_p \frac{D_p}{T_p} \frac{e^{-sT_p}}{|\Lambda_p|} \,.$$

Wrong in detail, this estimate is the crux of many a *Phys. Rev. Letter*, and in its essence the key result of this chapter, the 'trace formula.' Here we redo the argument in a bit greater depth, and derive the correct formula (23.23) for a long time average $\langle D \rangle$ as a weighted sum over periodic orbits. It will take three chapters, but it is worth it - the reward is an *exact* (i.e., not heuristic) and highly convergent and controllable formula for computing averages over chaotic flows.

21.1 A trace formula for maps

Our extraction of the spectrum of $\mathcal{L}$ commences with the evaluation of the trace formula for maps.

To compute an expectation value using (20.22) we have to integrate over all the values of the kernel $\mathcal{L}^n(x, y)$.

$$\mathrm{tr}\,\mathcal{L}^n = \int dx\,\mathcal{L}^n(x,x) = \int dx\,\delta(x - f^n(x))\,e^{\beta A(x,n)} \,. \tag{21.1}$$

On the other hand, by its matrix motivated definition, the trace is the sum over eigenvalues (20.28),

$$\mathrm{tr}\,\mathcal{L}^n = \sum_{\alpha=0}^{\infty} e^{s_\alpha n} . \tag{21.2}$$

We assume that spectrum of $\mathcal{L}$ is discrete, $s_0, s_1, s_2, \cdots$, ordered so that Re $s_\alpha \geq$ Re $s_{\alpha+1}$.

21.1.1 Hyperbolicity assumption

We have learned in sect. 19.2 how to evaluate the delta-function integral (21.1).

According to (19.8) the trace (21.1) picks up a contribution whenever $x - f^n(x) = 0$, i.e., whenever x belongs to a periodic orbit. The contribution of an isolated prime cycle p of period n_p for a map f can be evaluated by restricting the integration to an infinitesimal open neighborhood $\mathcal{M}_p$ around the cycle,

$$\begin{aligned}\mathrm{tr}_p\,\mathcal{L}^{n_p} &= \int_{\mathcal{M}_p} dx\,\delta(x - f^{n_p}(x)) \\ &= \frac{n_p}{\left|\det\left(\mathbf{1} - M_p\right)\right|} = n_p \prod_{i=1}^{d} \frac{1}{|1 - \Lambda_{p,i}|} .\end{aligned} \tag{21.3}$$

For the time being we set here and in (19.9) the observable $e^{\beta A_p} = 1$. Periodic orbit Jacobian matrix M_p is also known as the *monodromy matrix*, and its eigenvalues $\Lambda_{p,1}, \Lambda_{p,2}, \ldots, \Lambda_{p,d}$ as the Floquet multipliers.

We sort the eigenvalues $\Lambda_{p,1}, \Lambda_{p,2}, \ldots, \Lambda_{p,d}$ of the p-cycle $[d\times d]$ monodromy matrix M_p into expanding and contracting sets $\{e,c\}$ and factorize the trace (21.3) into a product over the expanding and the contracting eigenvalues

$$\left|\det\left(\mathbf{1} - M_p\right)\right|^{-1} = \frac{1}{|\Lambda_p|} \prod_e \frac{1}{1 - 1/\Lambda_{p,e}} \prod_c \frac{1}{1 - \Lambda_{p,c}} , \tag{21.4}$$

where $\Lambda_p = \prod_e \Lambda_{p,e}$ is the product of expanding eigenvalues. Both $\Lambda_{p,c}$ and $1/\Lambda_{p,e}$ are smaller than 1 in absolute value, and as they are either real or come in complex conjugate pairs we are allowed to drop the absolute value brackets $|\cdots|$ in the above products.

The *hyperbolicity assumption* requires that the stabilities of all cycles included in the trace sums be exponentially bounded away from unity:

$$\begin{array}{lcll} |\Lambda_{p,e}| & > & e^{\lambda_e T_p} & \text{any } p, \text{ any expanding } |\Lambda_{p,e}| > 1 \\ |\Lambda_{p,c}| & < & e^{-\lambda_c T_p} & \text{any } p, \text{ any contracting } |\Lambda_{p,c}| < 1 \,, \end{array} \tag{21.5}$$

where $\lambda_e, \lambda_c > 0$ are strictly positive bounds on the expanding, contracting cycle Lyapunov exponents. If a dynamical system satisfies the hyperbolicity assumption (for example, the well separated 3-disk system clearly does), the $\mathcal{L}^t$ spectrum will be relatively easy to control.

It follows from (21.4) that for long times, $t = rT_p \to \infty$, only the product of expanding eigenvalues matters, $\left|\det\left(\mathbf{1} - M_p^r\right)\right| \to |\Lambda_p|^r$. We shall use this fact to motivate the construction of dynamical zeta functions in sect.22.3.

21.1.2 A classical trace formula for maps

If the evolution is given by a discrete time mapping, and all periodic points have Floquet multipliers $|\Lambda_{p,i}| \neq 1$ strictly bounded away from unity, the trace $\mathcal{L}^n$ is given by the sum over all *periodic points i* of period n:

$$\mathrm{tr}\,\mathcal{L}^n = \int dx\,\mathcal{L}^n(x,x) = \sum_{x_i \in \mathrm{Fix} f^n} \frac{e^{\beta A_i}}{|\det\,(\mathbf{1} - M^n(x_i))|}\,. \tag{21.6}$$

Here $\mathrm{Fix}\, f^n = \{x : f^n(x) = x\}$ is the set of all periodic points of period n, and A_i is the observable (20.4) evaluated over n discrete time steps along the cycle to which the periodic point x_i belongs. The weight follows from the properties of the Dirac delta function (19.8) by taking the determinant of $\partial_i(x_j - f^n(x)_j)$. If a trajectory retraces itself r times, its monodromy matrix is M_p^r, where M_p is the $[d \times d]$ monodromy matrix (4.5) evaluated along a single traversal of the prime cycle p. As we saw in (20.4), the integrated observable A is additive along the cycle: If a prime cycle p trajectory retraces itself r times, $n = rn_p$, we obtain A_p repeated r times, $A_i = A(x_i, n) = rA_p$, $x_i \in \mathcal{M}_p$.

A prime cycle is a single traversal of the orbit, and its label is a non-repeating symbol string. There is only one prime cycle for each cyclic permutation class.

For example, the four periodic points $\overline{0011} = \overline{1001} = \overline{1100} = \overline{0110}$ belong to the same prime cycle $p = 0011$ of length 4. As both the stability of a cycle and the weight A_p are the same everywhere along the orbit, each prime cycle of length n_p contributes n_p terms to the sum, one for each periodic point. Hence (21.6) can be rewritten as a sum over all prime cycles and their repeats chapter 14

$$\mathrm{tr}\,\mathcal{L}^n = \sum_p n_p \sum_{r=1}^{\infty} \frac{e^{r\beta A_p}}{\left|\det\left(\mathbf{1} - M_p^r\right)\right|} \delta_{n,n_p r}\,, \tag{21.7}$$

with the Kronecker delta $\delta_{n,n_p r}$ projecting out the periodic contributions of total period n. A discrete Laplace transform rids us of the time periodicity constraint:

In the sum over all cycle periods,

$$\sum_{n=1}^{\infty} z^n \mathrm{tr}\,\mathcal{L}^n = \mathrm{tr}\,\frac{z\mathcal{L}}{1 - z\mathcal{L}} = \sum_p n_p \sum_{r=1}^{\infty} \frac{z^{n_p r} e^{r\beta A_p}}{\left|\det\left(\mathbf{1} - M_p^r\right)\right|}\,, \tag{21.8}$$

the constraint $\delta_{n,n_p r}$ is replaced by weight z^n. Such discrete time Laplace transform of $\mathrm{tr}\,\mathcal{L}^n$ is usually referred to as a 'generating function'. Why this transform? We are actually not interested in evaluating the sum (21.7) for any particular fixed period n; what we are interested in is the long time $n \to \infty$ behavior. The transform trades in the large time n behavior for the small z behavior. Expressing the trace as in (21.2), in terms of the sum of the eigenvalues of $\mathcal{L}$, we obtain the *trace formula for maps*:

$$\sum_{\alpha=0}^{\infty} \frac{z e^{s_\alpha}}{1 - z e^{s_\alpha}} = \sum_p n_p \sum_{r=1}^{\infty} \frac{z^{n_p r} e^{r\beta A_p}}{\left|\det\left(\mathbf{1} - M_p^r\right)\right|}\,. \tag{21.9}$$

This is our second example of the duality between the spectrum of eigenvalues and the spectrum of periodic orbits, announced in the introduction to this chapter. (The first example was the topological trace formula (18.8).)

Chapter 22

Spectral determinants

> "It seems very pretty," she said when she had finished it, "but it's rather hard to understand!" (You see she didn't like to confess, even to herself, that she couldn't make it out at all.) "Somehow it seems to fill my head with ideas — only I don't exactly know what they are!"
>
> —Lewis Carroll, *Through the Looking Glass*

THE PROBLEM with the trace formulas (21.9), (21.19) and (21.24) is that they diverge at $z = e^{-s_0}$, respectively $s = s_0$, i.e., precisely where one would like to use them. While this does not prevent numerical estimation of some "thermodynamic" averages for iterated mappings, in the case of the Gutzwiller trace formula this leads to a perplexing observation that crude estimates of the radius of convergence seem to put the entire physical spectrum out of reach. We shall now cure this problem by thinking, at no extra computational cost; while traces and determinants are formally equivalent, determinants are the tool of choice when it comes to computing spectra. Determinants tend to have larger analyticity domains because if $\mathrm{tr}\,\mathcal{L}/(1 - z\mathcal{L}) = -\frac{d}{dz}\ln\det(1 - z\mathcal{L})$ diverges at a particular value of z, then $\det(1 - z\mathcal{L})$ might have an isolated zero there, and a zero of a function is easier to determine numerically than its poles.

chapter 28

22.1 Spectral determinants for maps

The eigenvalues z_k of a linear operator are given by the zeros of the determinant

$$\det(1 - z\mathcal{L}) = \prod_k (1 - z/z_k)\,. \tag{22.1}$$

For finite matrices this is the characteristic determinant; for operators this is the Hadamard representation of the *spectral determinant* (sparing the reader from pondering possible regularization factors). Consider first the case of maps, for which the evolution operator advances the densities by integer steps in time. In this case we can use the formal matrix identity

exercise 4.1

$$\ln\det(1-M) = \operatorname{tr}\,\ln(1-M) = -\sum_{n=1}^{\infty}\frac{1}{n}\operatorname{tr}M^n\,, \tag{22.2}$$

to relate the spectral determinant of an evolution operator for a map to its traces (21.7), and hence to periodic orbits:

$$\begin{aligned}\det(1-z\mathcal{L}) &= \exp\left(-\sum_n \frac{z^n}{n}\operatorname{tr}\mathcal{L}^n\right)\\ &= \exp\left(-\sum_p\sum_{r=1}^{\infty}\frac{1}{r}\frac{z^{n_p r}e^{r\beta A_p}}{\left|\det\left(\mathbf{1}-M_p^r\right)\right|}\right).\end{aligned} \tag{22.3}$$

Going the other way, the trace formula (21.9) can be recovered from the spectral determinant by taking a derivative

$$\operatorname{tr}\frac{z\mathcal{L}}{1-z\mathcal{L}} = -z\frac{d}{dz}\ln\det(1-z\mathcal{L})\,. \tag{22.4}$$

Now we are finally poised to deal with the problem posed at the beginning of chapter 21; how do we actually evaluate the averages introduced in sect.20.1? The eigenvalues of the dynamical averaging evolution operator are given by the values of s for which the spectral determinant (22.5) of the evolution operator (20.24) vanishes. If we can compute the leading eigenvalue $s_0(\beta)$ and its derivatives, we are done. Unfortunately, the infinite product formula (22.8) is no more than a shorthand notation for the periodic orbit weights contributing to the spectral determinant; more work will be needed to bring such formulas into a tractable form. This shall be accomplished in chapter 23, but here it is natural to introduce still another variant of a determinant, the dynamical zeta function.

Résumé

The eigenvalues of evolution operators are given by the zeros of corresponding determinants, and one way to evaluate determinants is to expand them in terms of traces, using the matrix identity log det = tr log. Traces of evolution operators can be evaluated as integrals over Dirac delta functions, and in this way the spectra of evolution operators are related to periodic orbits. The spectral problem is now recast into a problem of determining zeros of either the *spectral determinant*

$$\det(s-\mathcal{A}) = \exp\left(-\sum_p\sum_{r=1}^{\infty}\frac{1}{r}\frac{e^{(\beta A_p - sT_p)r}}{\left|\det\left(\mathbf{1}-M_p^r\right)\right|}\right),$$

or the leading zeros of the *dynamical zeta function*

$$1/\zeta = \prod_p \left(1 - t_p\right), \qquad t_p = \frac{1}{|\Lambda_p|} e^{\beta A_p - s T_p}.$$

The spectral determinant is the tool of choice in actual calculations, as it has superior convergence properties (this will be discussed in chapter 28 and is illustrated, for example, by table 23.2). In practice both spectral determinants and dynamical zeta functions are preferable to trace formulas because they yield the eigenvalues more readily; the main difference is that while a trace diverges at an eigenvalue and requires extrapolation methods, determinants vanish at s corresponding to an eigenvalue s_α, and are analytic in s in an open neighborhood of s_α.

The critical step in the derivation of the periodic orbit formulas for spectral determinants and dynamical zeta functions is the hyperbolicity assumption (21.5) that no cycle stability eigenvalue is marginal, $|\Lambda_{p,i}| \neq 1$. By dropping the prefactors in (1.5), we have given up on any possibility of recovering the precise distribution of the initial x (return to the past is rendered moot by the chaotic mixing and the exponential growth of errors), but in exchange we gain an effective description of the asymptotic behavior of the system. The pleasant surprise (to be demonstrated in chapter 23) is that the infinite time behavior of an unstable system turns out to be as easy to determine as its short time behavior.

Chapter 23

Cycle expansions

Recycle... It's the Law!

—Poster, New York City Department of Sanitation

WHEN WE SET OUT on this journey, we had promised to teach you something profound that *your professor does not know*. Well, this chapter is the chapter. If your professor knows *cycle formulas for dynamical averages*, please send us her name, and we'll feature it in ChaosBook. They look like cumulants, but when you start to take them apart you realize how brilliant they are - your professor would not guess their form in 1 007 *Physical Review Letters*. Takes 20 some chapters of hard study to start to understand them, and who has time for that?

The Euler product representations of spectral determinants (22.8) and dynamical zeta functions (22.11) are really only a shorthand notation - the zeros of the individual factors are *not* the zeros of the zeta function, and the convergence of these objects is far from obvious. Now we shall give meaning to dynamical zeta functions and spectral determinants by expanding them as *cycle expansions*, which are series representations ordered by increasing topological cycle length, with products in (22.8), (22.11) expanded as sums over *pseudo-cycles*, products of weights t_p of contributing cycles. The zeros of correctly truncated cycle expansions yield the desired leading eigenvalues of evolution operators, and the expectation values of observables are given by the cycle averaging formulas obtained from the partial derivatives of dynamical zeta functions (or spectral determinants).

For reasons of pedagogy in what follows everything is first explained in terms of dynamical zeta functions: they aid us in developing 'shadowing' intuition about the geometrical meaning of cycle expansions. For actual calculations, we recommend the spectral determinant cycle expansions of sects. 23.2.2 and 23.5.2. While the shadowing is less transparent, and the weights calculation is an iterative numerical algorithm, these expansions use full analytic information about the flow, and can have better convergence properties than the dynamical zeta functions. For example, as we shall show in chapter 28, even when a spectral determinant (22.5) is entire and calculations are super-exponentially convergent, cycle expansion of the corresponding dynamical zeta function (22.28) has a finite radius of convergence and captures only the leading eigenvalue, at exponentially convergent rate.

23.1 Pseudo-cycles and shadowing

How are periodic orbit formulas such as (22.11) evaluated? We start by computing the lengths and Floquet multipliers of the shortest cycles. This always requires numerical work, such as searches for periodic solutions via Newton's method; we shall assume for the purpose of this discussion that the numerics is under control, and that *all* short cycles up to a given (topological) length have been found. Examples of the data required for application of periodic orbit formulas are the lists of cycles given in exercise 7.2 and table 33.3. Sadly, it is not enough to set a computer to blindly troll for invariant solutions, and blithely feed those into the formulas that will be given here. The reason that this chapter is numbered 23 and not 6, is that understanding the geometry of the non–wandering set is a prerequisite to good estimation of dynamical averages: one has to identify cycles that belong to a given ergodic component (whose symbolic dynamics and shadowing is organized by its transition graph), and discard the isolated cycles and equilibria that do not take part in the asymptotic dynamics. It is important not to miss any short cycles, as the calculation is as accurate as the shortest cycle dropped - including cycles longer than the shortest omitted does not improve the accuracy (more precisely, the calculation improves, but so little as not to be worth while).

chapter 16

Given a set of periodic orbits, we can compute their weights t_p and expand the dynamical zeta function (22.11) as a formal power series,

$$1/\zeta = \prod_p (1 - t_p) = 1 - \sum_{\{p_1 p_2 \dots p_k\}}{}' (-1)^{k+1} t_{p_1} t_{p_2} \dots t_{p_k} \tag{23.1}$$

where the prime on the sum indicates that the sum is over all distinct non-repeating combinations of prime cycles. As we shall frequently use such sums, let us denote by $t_\pi = (-1)^{k+1} t_{p_1} t_{p_2} \dots t_{p_k}$ an element of the set of all distinct products of the prime cycle weights t_p, and label each such *pseudo-cycle* by

$$\pi = p_1 + p_2 + \dots + p_k \tag{23.2}$$

The formal power series (23.1) is now compactly written as

$$1/\zeta = 1 - \sum_\pi{}' t_\pi \,. \tag{23.3}$$

For $k > 1$, the signed products t_π are weights of *pseudo-cycles*; they are sequences of shorter cycles that shadow a cycle with the symbol sequence $p_1 p_2 \dots p_k$ along the segments $p_1, p_2, \dots, p_k$, as in figure 1.12. The symbol $\sum'$ denotes the restricted sum, for which any given prime cycle p contributes at most once to a given pseudo-cycle weight t_π.

The pseudo-cycle weight, i.e., the product of weights (22.9) of prime cycles comprising the pseudo-cycle,

$$t_\pi = (-1)^{k+1} \frac{1}{|\Lambda_\pi|} e^{\beta A_\pi - s T_\pi} z^{n_\pi} , \tag{23.4}$$

depends on the pseudo-cycle integrated observable A_π, the period T_π, the stability Λ_π,

remark 5.1

$$\begin{aligned} \Lambda_\pi &= \Lambda_{p_1}\Lambda_{p_2}\cdots\Lambda_{p_k} , \qquad T_\pi = T_{p_1} + \ldots + T_{p_k} \\ A_\pi &= A_{p_1} + \ldots + A_{p_k} , \qquad n_\pi = n_{p_1} + \ldots + n_{p_k} , \end{aligned} \tag{23.5}$$

and, when available, the topological length n_π.

23.1.1 Curvature expansions

The simplest example is the pseudo-cycle sum for a system described by a complete binary symbolic dynamics. In this case the Euler product (22.11) is given by

$$\begin{aligned} 1/\zeta &= (1-t_0)(1-t_1)(1-t_{01})(1-t_{001})(1-t_{011}) \\ &\quad \times (1-t_{0001})(1-t_{0011})(1-t_{0111})(1-t_{00001})(1-t_{00011}) \\ &\quad \times (1-t_{00101})(1-t_{00111})(1-t_{01011})(1-t_{01111}) \ldots \end{aligned} \tag{23.6}$$

(see table 18.1), and the first few terms of the expansion (23.3) ordered by increasing total pseudo-cycle length are:

$$\begin{aligned} 1/\zeta &= 1 - t_0 - t_1 - t_{01} - t_{001} - t_{011} - t_{0001} - t_{0011} - t_{0111} - \ldots \\ &\quad + t_{0+1} + t_{0+01} + t_{01+1} + t_{0+001} + t_{0+011} + t_{001+1} + t_{011+1} \\ &\quad - t_{0+01+1} - \ldots \end{aligned} \tag{23.7}$$

We refer to such series representation of a dynamical zeta function or a spectral determinant, expanded as a sum over pseudo-cycles, and ordered by increasing cycle length and instability, as a *cycle expansion*.

The next step is the key step: regroup the terms into the dominant *fundamental* contributions t_f and the decreasing *curvature* corrections $\hat{c}_n$, each $\hat{c}_n$ split into prime cycles p of length $n_p{=}n$ grouped together with pseudo-cycles whose full itineraries build up the itinerary of p. For the binary case this regrouping is given by

$$\begin{aligned} 1/\zeta &= 1 - t_0 - t_1 - [(t_{01} - t_{0+1})] - [(t_{001} - t_{0+01}) + (t_{011} - t_{01+1})] \\ &\quad -[(t_{0001} - t_{0+001}) + (t_{0111} - t_{011+1}) \\ &\qquad +(t_{0011} - t_{001+1} - t_{0+011} + t_{0+01+1})] - \ldots \\ &= 1 - \sum_f t_f - \sum_n \hat{c}_n . \end{aligned} \tag{23.8}$$

All terms in this expansion up to length $n_p = 6$ are given in table 23.1. We refer to such regrouped series as *curvature expansions*, because the shadowed combinations $[\cdots]$ vanish identically for piecewise-linear maps with nice partitions, such as the 'full tent map' of figure 19.3.

The fundamental cycles t_0, t_1 have no shorter approximations; they are the "building blocks" of the dynamics in the sense that all longer orbits can be approx-imately pieced together from them. The fundamental part of a cycle expansion is given by the sum of the products of all non-intersecting loops of the associated transition graph, discussed in chapter17. The terms grouped in brackets $[\cdots]$ are the curvature corrections; the terms grouped in parentheses $(\cdots)$ are combinations of longer cycles and corresponding sequences of "shadowing" pseudo-cycles, as in figure 1.12. If all orbits are weighted equally ($t_p = z^{n_p}$), such combinations cancel exactly, and the dynamical zeta function reduces to the topological poly-nomial (18.17). If the flow is continuous and smooth, orbits of similar symbolic dynamics will traverse the same neighborhoods and will have similar weights, and the weights in such combinations will almost cancel. The utility of cycle expansions of dynamical zeta functions and spectral determinants, in contrast to naive averages over periodic orbits such as the trace formulas discussed in sect.27.4, lies precisely in this organization into nearly canceling combinations: cycle expansions are dominated by short cycles, with longer cycles giving exponentially decaying corrections.

Table 23.1: The binary curvature expansion (23.8) up to length 6, listed in such a way that the sum of terms along the pth horizontal line is the curvature $\hat{c}_p$ associated with a prime cycle p, or a combination of prime cycles such as the $t_{100101} + t_{100110}$ pair.

$-t_0$				
$-t_1$				
$-t_{10}$	$+t_1 t_0$			
$-t_{100}$	$+t_{10+0}$			
$-t_{101}$	$+t_{10+1}$			
$-t_{1000}$	$+t_{100+0}$			
$-t_{1001}$	$+t_{100+1}$	$+t_{110+0}$	$-t_{1+10+0}$	
$-t_{1011}$	$+t_{101+1}$			
$-t_{10000}$	$+t_{1000+0}$			
$-t_{10001}$	$+t_{1001+0}$	$+t_{1000+1}$	$-t_{0+100+1}$	
$-t_{10010}$	$+t_{100+10}$			
$-t_{10101}$	$+t_{101+10}$			
$-t_{10011}$	$+t_{1011+0}$	$+t_{1001+1}$	$-t_{0+101+1}$	
$-t_{10111}$	$+t_{1011+1}$			
$-t_{100000}$	$+t_{10000+0}$			
$-t_{100001}$	$+t_{10001+0}$	$+t_{10000+1}$	$-t_{0+1000+1}$	
$-t_{100010}$	$+t_{10010+0}$	$+t_{1000+10}$	$-t_{0+100+10}$	
$-t_{100011}$	$+t_{10011+0}$	$+t_{10001+1}$	$-t_{0+1001+1}$	
$-t_{100101}$	$-t_{100110}$	$+t_{10010+1}$	$+t_{10110+0}$	
	$+t_{10+1001}$	$+t_{100+101}$	$-t_{0+10+101}$	$-t_{1+10+100}$
$-t_{101110}$	$+t_{10110+1}$	$+t_{1011+10}$	$-t_{1+101+10}$	
$-t_{100111}$	$+t_{10011+1}$	$+t_{10111+0}$	$-t_{0+1011+1}$	
$-t_{101111}$	$+t_{10111+1}$			

Table 23.2: The 3-disk repeller escape rates computed from cycle expansions of the spectral determinant (22.5) and the dynamical zeta function (22.11), as functions of the maximal cycle length N. The disk-disk center separation to disk radius ratio is R:a, and the $\det(s - \mathcal{A})$ is an estimate of the classical escape rate computed from the spectral determinant cycle expansion in the fundamental domain. For larger disk-disk separations, the dynamics is more uniform, as illustrated by the faster convergence. Convergence of spectral determinant $\det(s - \mathcal{A})$ is super-exponential, see chapter 28. For comparison, the $1/\zeta(s)$ column lists estimates from the fundamental domain dynamical zeta function cycle expansion (23.8), and the $1/\zeta(s)_{\text{3-disk}}$ column lists estimates from the full 3-disk cycle expansion (25.54). The convergence of the fundamental domain dynamical zeta function is significantly slower than the convergence of the corresponding spectral determinant, and the full (unfactorized) 3-disk dynamical zeta function has still poorer convergence. (P.E. Rosenqvist.)

R:a	N	. $\det(s - \mathcal{A})$	$1/\zeta(s)$	$1/\zeta(s)_{\text{3-disk}}$
	1	0.39	0.407	
	2	0.4105	0.41028	0.435
	3	0.410338	0.410336	0.4049
6	4	0.4103384074	0.4103383	0.40945
	5	0.4103384077696	0.4103384	0.410367
	6	0.410338407769346482	0.4103383	0.410338
	7	0.4103384077693464892		0.4103396
	8	0.410338407769346489338468		
	9	0.4103384077693464893384613074		
	10	0.4103384077693464893384613078192		
	1	0.41		
	2	0.72		
	3	0.675		
	4	0.67797		
3	5	0.677921		
	6	0.6779227		
	7	0.6779226894		
	8	0.6779226896002		
	9	0.677922689599532		
	10	0.67792268959953606		

23.3 Periodic orbit averaging

The first cycle expansion calculation should always be the determination of the leading eigenvalue of the evolution operator, calculated as follows. After the prime cycles and the pseudo-cycles have been grouped into subsets of equal topological length, the dummy variable can be set equal to $z = 1$. With $z = 1$, the expansion (23.15) constitutes the cycle expansion (22.5) for the spectral determinant $\det(s - \mathcal{A})$. We vary s in cycle weights, and determine αth eigenvalue s_α (20.28) by finding $s = s_\alpha$ for which (23.15) vanishes. As an example, the convergence of a leading eigenvalue for a nice hyperbolic system is illustrated in table 23.2 by the list of pinball escape rates $\gamma = -s_0$ estimates computed from truncations of (23.8) and (23.15) to different maximal cycle lengths.

The pleasant surprise, to be explained in chapter 28, is that one can prove that the coefficients in these cycle expansions decay exponentially or even faster, because of the analyticity of $\det(s - \mathcal{A})$ or $1/\zeta(s)$, for s values well beyond those for which the corresponding trace formula (21.19) diverges.

Our next task will be to compute long-time averages of observables.

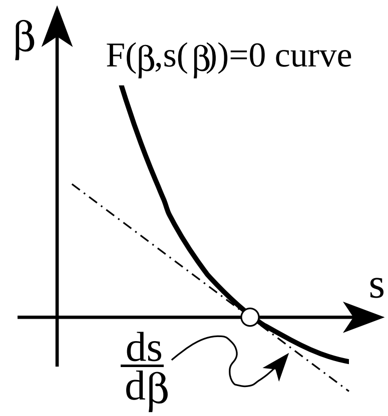

Figure 23.2: The eigenvalue condition is satisfied on the curve $F = 0$ on the (β, s) plane. The expectation value of the observable (20.11) is given by the slope of the curve.

23.5 Cycle formulas for dynamical averages

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The eigenvalue conditions for the dynamical zeta function (23.3) and the spectral determinant (23.15),

$$0 = 1 - \sum_{\pi}{}' t_\pi\,, \qquad t_\pi = t_\pi(\beta, s(\beta)) \tag{23.18}$$

$$0 = 1 - \sum_{n=1}^{\infty} Q_n\,, \qquad Q_n = Q_n(\beta, s(\beta))\,, \tag{23.19}$$

are implicit equations for an eigenvalue $s = s(\beta)$ of the form $0 = F(\beta, s(\beta))$. The eigenvalue $s = s(\beta)$ as a function of β is sketched in figure 23.2; this condition is satisfied on the curve $F = 0$. The cycle averaging formulas for the slope and curvature of $s(\beta)$ are obtained as in (20.11) by taking derivatives of the eigenvalue condition. Evaluated along $F = 0$, by the chain rule the first derivative yields

$$\begin{aligned} 0 &= \frac{d}{d\beta} F(\beta, s(\beta)) \\ &= \frac{\partial F}{\partial \beta} + \frac{ds}{d\beta}\frac{\partial F}{\partial s}\Big|_{s=s(\beta)} \quad \Longrightarrow \quad \frac{ds}{d\beta} = -\frac{\partial F}{\partial \beta} \Big/ \frac{\partial F}{\partial s}\,, \end{aligned} \tag{23.20}$$

and the second derivative of $F(\beta, s(\beta)) = 0$ yields

$$\frac{d^2 s}{d\beta^2} = -\left[\frac{\partial^2 F}{\partial \beta^2} + 2\frac{ds}{d\beta}\frac{\partial^2 F}{\partial\beta\partial s} + \left(\frac{ds}{d\beta}\right)^2 \frac{\partial^2 F}{\partial s^2}\right] \Big/ \frac{\partial F}{\partial s}\,. \tag{23.21}$$

Denoting expectations as in (20.14) by

$$\begin{aligned}
\langle A\rangle_F &= -\left.\frac{\partial F}{\partial \beta}\right|_{\beta,s=s(\beta)}, \qquad \langle T\rangle_F = \left.\frac{\partial F}{\partial s}\right|_{\beta,s=s(\beta)}, \\
\langle A^2\rangle_F &= -\left.\frac{\partial^2 F}{\partial \beta^2}\right|_{\beta,s=s(\beta)}, \qquad \langle TA\rangle_F = \left.\frac{\partial^2 F}{\partial s\partial \beta}\right|_{\beta,s=s(\beta)},
\end{aligned} \tag{23.22}$$

the mean cycle expectation value of A, the mean cycle period, and second derivatives of F computed for $F(\beta, s(\beta)) = 0$, we obtain the cycle averaging formulas for the expectation of the observable (20.11) and for its (generalized) diffusion constant (or, more generally, diffusion tensor):

$$\langle a\rangle = \frac{\langle A\rangle_F}{\langle T\rangle_F} \tag{23.23}$$

$$\Delta = \frac{1}{\langle T\rangle_F}\langle (A - T\langle a\rangle)^2\rangle_F\,, \tag{23.24}$$

and so forth for higher cumulants. These formulas are the central result of periodic orbit theory. We now show that for each choice of the function $F(\beta, s)$ in (23.3) and (23.15) (also the trace, or 'level sum' of (27.15)), the above quantities have explicit cycle expansions.

section 20.2

23.5.1 Dynamical zeta function cycle averaging formulas

For the dynamical zeta function condition (23.18), the cycle averaging formulas (23.20), (23.24) require one to evaluate derivatives of dynamical zeta functions at a given eigenvalue. Substituting the cycle expansion (23.3) for the dynamical zeta function we obtain

$$\langle A\rangle_\zeta := -\frac{\partial}{\partial\beta}\frac{1}{\zeta} = \sum{}' A_\pi t_\pi \tag{23.25}$$

$$\langle T\rangle_\zeta := \frac{\partial}{\partial s}\frac{1}{\zeta} = \sum{}' T_\pi t_\pi\,, \quad \langle n\rangle_\zeta := -z\frac{\partial}{\partial z}\frac{1}{\zeta} = \sum{}' n_\pi t_\pi\,,$$

where the subscript in $\langle\cdots\rangle_\zeta$ stands for the dynamical zeta function average over prime cycles, A_π, T_π, and n_π given by (23.4) are evaluated on pseudo-cycles (23.5), and pseudo-cycle weights $t_\pi = t_\pi(z, \beta, s(\beta))$ are evaluated at the eigenvalue $s(\beta)$. In most applications $\beta = 0$, and $s(\beta)$ of interest is typically the leading eigenvalue $s_0 = s_0(0)$ of the evolution generator $\mathcal{A}$.

For bounded flows the leading eigenvalue (the escape rate) vanishes, $s(0) = 0$, the exponent $\beta A_\pi - sT_\pi$ in (23.4) vanishes, so the cycle expansions take a simple form

$$\langle A\rangle_\zeta = \sum_\pi{}'(-1)^{k+1}\frac{A_{p_1} + A_{p_2}\cdots + A_{p_k}}{|\Lambda_{p_1}\cdots\Lambda_{p_k}|}\,, \tag{23.26}$$

where analogous formulas hold for $\langle T\rangle_\zeta$, $\langle n\rangle_\zeta$.

23.6 Cycle expansions for finite alphabets

A finite transition graph like the one given in figure 17.3 (d) is a compact encoding of the transition matrix for a given subshift. It is a sparse matrix, and the associated determinant (18.32) can be written by inspection: it is the sum of all possible partitions of the graph into products of non-intersecting loops, with each loop carrying a minus sign:

$$\det(1-T) = 1 - t_0 - t_{0011} - t_{0001} - t_{00011} + t_{0+0011} + t_{0011+0001} \tag{23.30}$$

The simplest application of this determinant is the evaluation of the topological entropy; if we set $t_p = z^{n_p}$, where n_p is the length of the p-cycle, the determinant reduces to the topological polynomial (18.33).

The determinant (23.30) is exact for the finite graph figure 17.3 (e), as well as for the associated finite-dimensional transfer operator of example 20.4. For the associated (infinite dimensional) evolution operator, it is the beginning of the cycle expansion of the corresponding dynamical zeta function:

$$\begin{aligned}1/\zeta &= 1 - t_0 - t_{0011} - t_{0001} + t_{0001+0011} \\ &\qquad -(t_{00011} - t_{0+0011} + \ldots \text{curvatures})\ldots\end{aligned} \tag{23.31}$$

The cycles $\overline{0}$, $\overline{0001}$ and $\overline{0011}$ are the *fundamental* cycles introduced in (23.8); they are not shadowed by any combinations of shorter cycles. All other cycles appear together with their shadows (for example, the $t_{00011} - t_{0+0011}$ combination, see figure 1.12) and yield exponentially small corrections for hyperbolic systems. For cycle counting purposes, both t_{ab} and the pseudo-cycle combination $t_{a+b} = t_a t_b$ in (23.3) have the same weight $z^{n_a+n_b}$, so all curvature combinations $t_{ab} - t_{a+b}$ vanish exactly, and the topological polynomial (18.17) offers a quick way of checking the fundamental part of a cycle expansion.

The splitting of cycles into the fundamental cycles and the curvature corrections depends on balancing long cycles t_{ab} against their pseudo-trajectory shadows $t_a t_b$. If the $\overline{ab}$ cycle or either of the shadows $\overline{a}$, $\overline{b}$ do not to exist, such curvature cancelation is unbalanced.

The most important lesson of the pruning of the cycle expansions is that prohibition of a finite subsequence imbalances the head of a cycle expansion and increases the number of the fundamental cycles in (23.8). Hence the pruned expansions are expected to start converging only *after* all fundamental cycles have been incorporated - in the last example, the cycles $\overline{1}$, $\overline{10}$, $\overline{10100}$, $\overline{1011100}$. Without cycle expansions, no such crisp and clear cut definition of the fundamental set of scales is available.

Because topological zeta functions reduce to polynomials for finite grammars, only a few fundamental cycles exist and long cycles can be grouped into curvature combinations. For example, the fundamental cycles in exercise 11.1 are the three 2-cycles that bounce back and forth between two disks and the two 3-cycles that visit every disk. Of all cycles, the 2-cycles have the smallest Floquet exponent, and the 3-cycles the largest. It is only after these fundamental cycles have been included that a cycle expansion is expected to start converging smoothly, i.e., only for n larger than the lengths of the fundamental cycles are the curvatures $\hat{c}_n$ (in expansion (23.8)), a measure of the deviations between long orbits and their short cycle approximations, expected to fall off rapidly with n.

Résumé

A *cycle expansion* is a series representation of a dynamical zeta function, trace formula or a spectral determinant, with products in (22.11) expanded as sums over *pseudo-cycles*, which are products of the prime cycle weights t_p.

If a flow is hyperbolic and has the topology of the Smale horseshoe (a subshift of finite type), dynamical zeta functions are holomorphic (have only poles in the complex s plane), the spectral determinants are entire, and the spectrum of the evolution operator is discrete. The situation is considerably more reassuring than what practitioners of quantum chaos fear; there is no 'abscissa of absolute convergence' and no 'entropy barrier', the exponential proliferation of cycles is no problem, spectral determinants are entire and converge everywhere, and the topology dictates the choice of cycles to be used in cycle expansion truncations.

In this case, the basic observation is that the motion in low-dimensional dynamical systems is organized around a few *fundamental* cycles, with the cycle expansion of the Euler product

$$1/\zeta = 1 - \sum_f t_f - \sum_n \hat{c}_n ,$$

regrouped into dominant *fundamental* contributions t_f and decreasing *curvature* corrections $\hat{c}_n$. The fundamental cycles t_f have no shorter approximations; they are the 'building blocks' of the dynamics in the sense that all longer orbits can be approximately pieced together from them. A typical curvature contribution to $\hat{c}_n$ is the *difference* of a long cycle $\{ab\}$ and its shadowing approximation by shorter cycles $\{a\}$ and $\{b\}$, as in figure 1.12:

$$t_{ab} - t_a t_b = t_{ab}(1 - t_a t_b / t_{ab})$$

Orbits that follow the same symbolic dynamics, such as $\{ab\}$ and a 'pseudo-cycle' $\{a\}\{b\}$, lie close to each other, have similar weights, and for increasingly long orbits the curvature corrections fall off rapidly. Indeed, for systems that satisfy the 'axiom A' requirements, such as the 3-disk billiard, curvature expansions converge very well.

Once a set of the shortest cycles has been found, and the cycle periods, stabilities, and integrated observable have been computed, the cycle averaging formulas such as (23.25) for the dynamical zeta function

$$\begin{aligned} \langle a \rangle &= \langle A \rangle_\zeta / \langle T \rangle_\zeta \,, \qquad \text{where for the zeta function expansions:} \\ \langle A \rangle_\zeta &= -\frac{\partial}{\partial \beta}\frac{1}{\zeta} = \sum{}' A_\pi t_\pi \,, \qquad \langle T \rangle_\zeta = \frac{\partial}{\partial s}\frac{1}{\zeta} = \sum{}' T_\pi t_\pi \end{aligned}$$

yield the expectation value of the observable $a(x)$, i.e., the long time average over the chaotic non–wandering set).