Abbreviations and Synonyms

SIS: Strange Invariant Set, an invariant set that has a fractal dimension.
UPO: Unstable Periodic Orbit.
cycle: a periodic orbit.
PDE: Partial Differential Equation.
ODE: Ordinary Differential Equation.
KSe: Kuramoto-Sivashinsky equation.
CGLe: Complex Ginzburg-Landau equation.
NSe: Navier-Stokes equation

SUMMARY

We propose a dynamical systems approach to study of turbulence (spatiotemporal chaos) based on the periodic orbit theory. The role of recurrent patterns and coherent structures is emphasized in the description. After a brief review of the periodic orbit theory in low dimensions, we discuss its possible application to the dynamics of spatially extended systems. The discussion is three-fold. First, we introduce a novel variational scheme for finding periodic orbits in general flows. Second, we check the periodic structures near the first instability of the complex Ginzburg-Landau equation and talk about its role in pattern formation. Third, we discuss the extensive numerical explorations that we have done to the Kuramoto-Sivashinsky system in the chaotic regime, including searching for periodic orbits, constructing symbolic dynamics and describing the chaotic invariant set in terms of intrinsic coordinates. In these investigations, we hope to identify and rank the nonlinear instabilities according to their relative importance.

CHAPTER II

periodic
orbit
theory—(tex

PERIODIC ORBIT THEORY

The theme of the whole thesis is the periodic orbit theory applied to the study of spatiotemporal dynamics of extended systems. Even in low-dimensional dynamical systems, the theory is still under development although the main ingredients are ready. In this chapter, we will review the theory and point out open problems (obstacles in applications) in the end. After reviewing the basic properties and symbolic dynamics description of a dynamical system in sect. 2.1, we discuss the space and time averages and introduce operator formulation of invariant measures in sect. 2.2. In sect. 2.3, the main object in the periodic orbit theory - trace formula, spectral determinant, dynamical zeta functions are derived and their physical interpretation is given. The calculation of physical averages through cycle expansions is discussed in sect. 2.4. Finally, we point out the difficulties and open problems of the periodic orbit theory in sect. 2.5. A comprehensive presentation of the theory is given in [51].

2.1 Dynamical systems

A deterministic dynamical system maps a point in its phase space $\mathcal{M}$ to another point in a discrete (maps) or continous (flows) manner. In this dissertation, we restrict our attention to the dynamical systems with the phase space $\mathcal{M}$ being Euclidean, *i.e.*, $\mathcal{M} \subset \mathbb{R}^n\,, n \in \mathbb{N}$. Let $x \in \mathcal{M}$, then the phase space dynamics consists of a family of continuous mappings

$$f^t : x \to f^t(x)\,,\ t \in \mathcal{S}\,, \tag{1}$$

where $\mathcal{S} \subseteq \mathbb{N}$ or $\mathbb{R}$ is the domain of the evolution parameter t, satisfying: $(1) f^0(x) = x\,; (2) f^{t_2} \circ f^{t_1}(x) = f^{t_1+t_2}(x)\,, \forall t_1\,, t_2 > 0$. If these mappings are homeomorphisms, then they form a group; otherwise, a semigroup. An invariant set $V \subset \mathcal{M}$ is a set that satisfies $f^t(V) = V\,, \forall t$. An orbit is a subset of $\mathcal{M}$ defined as $\iota = \{f^t(x) \in \mathcal{M} : t \in \mathcal{S}\,,\ \text{for any fixed } x \in \mathcal{M}\}$. An orbit is an invariant set and a general invariant set is a collection of orbits.

In chaotic dynamical systems, sensitive dependence on initial conditions precludes the long-time prediction of system behavior, and any open set on the SIS spreads over the whole SIS in finite time. If the dynamics takes place in a compact subset (the SIS) of the phase space, then there is an upper bound over distances between any two points on the SIS, so trajectories have to bend back and mix with each other. Local instability and global mixing creates very complex dynamics. For example, a (typical) point can visit neighborhood of any point infinitely many times. We say that the dynamics is topologically transitive. Specifically, a point can visit its own neighborhood arbitrarily often, which is the recurrence property proved first in Hamiltonian systems by Poincaré. It is natural to ask whether there are points whose orbit actually comes back to itself exactly and forms a periodic orbit. For

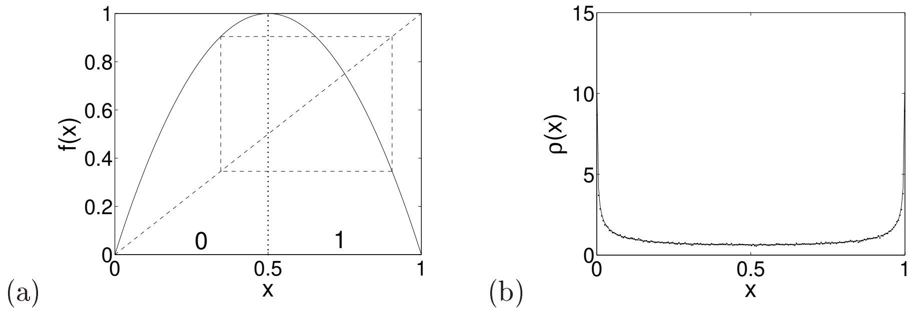

Figure 1: The Ulam map $f(x) = 4x(1-x)$ on the unit interval. (a) The graph of the map with its symbolic regions denoted by 0 and 1. (b) The invariant measure: analytic result is depicted by the solid line; numerical result by the dots.

a typical chaotic system, there are infinitely many such orbits (closing lemma [209]). They cover the SIS densely. A good knowledge of their properties reveals the system dynamics in a hierarchical way.

Though in a chaotic system, the asymptotic dynamics is complicated and unpredictable in the long run, symbolic dynamics is a good description at the global level which encodes all the possible orbits and their topological layout. It is an invariant characterization of the dynamics, independent of the underlying coordinate system. To build a symbolic dynamics, we partition the SIS into units and assign a symbol to each partitioning unit such that a trajectory is uniquely associated with a symbol sequence called itinerary according to the units it visited. A good partition insures that two different trajectories have distinct itineraries. It is possible that no trajectory corresponds to certain symbol sequence, and we then say that there exist pruning rules. A phase point corresponds to the itinerary of its trajectory and the dynamics is described by a shift of the symbols. Periodic orbits correspond to itineraries with repeating symbol blocks. This symbolic dynamics description of a chaotic system is extremely convenient and reveals much about the dynamics of the original system although it takes time and effort to find a good partition in a general dynamical system.

Consider the Ulam map

$$f(x) = 4x(1-x)\,,\ x \in [0,1]\,. \tag{2}$$

This is a quadratic map with the critical point sitting at $x = 0.5$. The non-wandering set is the whole unit interval and the symbolic dynamics of the system is a full shift on two symbols, say $\Sigma = \{0, 1\}$, with 0 corresponding to the subinterval on the left and 1 to that on the right of the critical point $x = \frac{1}{2}$, respectively (see figure 1). According to its itinerary, any orbit correponds uniquely to an infinite sequence $s_1 s_2 s_3 \cdots$, with $s_i \in \Sigma$, and vice versa. A periodic orbit is given by a periodic sequence. For example, the period two orbit in figure 1(a) is described by the sequence $010101\cdots$, which may be denoted by $\overline{01}$. The *topological length* of this orbit is 2, as its symbol sequence is a repeat of two symbols. A prime cycle is a periodic orbit that can not be decomposed to shorter ones. For example, $\overline{0101}$ is not a prime cycle as it is a repeat of $\overline{01}$.

In applications, often instead of the detailed dynamics averages of physical quantities are the only thing we care about. Due to the vastly different time scales, our observation or measurement is usually time average of the physical quantity under check. In gas dynamics, the pressure is just the average collision force exerted by the gas molecules on the container wall. In quantum mechanics, the only measurable quantities are the averages of observables. In fluid mechanics, a good many statistical quantities are used to characterize a turbulent flow. They are determined by the system control parameters and reproducible in observations. Usually, statistical models are proposed to explain the experimental observations. Though they capture ingradients of essential dynamics, their extra assumptions may severely restrict the applicability. In the following, we discuss how to use periodic orbits to do these calculations from first principles.

2.2 *Physical averages in a dynamical system*

2.2.1 Space, time averages and ergodicity

In classical or semiclassical mechanics, observables are (scalar, vector or tensor) functions $a(x)$ defined in $\mathcal{M}$. The integrated quantity $A^t(x_0)$ on an orbit segment is defined as

$$A^t(x_0) = \sum_{k=0}^{t} a(f^k(x_0)) \,. \tag{3}$$

This limit may not exist for all $x_0 \in \mathcal{M}$, but it does exist for almost all x_0 as the distribution of orbits from these points approach a definite limit. For flows the summation is replaced by integration over time. The time average of the observable a along a trajectory is

$$\bar{a}(x_0) = \lim_{t\to\infty} \frac{1}{t} A^t(x_0) \,. \tag{4}$$

Specifically, on a periodic orbit p, we may define

$$A_p = A^{T_p}(x_0) \,, \; a_p = \frac{1}{T_p} A_p \,,$$

where T_p is the period of the periodic orbit. Notice that $A_p \,, a_p$ does not depend on the starting point x_0 on the periodic orbit. The space average of $a(x)$ on a ensemble of phase points is

$$\langle a(t) \rangle = \int_{\mathcal{M}} dx\, \omega(x) a(f^t(x)) \,, \tag{5}$$

where $\omega(x)$ is the initial distribution of these phase points and normalized such that

$$\int_{\mathcal{M}} dx\, \omega(x) = 1 \,.$$

If the dynamics is ergodic, then for almost all $x_0 \in \mathcal{M}$, $\bar{a}(x_0)$ exists and *equals* to a constant value (independent of x_0). This is easily understood from a symbolic dynamics point of view. Suppose that the phase space is partitioned into m regions and the dynamics is a full shift of m symbols. in each region the observable has a value, so A is determined by the number (frequency) of each symbol but not their order in the symbol sequence of a trajectory. The itineraries with the m symbols occuring almost equally frequently dominate, which means that the corresponding phase points dominate and will have equal $\bar{a}$. To exclude the effect of the zero-measure bad set, we may take the space average of the time average and thus define the expectation value

$$\langle a\rangle = \lim_{t\to\infty}\frac{1}{t}\int_{\mathcal{M}} dx\, A^t(x)\,. \tag{6}$$

The space-time averaging is linear functional of the observale, since $\langle c_1 a + c_2 b\rangle = c_1\langle a\rangle + c_2\langle b\rangle$. If the system is ergodic [231, 74], there exists a measure $\rho(x)$ defined on $\mathcal{M}$ such that

$$\langle a\rangle = \int_{\mathcal{M}} dx\, \rho(x)a(x)\,. \tag{7}$$

In this way, the typical time average becomes a space average with a particular weight function $\rho(x)$. In a chaotic system, $\rho(x)$ is usually a non-differentiable function supported on a fractal set. The example given in figure 1 is an exceptional case where $\rho(x)$ is a smooth function defined on $(0,1)$,

$$\rho(x) = \frac{1}{\pi x\sqrt{1-x}}\,. \tag{8}$$

The profile of (8) is depicted in figure 1(b) in solid line. The dots in the graph represent the approximation of $\rho(x)$ obtained from numerical evolution of a typical phase point for 10^5 steps. From (8), it is easy to get the moments

$$\langle x^n\rangle = \frac{B(n+1/2,1/2)}{\pi} = \frac{(2n-1)!!}{2^n n!}\,,$$

where $B(n+1/2,1/2)$ is the Beta function. In particular, we get $\langle x\rangle = 1/2\,, \langle x^2\rangle = 3/8$.

Though the existence of $\rho(x)$ is easy to prove, its exact form is hard to obtain. Like in equilibrium statistical thermodynamics, we can conveniently define a generating functional such that all the statistical information of a particular dynamical variable is contained in it. Let's define

$$s(\beta) = \lim_{t\to\infty}\frac{1}{t}\ln\langle e^{\beta A^t}\rangle\,, \tag{9}$$

where β is an auxilliary variable and the ln is used to normalize the measure. The averaged quantity $\exp\beta A^t$ is multiplicative along an orbit, which is essential to the formulation below. Due to ergodicity, any smooth measure can be used in (9) to take the space average. For example, the uniform distribution will be used later. It is easy to see that

$$\begin{aligned}\langle a\rangle &= \lim_{t\to\infty}\frac{1}{t}\langle A^t\rangle = \left.\frac{\partial s}{\partial\beta}\right|_{\beta=0}\\ \langle a^2\rangle - \langle a\rangle^2 &= \lim_{t\to\infty}\frac{1}{t^2}(\langle A^t A^t\rangle - \langle A^t\rangle\langle A^t\rangle) = \left.\frac{\partial^2 s}{\partial\beta^2}\right|_{\beta=0}\,.\end{aligned} \tag{10}$$

Any moment of a is obtainable by taking derivatives of S.

2.2.2 Evolution operators and invariant measures

In the dynamical system (1), a time evolution operator $\mathcal{L}^t$ can be defined for continuous function $h(x)$ on $\mathcal{M}$,

$$\mathcal{L}^t\circ h(x) = \int_{\mathcal{M}} dy\, \delta(x - f^t(y))e^{\beta A^t}h(y)\,. \tag{11}$$

Physically, the evolution can be viewed as a passive transport of some quantity $h(x)$ attached to each phase point. The function

$$\mathcal{L}^t(x,y) = \delta(x - f^t(y))e^{\beta A^t} \tag{12}$$

is called the kernel of the evolution operator $\mathcal{L}^t$. It depends on the integrated quantity A^t. The delta function collects points y which evolves to x in time t. The usual evolution operator depends only on the flow, for example, when $\beta = 0$, $\mathcal{L}^t(x,y)$ reduces to the familiar Frobenius-Perron kernel. Note that the evolution operator has semigroup property for a general flow, *i.e.*,

$$\mathcal{L}^{t_1} \circ \mathcal{L}^{t_2} \circ h(x) = \mathcal{L}^{t_1+t_2} \circ h(x)\,, t_1, t_2 \in \mathbb{R}^+\,.$$

If the original dynamics f^t is a diffeomorphism, then the above relation holds for any $t_1, t_2 \in \mathbb{R}$ and thus the set of operators $\mathcal{L}^t$ form an Abelian group.

In a closed system, the Frobenius-Perron operator $\mathcal{L}^t|_{\beta=0}$ does not change the average of the function $h(x)$, since

$$\int_{\mathcal{M}} dx\, \mathcal{L}^t|_{\beta=0} \circ h(x) = \int_{\mathcal{M}} dx \int_{\mathcal{M}} dy\, \delta(x - f^t(y))h(y) = \int_{\mathcal{M}} dy\, h(y)\,.$$

Furthermore, if the system is autonomous, for any smooth function $a(x)$, $\langle a \rangle$ is independent of time, so $\rho(x)$ is invariant in time,

$$\mathcal{L}^t|_{\beta=0} \circ \rho(x) = \rho(x)\,. \tag{13}$$

We call $\rho(x)$ an invariant measure of dynamical system (1). For the Ulam map, (13) becomes

$$\frac{\rho(\frac{1+\sqrt{1-x}}{2})}{4\sqrt{1-x}} + \frac{\rho(\frac{1-\sqrt{1-x}}{2})}{4\sqrt{1-x}} = \rho(x)\,.$$

It is a functional equation which can be used to determine $\rho(x)$ if it is unknown. In a chaotic system, infinitely many invariant measures can exist. For example, the delta measure defined on a compact invariant set is an invariant measure. $\rho(x)$ discussed above is the one most relevant to the dynamics. Any smooth distributions will evolve asymptotically to $\rho(x)$. If a typical phase point is evolved for a long time on the computer, the phase space density of the points on its trajectory is proportional to $\rho(x)$. In the following, we will analyze the invariant measure $\rho(x)$ in the neighborhood of any periodic orbit and use the trace formula to piece together the useful information. The ensuing spectral determinants and dynamical zeta functions then provide basis for fast-convergent calculations - cycle expansions.

2.3 *Trace formula, spectral determinant and dynamical zeta function*

2.3.1 Trace formula

In terms of the evolution operator, we may write

$$\langle e^{\beta A^t} \rangle = \langle \mathcal{L}^t \circ \mathcal{I}(x) \rangle\,,$$

where $\mathcal{I}(x) \equiv 1$ is the identity function. According to (6), we mainly care about the long (infinite) time behavior of $\mathcal{L}^t$. In view of the semi-group property and linearity of $\mathcal{L}^t$, it is clear that the asymptotic state is dominated by the eigenstate of the "differential" of $\mathcal{L}^t$ that has the maximum eigenvalue. Under quite general assumptions, we may take the ansatz (for flows)

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

where $\mathcal{A}$ is called the generator of the evolution operator $\mathcal{L}^t$ and is the "differential" just mentioned. It is a linear operator independent of t and its spectrum determines the property of $\mathcal{L}^t$. Why is it so? Let's suppose that the eigenvalues and the eigenfunction of $\mathcal{A}$ are ordered as following (assume no degeneracy exists),

$$\begin{array}{ccccccc} s_0 & , & s_1 & , & s_2 & , & \cdots \\ \phi_0 & , & \phi_1 & , & \phi_2 & , & \cdots \end{array}$$

where $Re(s_k) > Re(s_{k+1})$, such that $\mathcal{A} \circ \phi_k = s_k \phi_k$. If we expand the identity function $\mathcal{I}(x)$ in terms of the eigenfunctions

$$\mathcal{I} = \sum_k I_k \phi_k\,,$$

then

$$\langle e^{\beta\,A^t} \rangle = \langle \mathcal{L}^t \circ \mathcal{I} \rangle = \langle \sum_k I_K e^{t\,s_k} \phi_k \rangle\,. \tag{14}$$

So, $\langle e^{\beta\,A^t} \rangle \sim e^{t\,s_0}$, for $t \to \infty$. The average is dominated by the maximum eigenvalue in the large time limit. In the following, we will study how to extract the spectrum of $\mathcal{A}$ from the set of periodic orbits. We will derive the formula for maps and write out the formula for flows directly.

For maps, we may write $\mathcal{L} = \exp(\mathcal{A})$. The notation is consistent as $\mathcal{L} = \mathcal{L}^1$. In analogy to the matrix calculation, the spectrum of the linear operator $\mathcal{L}$ is determined by solving the determinant equation $\det(\mathbb{1} - z\mathcal{L}) = 0$. But how to compute the determinant of an operator? Note the following identity in the matrix algebra

$$\det(M) = \exp(\mathrm{tr} \ln M)\,, \tag{15}$$

where M is an arbitrary square matrix and tr takes the trace of a matrix. Using (15), we can write

$$\begin{aligned} \det(\mathbb{1} - z\mathcal{L}) &= \exp(\mathrm{tr} \ln(\mathbb{1} - z\mathcal{L})) \\ &= \exp(-\sum_{k=1}^{\infty} \frac{z^k}{k} \mathrm{tr}(\mathcal{L}^k))\,, \end{aligned} \tag{16}$$

where we have used the Taylor expansion of the logrithmic function. This determinant is called spectral determinant as its zeros give the spectrum of the operator. So, in order to get the spectrum of the operator $\mathcal{L}$, we only need to calculate the trace $\mathrm{tr}(\mathcal{L}^k))\,, \forall k \in \mathbb{N}$. If we know the spectrum $\{s_m\}_{m \in \mathbb{Z}^+}$ of $\mathcal{L}$, then the trace

$$\mathrm{tr}(\mathcal{L}^k) = \sum_m e^{k s_m} \sim e^{k s_0}\,, k \to \infty\,,$$

increases exponentially if s_0 is the largest eigenvalue of $\mathcal{L}$.

The trace of an operator is defined in analogy with the marix case as the sum of diagonal terms, *i.e.*,

$$\begin{aligned}\mathrm{tr}(\mathcal{L}^k) &= \int_{\mathcal{M}} dx \int_{\mathcal{M}} dz\, \delta(z-x) \int_{\mathcal{M}} dy\, \delta(z - f^k(y)) e^{\beta A^k} \delta(y-x) \\ &= \int_{\mathcal{M}} dx\, \delta(x - f^k(x)) e^{\beta A^k}\,. \end{aligned} \tag{17}$$

Here, delta functions are used as the basis functions to calculate the trace. Sometimes, *i.e.*, like in the intermittency case this is not well defined as we we will explain. We may now directly integrate the delta function to get the trace. Notice that every time $f^k(x) = x$, *i.e.*, x is a periodic point of period k, the delta function contributes a term. So, we write the trace as a summation over periodic points

$$\mathrm{tr}(\mathcal{L}^k) = \sum_{f^k(x_i)=x_i} \frac{e^{\beta A^k(x_i)}}{|\det(1 - J_k(x_i))|}\,, \tag{18}$$

where $J_k(x_i)$ is the Jacobian matrix of f^k evaluated at x_i. Notice that (18) only holds for hyperbolic periodic orbits. If a neutral direction exists for the Jacobian, then $|\det(1 - J_k(x_i))| = 0$ and (18) has a zero denominator. This intermittency case even invalidates (17) since the delta function is not defined at degenerate zeros of function $x - f^k(x)$. With special care, the trace of the evolution operator is still computable but found to depend on powers of k. [10] We may now write the following generating functional for the trace

$$\begin{aligned}\mathrm{tr}\frac{z\mathcal{L}}{1 - z\mathcal{L}} &= \sum_{k=1}^{\infty} z^k \mathrm{tr}(\mathcal{L}^k) \\ &= \sum_p n_p \sum_{r=1}^{\infty} z^{rn_p} \frac{e^{\beta A_p}}{|\det(1 - J_p^r)|}\,, \end{aligned} \tag{19}$$

where the summation has been decomposed into summation over prime cycles p and their repeats. A_p, J_p are the integrated quantity and the Jacobian along the prime cycle p, and $A_p, \det(1 - J_k(x_i))$ depend only on the cycle but not the starting point on the cycle. (19) may be viewed as a generating function for the trace $\mathrm{tr}(\mathcal{L}^k)$. The spectral determinant is now easily calculated to be

$$\det(\mathbb{1} - z\mathcal{L}) = \exp\left[- \sum_p \sum_{r=1}^{\infty} \frac{z^{rn_p}}{r} \frac{e^{\beta A_p}}{|\det(1 - J_p^r)|} \right]. \tag{20}$$

The trace formula for flows is derived as [53]

$$\mathrm{tr}\mathcal{L}^t = \sum_p T_p \sum_{r=1}^{\infty} \frac{e^{r\beta\cdot A_p}}{|\det(1 - J_p^r)|} \delta(t - rT_p)\,, \tag{21}$$

where T_p is the period of the period orbit p. Now we have a continuous family of operators. So, to obtain the corresponding generating function we have to use integration instead of summation,

$$\int_{0^+}^{\infty} dt\, e^{-st} \mathrm{tr}\mathcal{L}^t = \mathrm{tr}\frac{1}{s - \mathcal{A}} = \sum_p T_p \sum_{r=1}^{\infty} \frac{e^{r(\beta\cdot A_p - sT_p)}}{|\det(1 - J_p^r)|}\,, \tag{22}$$

where J_p is the restriction on a transverse section of the monodromy matrix associated with the orbit p. The neutral direction along the cycle is excluded. In Appendix A, it is shown that the eigenvalues of J_p does not depend on the choice of the section. The spectral determinant is

$$F(s) = \det(s - \mathcal{A}) = \exp\left[-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{e^{\beta \cdot A_p - sT_p}}{|\det(1 - J_p^r)|}\right] . \tag{23}$$

It is easy to check that

$$\operatorname{tr}\frac{1}{s - \mathcal{A}} = \frac{d}{ds}\ln\det(s - \mathcal{A}) = \frac{d}{ds}\ln F(s) .$$

Note that the spectral determinants for maps and flows are very similar. Under the subsitution

$$z \to e^{-s} \, , \; n_p \to T_p$$

(20) becomes (23). In fact, in all the general expressions related to the spectral properties of the evolution operator, this substitution relates the map version to the flow version.

Very often, we are only interested in the leading eigenvalue of the evolution operator. In this case, only the dominant asymptotic behavior is of interest. If the flow is hyperbolic, a further simplification is possible,

$$\frac{1}{|\det(1 - J_p^r)|} \approx \frac{1}{|\Lambda_p|^r} , \tag{24}$$

where $\Lambda_p = \Pi_e \Lambda_{p,e}$ is a product of expanding eigenvalues $\{\Lambda_{p,e}\}_e$ of the matrix J_p. With $r \to \infty$, the relative difference between the two sides of (24) becomes exponentially small, and (20) leads to the dynamical zeta function

$$\frac{1}{\xi(z)} = \exp\left(-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} t_p^r\right) = \prod_p (1 - t_p) , \tag{25}$$

where $t_p = z^{n_p} \exp(\beta A_p)/|\Lambda_p|$. In practice, the spectral determinant (20) has better convergence properties [51] and if we need more eigenvalues other than the leading one, the spectral determinant gives the correct result.

2.3.2 Geometrical interpretation

We now give an intuitive explanation to (25) from a geometrical point of view. Consider the set $\mathcal{P}_n = \{p_{i,n} : f^n(p_{i,n}) = p_{i,n}\}$ of fixed points of f^n and assume that there are m of them. The SIS in the phase space is partitioned by the neighborhoods $\{\mathcal{M}_{i,n}\}$ of these periodic points. For simplicity, suppose that each of the neighborhoods $\mathcal{M}_{i,n}$ expands to cover the whole SIS in a one-to-one manner under the map f^n. So, if $n \to \infty$, the size of each $\mathcal{M}_{i,n}$, denoted by $V(\mathcal{M}_{i,n})$ goes to zero exponentially. If n is large, then $V(\mathcal{M}_{i,n}) \propto 1/\Lambda_{i,n}$, where $\Lambda_{i,n}$ is the product of expanding eigenvalues of $Df^n(p_{i,n})$, and to a high accuracy f^n can be treated as linear in each $\mathcal{M}_{i,n}$. The SIS has each component $\mathcal{M}_{i,n}$ as a preimage, so f^n will map m different pieces to $\mathcal{M}_{i,n}\, , \forall i$, one piece from each $\mathcal{M}_{j,n}\, , j = 1, \cdots , m$.

Put a uniform density defined by $\mathcal{I}(x)$ on the SIS. After the action by f^n, we see that *mass* contained in $\mathcal{M}_{i,n}$ (the integral of $\mathcal{I}(x)$ over $\mathcal{M}_{i,n}$) is proportional to its size $V(\mathcal{M}_{i,n})$ because the mass contained in each of its m preimages is proportional to the size of the preimage in the corresponding $\mathcal{M}_{j,n}$. We know that $\mathcal{I}^n(x) = \mathcal{L}^n \circ \mathcal{I}(x)$ tends to the natural invariant measure $\rho(x)$ for large n, so correlation!tim

$$\begin{aligned}\langle a \rangle &= \int_{\mathcal{M}} dx\, \rho(x)a(x) \approx \int_{\mathcal{M}} dx\, \mathcal{I}^n(x)a(x) \\ &\approx C \sum_{i=1}^{m} \frac{a(x_i)}{\Lambda_{i,n}}\,,\end{aligned}$$

where C is a constant and $x_i \in \mathcal{M}_{i,n}$ is a representative point. The deviation comes from the non-uniform expansion of f^n and non-constancy of $a(x)$ inside each $\mathcal{M}_{i,n}$, which become vanishingly small when n is large. So, we may interpret (25) as the natural weight of each periodic point. The trace formula (18) is just a weighted summation over the linear neighborhood of all the periodic points. The weight is given by (24), and it is an invariant quantity determined by the dynamics f, independent of the choice of coordinate system.

2.3.3 Correlation functions

We know that the largest eigenvalue of the evolution operator dominates $s(\beta)$, thus determines the statistical properties of an observable. What is the physical significance of the rest eigenvalues? Below, we will see that they determine the correlation of two or more observables.

The *time correlation function* $C_{ab}(t)$ of two observables a and b along the trajectory $x(t) = f^t(x_0)$ is defined as

$$C_{ab}(t; x_0) = \lim_{T\to\infty} \frac{1}{T} \int_0^T d\tau a(x(\tau+t))b(x(\tau))\,, \qquad x_0 = x(0)\,. \tag{26}$$

If the system is ergodic [271], with invariant continuous measure $\rho(x)$, then correlation functions do not depend on x_0 (apart from a set of zero measure), and may be computed by a space average as well

$$C_{ab}(t) = \int_{\mathcal{M}} dx_0\, \rho(x_0)a(f^t(x_0))b(x_0)\,. \tag{27}$$

For a chaotic system we expect that time evolution will lose the information contained in the initial conditions, so that $C_{ab}(t)$ will approach the *uncorrelated* limit $\langle a\rangle\langle b\rangle$. As a matter of fact, the asymptotic decay of correlation functions

$$\hat{C}_{ab} := C_{ab} - \langle a\rangle\,\langle b\rangle \tag{28}$$

for any pair of observables coincides with the definition of *mixing*, a fundamental property in ergodic theory. We now assume $\langle b\rangle = 0$ (otherwise we may define a new observable by $b(x) - \langle b\rangle$). Our purpose is now to connect the asymptotic behavior of correlation functions with the spectrum of $\mathcal{L}$. We can write (27) as

$$C_{ab}(t) = \int_{\mathcal{M}} dx \int_{\mathcal{M}} dy\, a(y)b(x)\rho(x)\delta(y - f^t(x)),$$

and recover the evolution operator

$$C_{ab}(t) \;=\; \int_{\mathcal{M}} dx \int_{\mathcal{M}} dy\; a(y)\mathcal{L}^t(y,x)|_{\beta=0} b(x)\rho(x)$$

We showed that $\rho(x)$ is the eigenvector of $\mathcal{L}$ corresponding to probability conservation

$$\int_{\mathcal{M}} dy\; \mathcal{L}^t(x,y)\rho(y) \;=\rho(x)\,.$$

The corresponding leading eigenvalue is 0. Now, we can expand the x dependent part in terms of the eigenbasis of $\mathcal{L}$:

$$b(x)\rho(x) = \sum_{\alpha=0}^{\infty} c_\alpha \phi_\alpha(x),$$

where $\phi_0 = \rho(x)$. Let $\mathcal{L}^t(y,x)|_{\beta=0\,,t\to\infty}$ acts on both sides. The average of the left hand side is zero since the evolution operator does not change the average. The average of the right hand side is equal to c_0, since other eigenmodes decay exponentially during the evolution as their eigenvalues are smaller than zero. So $c_0 = 0$ and the action of $\mathcal{L}$ then can be written as

$$C_{ab}(t) \;=\; \sum_{m\neq 0} e^{s_m t} c_\alpha \int_{\mathcal{M}} dy\; a(y)\phi_k(y). \tag{29}$$

We see immediately that if the spectrum has a *gap*, that is the second largest leading eigenvalue is isolated from the largest eigenvalue ($s_0 = 0$) then (29) implies an *exponential* decay of correlations

$$C_{ab}(t) \sim e^{\nu t}.$$

The correlation decay rate $\nu = s_1$ then depends only on intrinsic properties of the dynamical system (the position of the next-to-leading eigenvalue of the Perron-Frobenius operator), while the choice of particular observables determines the prefactor.

Correlation functions are important because they are often accessible from time series measurable in laboratory experiments and numerical simulations: moreover they are linked to transport exponents.

2.4 Cycle expansions

The spectral determinant (20) and (23) or the dynamical zeta function (25) are just formal infinite product expressions, and a effective way to evaluate them has to be presented in practice. To achieve this goal, in this section the cycle expansion method will be introduced and discussed. It reexpresses the formal product in terms of a convergent sum over periodic orbits ordered with a hierarchical way with contributions from long cycles decaying rapidly.

It is easiest to illustrate the cycle expansion by the dynamical zeta function. Consider the dynamical zeta function for a system whose symbolic dynamics is a full shift on two symbols $\{0,1\}$:

$$\frac{1}{\xi(x)} = (1-t_0)(1-t_1)(1-t_{01})(1-t_{001})(1-t_{011})(1-t_{0001})(1-t_{0011})(1-t_{0111})\cdots\,.$$

Expanded into a sum over cycles of increasing total length this becomes:

$$\begin{aligned}\frac{1}{\xi(z)} &= 1 - t_0 - t_1 - t_{01} - t_{001} - t_{011} - \cdots \\ &\quad + t_0 t_1 + t_0 t_{01} + t_1 t_{01} + t_0 t_{001} + \cdots \\ &\quad - t_0 t_1 t_{01} - t_0 t_1 t_{001} - \cdots ,\end{aligned} \tag{30}$$

where the products of t_*'s are called pseudocyles, *e.g.*, $t_0 t_1$, $t_0 t_1 t_{001}$ are pseudocycles. Such series representation of a dynamical zata function or spectral derterminant, expanded as a sum over pseudocycles and ordered by increasing cycle length and instability, is called *cycle expansion*. In a uniformly hyperbolic map like the Ulam map (quadratic map) or tent map (piecewise linear map), $|t_p|\rangle C/\Lambda^n$, where $C > 0$ and $\Lambda > 1$ are constants, and n is the length of the cycle. Let

$$F_1 = |t_0| + |t_1| + |t_{01}| + |t_{001}| + |t_{011}| + \cdots . \tag{31}$$

As the number of prime cycles of period n is less than $2^n/n$, the series in (31) converges and F_1 can be made to be smaller than 1 if z in t_p is chosen sufficiently small. It follows that

$$\left|\frac{1}{\xi(z)}\right| < 1 + F_1 + F_1^2 + F_1^3 + \cdots = \frac{1}{1 - F_1} . \tag{32}$$

From (32), we see that the dynamical zeta function $1/\xi(z)$ is well defined and is an analytic function of z for z sufficiently small. $1/\xi(z)$ may be extended to bigger domains in the complex plane by analytic continuation. This proof of convergence can be easily extended to general hyperbolic systems with more complex symbolic dynamics or higher phase space dimensions.

While we proved the convergence of (30), the summation scheme used in the proof is not the best. A better one is to regroup the terms into the dominant *fundamental* contributions t_f and the decreasing *curvature* corrections c_n:

$$\begin{aligned}\frac{1}{\xi(z)} &= 1 - t_0 - t_1 - [t_{01} - t_0 t_1] - [t_{001} - t_0 t_{01} + t_{011} - t_{01} t_1] - \cdots \\ &= 1 - \sum_f t_f - \sum_n c_n .\end{aligned} \tag{33}$$

We refer such regrouped series as *curvature expansion.* The fundamental contribution originates from the symbolic dynamics partition and reflects the qualitative dynamics of the system at the coarsest level. The curvature correction is due to the non-uniform expansion of the map. Longer cycles correspond to finer partitions of the phase space, and the curvature corrections are the difference between locally linear approximations of f^t in the coarse and the fine partitions. For example, the curvature term $[t_{01} - t_0 t_1]$ in (33) accounts for the difference of weights between the partitions of unit interval into two parts (centered around periodic points p_0 , p_1) and into four parts (centered around p_0 , p_1 , p_{01} , p_{10}) [57]. For uniformly hyperbolic systems, the curvature corrections decay exponentially fast with the cycle length, with convergence controled by the second derivatives (curvatures) of f^t. In this case, we say that that the long cycles are *shadowed* by shorter ones. Shadowing is an important observation to justify the numerical calculation when the dynamics is chaotic [107, 103]. Here, shadowing between periodic orbits is an intrinsic property and reveals the existence of the underlying hierarchical structure in the dynamical system. For the tent map (Eq. (2) in Chapter 3), the curvature corrections c_n are identically zero as its expansion rate is uniform everywhere.

If we write out (33) in a polynomial series of z, it is clear that the terms which have the same powers of z are grouped. Here z can be viewed as a kind of topological index, the powers of which indicate the topological length of cycles or psudocycles. By applying the same technique to the spectral determinant, we group terms of same powers of z in the cumulant expansion of the exponential in (20). In the flow case, we need to introduce some topological length (integers) to each cycle p. For example, the flow may be viewed as a map on some Poincaré section and we assign the topological length of a cycle in the map to its correspondent in the flow. Usually, this is simultaneously done with the symbolic dynamics established on the Poincaré section. One example is the 3-disk billiard [51], every collision of the billiard with a disk increases the topological length by one. Once the topological length of each cycle is known, we may encode this information to the spectral determinant (23) by adding an auxiliary variable z such that (23) becomes

$$F(s) = \exp\left[-\sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{z^{rn_p} e^{r\beta A_p - sT_p}}{|\det(1 - J_p^r)|}\right], \tag{34}$$

where n_p is the topological length of the prime cycle p. The symbolic dynamics as well as the topological length assignment is no way unique. A good choice should exhibit maximal shadowing and thus lead to a fast convergence of the curvature expansion. After the curvature expansion is implemented, we may set $z = 1$ and solve $F(s) = 0$ for the eigenvalues s of the evolution operator.

2.4.1 Cycle formula for dynamical averages

In view of (14) and (9), we have

$$s(\beta) = s_0(\beta)\,,$$

where $s_0(\beta)$ is the largest eigenvalue of $\mathcal{L}$ (or $\mathcal{A}$ for the flow) and depends on the parameter β. Here we have assumed that $s_0(\beta)$ is seperated from other eigenvalues by a finite gap. In general, there is no analytic expression for $s(\beta)$, and all calculations have to be carried out numerically. Once we calculate $s_0(\beta)$, the corresponding dynamical averages are obtained through (10). The computation requires taking derivatives of $s_0(\beta)$ with respect to β, which inevitably lowers the accuracy of the calculation if numerical differentiation is used. Moreover several $s_0(\beta)$ values have to be calculated for different β's near $\beta = 0$.

Such numerical derivatives are not needed, as we can use the spectral determinant or dynamical zeta function directly to compute the derivatives. In both formulations, $s_0(\beta)$ satisfies equations of the form $G(\beta, s(\beta)) = 0$. The first and second derivative of $G(\beta, s(\beta)) = 0$ yields respectively

$$\frac{\partial s}{\partial \beta} = -\frac{\partial G/\partial \beta}{\partial G/\partial s} \tag{35}$$

$$\frac{\partial^2 s}{\partial \beta^2} = -\left[\frac{\partial^2 G}{\partial \beta^2} + 2\frac{\partial^2 G}{\partial \beta \partial s}\frac{\partial s}{\partial \beta} + \frac{\partial^2 G}{\partial s^2}\left(\frac{\partial s}{\partial \beta}\right)^2\right] / \frac{\partial G}{\partial s}\,, \tag{36}$$

where all the terms are evaluated at $s = s_0(\beta = 0)$. Note that all the quantities on the right hand side can be calculated directly through the spectral determinant or the dynamical zeta function. So, the accuracy of the evaluation is not lost and only $s_0(\beta = 0)$ has to be solved for.

2.5 Summary

One advantage of the periodic orbit theory is that all the eigenvalues of an evolution operator are obtained without explicitly constructing the singular eigenfunctions defined on a fractal set. Second, only short UPOs are needed for any finite precision calculation. Furthermore, UPOs and their stabilites are intrinsic properties of a dynamical system. They are independent of the representation coordinates, *i.e.*, invariant under smooth conjugacies [63]. We may choose the best representation that meets our needs. Third, if the chaotic system is uniformly hyperbolic, cycle expansions converge exponentially fast. If in addition a Markov partition [107] exists, the cycle expansion converges super-exponentially.

There are also many open problems in this periodic orbit approach. Establishing and controling the rate of convergence of cycle expansions remains the biggest problem. What is proven in literature is that cycle expansions are convergent if the nonlinear system is uniformly hyperbolic. Most physical systems we encounter are not uniformly hyperbolic, indeed they are almost never purely hyperbolic. Though cycle expansions are a useful tool in many cases, they fail (converge extremely slowly) on other occasions. The failure is mainly due to the bad shadowing of certain long cycles by the short ones. Some procedures have been proposed to improve the convergence, for example, a symbolic dynamics of infinite alphabet has been used in the $1 - d$ intermittent map [10], or special ordering is used to do the grouping and truncation [62]. The problem is far from solved. For example, we still do not know how to treat the intermittency in general high-dimensional systems, how to give correct weights to each component in a mixed phase space, or have trace formulas for invariant sets other than the perodic orbits, like the invariant tori.

Another problem is associated with the complexity of the phase space structure. In all cycle expansion calculations, the UPOs have to be classified and ordered in a hierarchical way, so the establishment of a symbolic dynamics is necessary. Unfortunately, only one- or two-dimensional maps can be treated fairly completely [51, 118]. Little has been done to deal with the high-dimensional case. For example, in the applications discussed in this thesis we never know whether all the periodic orbits up to some given length are found. Even one omitted short orbit could undermine the accuracy considerably [51]. The hope for which we offer some evidence in what follows, is that we may use UPOs and other invariant sets like equilibria or heteroclinic orbits to unfold the structure of the phase space level by level.

Except for a few exceptional cases, the theory requires efficient numerical determination of the shortest periodic orbits in a given nonlinear system. If the system is strongly chaotic or has a high-dimensional phase space, many existing methods either fail or are inefficient. Development of reliable and efficient numerical schemes for locating periodic orbits is a big challenge in the application of periodic orbit theory. In the next chapter, we will introduce a new set of numerical methods for detecting UPOs, taylored to high (and infinite-) dimensional dynamical flows. periodic orbit theory—)