Hamiltonian Chaos: Classical and Quantum Aspects

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Prerequisites:

1. You don't think that Hamiltonian is a type of pizza.
2. You don't think that Schrödinger is the guy who races Formula-1 Cars.
3. You have lots of faith.
4. You can do some basic programming and have access to a pentium3 or better PC, preferably with the Linux OS.

Chapter 1

Hamiltonian Chaos: Classical Mechanics

1.1 Preliminaries

Hamiltonian systems are a very special class of dynamical systems that are of central concern to physics. They encompass the classical mechanics of Newton and are the starting point for quantum mechanics.

The dynamics is completely specified by specifying the values of a minimum number of coordinates of the particles involved and their conjugate momenta. This minimum number, the *number of degrees of freedom*, or DoF, may require some thought to figure out.

Degrees of Freedom:

1. *The number of degrees of freedom of a planar pendulum is* **one***, the angle it makes with the vertical say is enough to specify its position.*

2. *If we suspend the planar pendulum on a spring then the length is not a constant and therefore this system has* **two** *DoF.*

3. *A rigid rotator with a ball-and-socket joint has ?? DoF. If the rotator is no more rigid but is actually a spring. How many DoF?*

4. *How many DoF in a water molecule?*

5. *How many degrees of freedom does your arm have?! Without physically harming your neighbours, extend your arms out and check on first the number of DoF for your shoulders, then elbow joint, and then the wrists. According to one source the total is seven. Do you agree?*

6. *Speculative: Number of DoF of a swan's neck.*

Let the number of DoF be d. Let us state at the very outset that this is a very critical number. All that we understand reasonably well today are utmost 2 DoF systems! Detailed structures and behaviour of say even 3 DoF systems is beyond the scope of modern science. The key reason for this surprising inability is "chaos", which is potentially present for any system whose $d > 1$. It therefore remains a deep mystery as to how we have anything at all to say about complex systems such as liquids and gases.

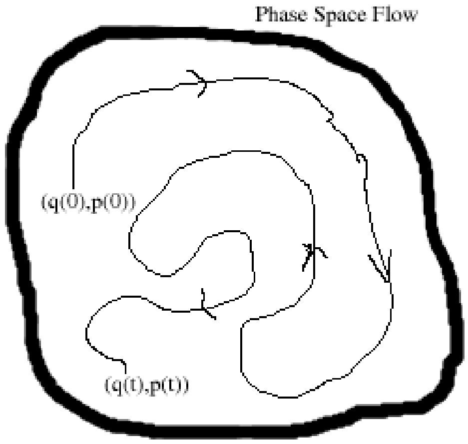

Figure 1.1: A phase space doodle

Let the coordinates that make up the DoF be labelled $(q_1, q_2, \ldots, q_d)$. Then the *phase-space* is the space that also includes the conjugate momenta $(p_1, p_2, \ldots, p_d)$. Thus the phase-space is has $2d$ dimensions. This is the proper space in which Hamiltonian mechanics is to be studied. Every physical system is assumed to be described by an Hamiltonian H which is a scalar function on the phase-space and completely determines the future and past of the $2d$ variables. The central equations are the Hamilton equations of motion:

$$\boxed{\begin{aligned} \frac{dq_i}{dt} &= \frac{\partial H}{\partial p_i} \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial q_i} \qquad (1.1) \end{aligned}}$$

These $2d$ first order ordinary differential equations are determined by the *single* phase-space function H. Note the $-$ sign in the momentum equation. Given any initial point $(q(0), p(0))$ it evolves to $(q(t), p(t))$ after a time t under the Hamiltonian equations of motion. Here $q(0)$ is written for the d position variable collectively, and similarly for momentum. Thus the Hamitonian generates a **flow** in the phase-space and classical mechanics is all about studying this flow. The Hamiltonian H could in general depend on all the $2d$ phase space variables as well as time t. If it depends on time t, the system is said to be non-autonomous, otherwise it is autonomous. For autonomous Hamiltonian systems, **trajectories in phase-space do not cross**. This follows from uniqueness of solutions of the set of first order o.d.e.s in Eq. (1.1).

If the trajectories crossed, then the partial derivatives of the Hamiltonian would have to be multi-valued at a given phase-space point. In fact they can be multivalued at different times if the system is non-autonomous and therefore phase-space trajectories can cross in this case. For such systems an extended $2d + 1$ space which is phase-space plus time space is such that trajectories don't cross here. It is easy to see that the no-crossing condition places severe restriction for a flow in a plane, i.e. for $d = 1$ cases. Refer to the phase-space doodle in Fig. (1.1) . It is easy to see that for spaces where the phase-space is higher than 2 there is a possibility for fairly complicated trajectories. In fact all $d = 1$

Hamiltonian systems are trivially *integrable*, $H = constant$ will give the phase space trajectories. There is no chaos.

The moment we step out of $d = 1$ we see interesting physics, in particular deterministic "randomness" or "chaos" appears as a generic (meaning usual) phenomena. For instance take the class of Hamiltonians $H(q, p, t)$, with $d = 1$, that is nonautonomous one degree of freedom systems, the extended phase-space is 3D, (q,p,t). Sometimes these systems are referred to as "one and a half" degree of freedom systems.

As somebody said "generalities are for wimps, real scientists study examples", lets study examples.

Elementary Examples:

1. *1-d Harmonic oscillator:* $H = p^2/2 + \omega^2 q^2/2$. *The Hamiltonian equations of motion are linear. The phase space trajectories are nested ellipses. There is one equilibrium point at the origin. If any of these things are not clear, clarify before proceeding.*

2. *The simple pendulum Hamiltonian is* $H = p^2/2 - gl\cos(q)$. *Notice that the equations are now nonlinear. There are stable equilibrium points at the origin and for every* $(q = 2\pi k, p = 0)$, *phase space point, there are unstable, hyperbolic points at* $(q = \pi(2k+1), p = 0)$, *where* k *is any integer.*

3. **Exercise:** *Draw the phase-space trajectories of the so-called Harper Hamiltonian* $H = \cos(2\pi p) + g\cos(2\pi q)$ *for some constant* g. *In particular analyze the cases as* g *crosses unity.*

1.2 Welcome to 1.5 degrees of freedom

1.2.1 Examples

All this is autonomous so far. Lets step out of $d = 1$ into $d = 1.5$, that is nonautonomous 1 DoF systems. We will take our elementary examples and modify them slightly. We will parametrically force them, i.e. change their parameters, like the restoring force, the length of the pendulum, gravity etc., in time. The harmonic oscillator case is well-known, the solutions are the *Mathieu* functions, the oscillator can be stable or unstable depending on the forcing amplitude and frequency. The case of the pendulum and the Harper Hamiltonian leads to chaos. These are *nonlinear* systems, and it may be expected that almost all nonlinear systems that are parametrically forced, even if they have only one-degree of freedom, will be chaotic. Surprisingly very little material is found on parametrically forced pendulum and it has been the subject of a Ph.D. thesis very recently!

Consider the general $d = 1.5$ Hamiltonian, for some functions f and h

$$H(q, p, t) = f(p) \; + \; g(t)\, V(q) \tag{1.2}$$

where $g(t)$ is some smooth function of time t. In the case when $g(t)$ is a periodic function, of period T say, important simplifications occurs. As an illustration consider the cases when the kinetic energy term is of the usual form, i.e. $f(p) = p^2/2$ and the case $g(t) = g(1 + \epsilon\sin(2\pi t))$, for the two potential, the simple harmonic oscillator $(V(q) = q^2/2)$ and the planar pendulum $(V(q) = \sin(q(t)))$.

In Fig. (1.2) we see what happens to such parametrically forced oscillators. Firstly, due to the nonautonomous nature of the systems, the phase-space trajectories cross. However they seem to be forming much more regular patterns in the case of the harmonic oscillator, but the pendulum behaviour starts looking complicated for increasing forcing. Before going any further let us illustrate with the pendulum an important feature: *sensitivity to initial conditions*. Shown in Fig. (1.3) are now the fate of *two* initial conditions that are separated initially by a small amount. We see that the parametrically

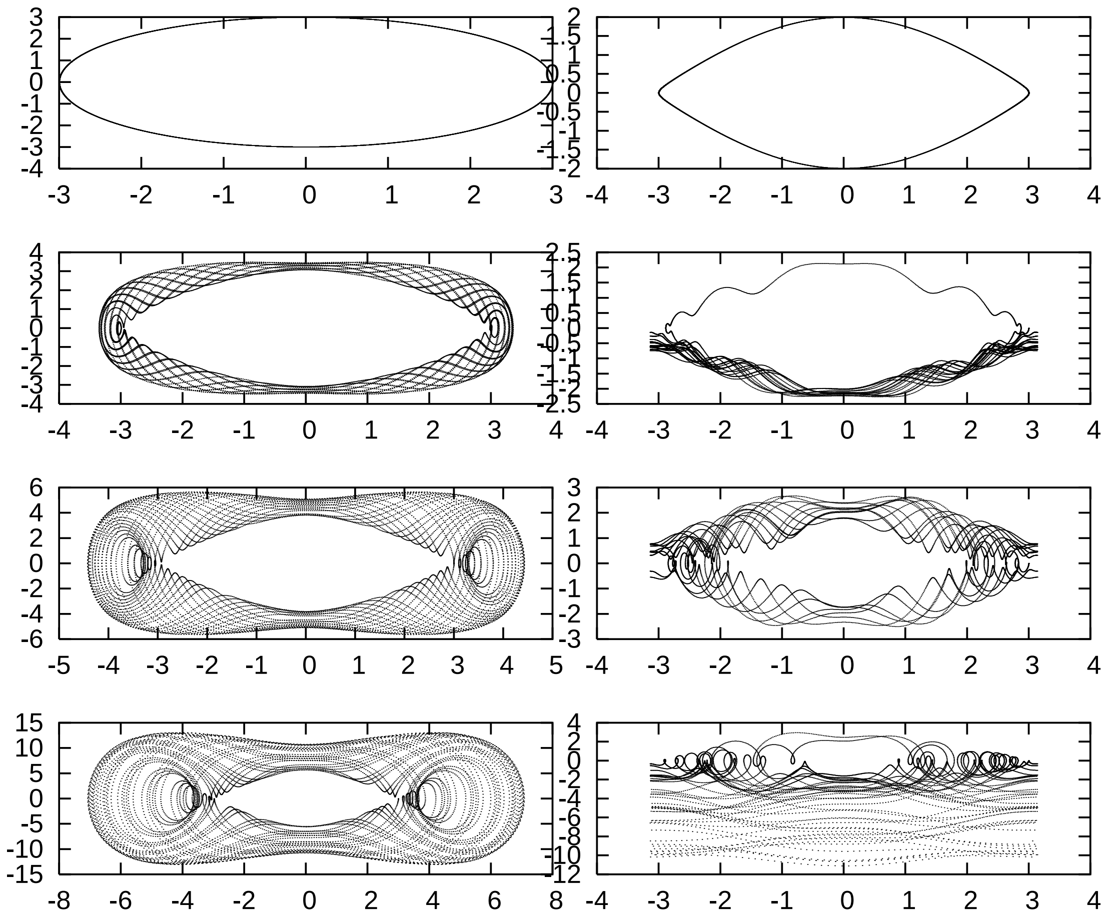

Figure 1.2: One phase-space trajectory of the parametrically forced harmonic oscillator (left) and the pendulum (right). Plotted is (q, p) as a function of time, all plots having the same initial condition $(q(0) = 3.0, p(0) = 0)$, and running for a time=100 (arb. units). The forcing function is $g(1+\epsilon\sin(2\pi t))$, and the parameters are $g = 1.0$, $\epsilon = 0, 2, 5, 10$ from top to bottom.

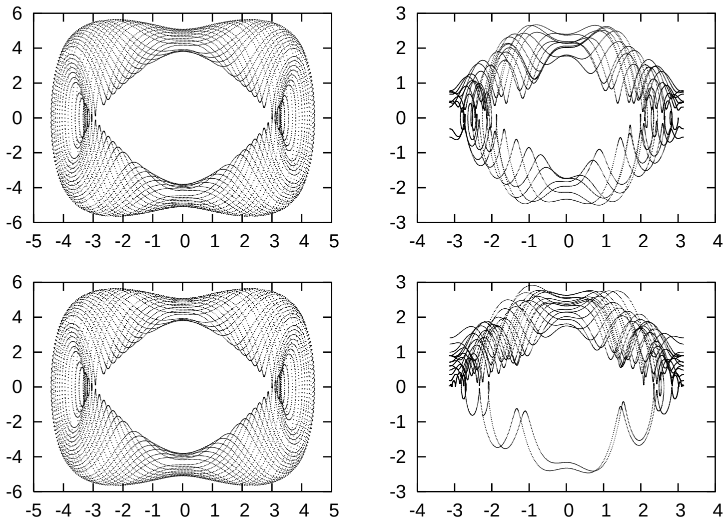

Figure 1.3: Tale of two initial conditions. On the left is the harmonic oscillator and the right is the pendulum. The initial conditions were $(q(0) = 3, p(0) = 0)$ (top) and $(q(0) = 3.0, p(0) = 0.001)$ (bottom). In both cases $\epsilon = 5$ and $g = 1$. The forcing function is same as that in Fig (1.2).

forced pendulum appears unstable, in the sense that these two trajectories quickly depart from each other, while the harmonic oscillator looks stable.

There is at best a statistical resemblance between the two initially nearby trajectories in the case of the pendulum, while the eye can discern no difference in the case of the harmonic oscillator. The harmonic oscillator can also be driven to instability, but the instability in the pendulum is of a very different nature. The instability that may arise in the harmonic oscillator is like the instability of a hill-top, anything dropped at the top runs away to infinity, while the pendulum instability seems to be there in *bounded* space. Even in the case when unboundedness arise, there is possibility of random looking recurrences in a very complicated manner. Thus this illustrates one of the central features of chaos in Hamiltonian systems:*instability coupled with confinement in finite regions of phase-space.* It should be remarked that there is Hamiltonian chaos in scattering systems as well, although we will not go into this aspect here.

While the pictures above are instructive, they are not terribly so. We have inferred that the harmonic oscillator is allegedly simpler, the pendulum is more complicated and perhaps sensitive to initial conditions. The pictures above have a disadvantage: this is only one trajectory, if we went ahead and plotted say 100 of them, so as to get a global understanding of phase-space behaviour, we will get some picture that looks worse than the Tamil Nadu Assembly in an excited state.

1.2.2 Stroboscopic Map

This is where we are helped by the fact that the forcing is periodic. We will choose to monitor the phase-space only at times separated by a period of the forcing. This will give us a discrete set of points, and the dynamics is specified by specifying where one point maps into the next time, the **stroboscopic**

map. Although the equations of motion are invariant under a time translation by T, the solutions are in general not periodic, let alone periodic with period T (see the pendulum pictures! Also *more generally the system's symmetries need not be shared by the solutions*). Let $f_{t_0}^t$ map evolve phase-space points at time t_0 by time t, i.e.

$$f_{t_0}^t(x(t_0), p(t_0)) \;=\; (x(t_0+t), p(t_0+t)) \tag{1.3}$$

$f_{t_0}^t$ does not have have the continuous semigroup structure seen for autonomous systems, in the sense that $f_{t_0}^t \circ f_{t_0}^t \neq f_{t_0}^{2t}$. We cannot use the same map to propagate further by the same time t, as the map will depend on the base time, so that it is true that $f_{t_0+t}^t \circ f_{t_0}^t = f_{t_0}^{2t}$. However due to the time-periodicity of the Hamiltonian, the map over a time T will possess a discrete simple Abelian group structure.

$$f_{t_0}^T \circ f_{t_0}^T \;=\; f_{t_0}^{2T} \tag{1.4}$$

The map $f_{t_0}^T$ propagates phase-space at time t_0 by T and repeated applications n times gives us $(x(t_0+nT), p(t_0+nT))$. Also clearly we have $f_{t_0}^T = f_{t_0+T}^T$, so that we have to only consider stroboscopic maps with base points between any two periods, say $[0, T]$. There is still an *infinity* of such stroboscopic mappings, however all of these are equivalent in a strong mathematical sense, they are *topologically conjugate* to each other. This means that the maps produce qualitatively identical structures, if there is a periodic orbit in one, there will be a corresponding periodic orbit in the other. This is a generalization of what we study in a first course (and for many of us, last) of classical mechanics as a property of homogeneous potentials.

The stroboscopic $2-dim$ map has *all* the information present in the extended phase-space, in a faithful manner. If there are periodic orbits in the phase-space, it will show up as a finite periodic collection of points on the map. In Fig. (1.4) we see how the map looks for the forced harmonic oscillator, and the forced pendulum.

Of Floquet and the Harmonic Oscillator.

The simplicity of the map for the parametrically forced harmonic oscillator is due to the fact that whatever may be the type of forcing function, $g(t)$, the stroboscopic map is a **linear** *one. This follows from because if $(x(t), p(t))$ is a solution then so is $x(t+T), p(t+T))$, but from the linearity of the differential equation the latter solution cannot be new, but must be a linear combination of the former. Thus we must have:*

$$\begin{aligned} x(n+1) &= a(t_0, T)x(n) + b(t_0, T)p(n) \\ p(n+1) &= c(t_0, T)x(n) + d(t_0, T)p(n), \end{aligned} \tag{1.5}$$

where $x(n) \equiv x(t_0 + nT)$ etc. This is a autonomous linear map, in the sense that the coefficients (a, b, c, d) don't depend on the iterate n, but they can depend on the base point t_0, and the period T. Also a very general property of Hamiltonian systems is reflected in the area-preserving condition that $ad - bc = 1$. Try to prove all these statements!

Floquet theory of linear differential equations with periodic coefficients, which predates a similar theorem due to Bloch which is applied for spatially periodic potentials in the Schrödinger equation and determines electronic band structure in solids, can be applied here, and the the Floquet exponents are the eigenvalues of the matrix $\{(a, b), (c, d)\}$. If the eigenvalues are complex and lie on the unit circle,

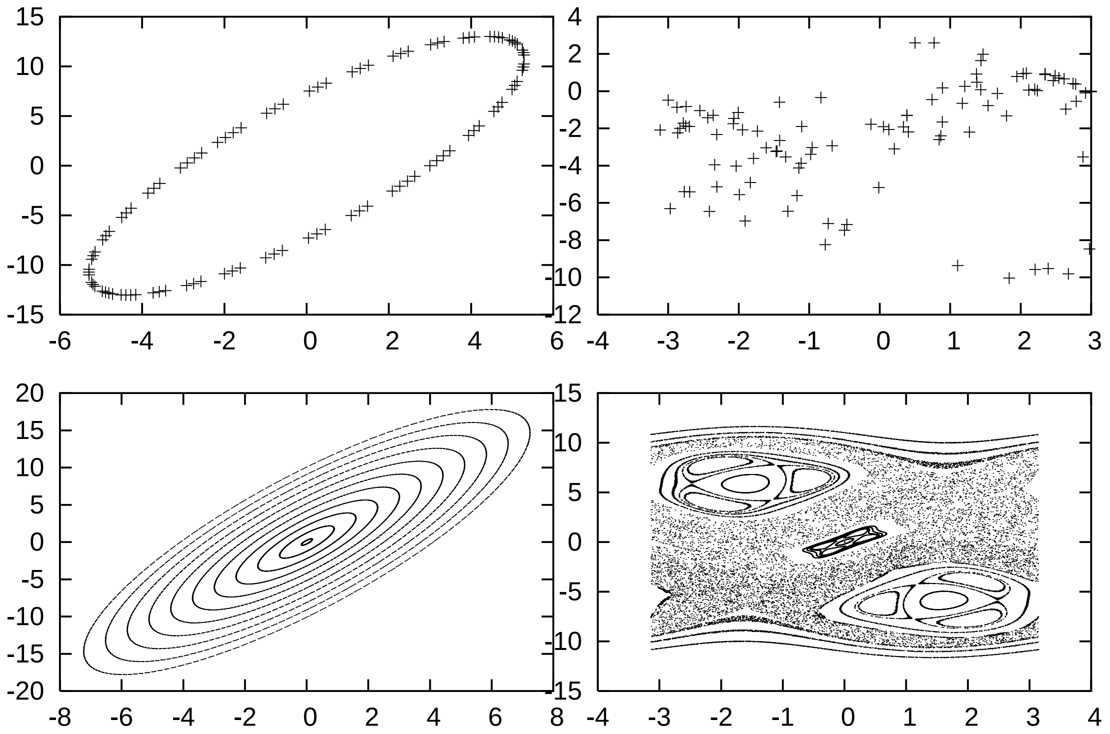

Figure 1.4: On the left is the harmonic oscillator and the right is the pendulum, stroboscopic maps. The top panel is for one hundred iterations with the initial conditions were $(q(0) = 3, p(0) = 0)$, while the bottom one features about 10000 iterations and many more initial conditions. In both cases $\epsilon = 10$ and $g = 1$. The forcing function is same as that in Fig. (1.2)

the system is stable and gives rise to elliptic orbits as illustrated above. Otherwise they will appear as pairs of real numbers whose product is unity and in this case the orbits will generically be hyperbolas.

The exact expression (a, b, c, d) depend on the forcing function $g(t)$ and are in general quite hard to find. For instance if $g(t)$ is a cosine function, the solutions are not elementray functions, but special ones, the Mathieu functions. However there are important cases where we can write down analytically the stroboscopic map. As a fairly extensive warm up the exercise below recommended.

Problem. *Consider the Hamiltonian:*

$$H = p^2/2 + s_T(t)\omega^2 q^2/2, \tag{1.6}$$

where $s_T(t)$ is the periodic function:

$$s_T(t) = \begin{cases} 1 & 0 < t \leq T/2 \\ -1 & T/2 < t \leq T \end{cases}. \quad s_T(t) = s_T(t+T).$$

Find the linear stroboscopic map. Analyze it for stability. Note that we are periodically switching from a stable harmonic oscillator to an inverted "oscillator" and back again. Thus we may expect that overall stability may be crucially dependent on the switching time T. Verify that the stroboscopic map is area-preserving.

The simplicity of the forced harmonic oscillator is lost in the case of the forced pendulum in many ways. Firstly, as is clear from the figures we are talking of qualitatively different behaviour. The simple elliptic orbits are replaced by a mixture of random splatter of points and regular looking curves. These are intermixed in an intricate manner that is not readily visible to our eye. This is in fact the generic phase-space of $d = 2$ (or $d = 1.5$) Hamiltonian systems: there is a mixture of chaos and regularity, what is called (naturally) a "mixed phase-space". Complete chaos, and complete regularity are exceptional. There is a rigorous mathematical statement to this effect.

But apart from the complexity of the phase-space, even writing down the stroboscopic maps are difficult in general. This is because we need to be able to integrate the equations of motion over one time period. For example if you attempt the corresponding boxed exercise for the pendulum, you will learn a lot about Elliptic functions, and yet the map will not be simple enough. The map will be *nonlinear* in general. However we can in fact write down nonlinear stroboscopic maps for one kind of forcing function, which is essentially the derivative of the step function s_T, namely a train of *delta* functions. This amounts to impulses at regular intervals of time. This case is often referred to as the "kicked" Hamiltonians and form a very important and well-studied genre of low-dimensional Hamiltonian chaos problems.

1.3 Kicked Hamiltonian Systems, Justforkix.

Consider Hamiltonians of the form

$$H = f(p) + \sum_{n=-\infty}^{\infty} \delta(t/T - n)\, V(q). \tag{1.7}$$

The Dirac delta function train is denoted in short as $\delta_T(t)$. The Hamiltonian equations of motion are:

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} = f'(p) \tag{1.8}$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q} = -\delta_T(t) V'(q) \tag{1.9}$$

We need to now integrate these equations over one period. Let us choose as $t_0 = 0^+$, so that we are going to consider the stroboscopic map just *after* each kick. The variables just after the n^{th} kick (q_n^+, p_n^+) are to be evolved to the next kicked. Just after the kick, there is no force till just before the next kick. Therefore we can write:

$$p_{n+1}^- = p_n^+, \quad q_{n+1}^- = q_n^+ + Tf'(p_n^+) \tag{1.10}$$

We have to now integrate over the kick number $n+1$ to arrive at q_{n+1}^+, p_{n+1}^+. Assuming that $f(p)$ is some smooth function of p, which does not itself have delta function dependencies, integrating the first of the equations of motion over the infinitesimal interval about the $n+1$ kick implies that the position of the particle is frozen. Integrating the second (force) equation gives us the impulse that is imparted, thus we can write:

$$q_{n+1}^+ = q_{n+1}^-, \quad p_{n+1}^+ = p_n^- - TV(q_{n+1}^+). \tag{1.11}$$

Finally combining the two sets of equations we get the stroboscopic map as:

$$\begin{aligned} q_{n+1} &= q_n + + Tf'(p_n) \\ p_{n+1} &= p_n - TV'(q_{n+1}). \end{aligned} \tag{1.12}$$

We have dropped the + superscript, as now every variable is defined as just after the respective kicks. Note that the second equation has the force $(-V'(q))$ evaluated at the *new* time. This follows from the equations of motion and make the above class of maps area-preserving for any functions f and V.

Exercises.
(a) Prove that map given in Eq. (??) is area-preserving. That is find the Jacobian of the transformation:

$$J = \begin{pmatrix} \partial q_{n+1}/\partial q_n & \partial q_{n+1}/\partial p_n \\ \partial p_{n+1}/\partial q_n & \partial p_{n+1}/\partial p_n \end{pmatrix}, \tag{1.13}$$

and show that $Det(J) = 1$.

(b) Find the stroboscopic maps in the case where the variables are monitored from just before the kicks, and in the case where they are monitored midway between kicks.

The stroboscopic maps in the family Eq. (??) present a very rich source of dynamical systems and it is quite accurate to say that we only partially understand them. Also while we have derived them from 1.5 dimensional systems, that is one-degree of freedom nonautonomous systems, it is important to note that they share the same phenomenology as the *Poincaré surface of section (PSOS) for two-degree of freedom autonomous Hamiltonian systems.* The PSOS of such systems are also area-preserving transformation of the same kind. PSOS are obtained by restricting ourselves to a given energy shell $H = E$ and observing the orbits as they cross a given section, traditionally as $x = 0$ in the positive $(p_x > 0)$ sense. The only difference between the PSOS and the stroboscopic maps is that the time of return to the PSOS is in general not the same and itself is a very complex, and ill-understood, function of phase-space. The popularity of maps such as in Eq. (??) is the simplicity of numerical work: we only have to iterate now and in principle there are no errors introduced due to truncation in integration schemes. Also certainly more analytical work is feasible in this approach.

1.3.1 Important Area-Preserving Maps in 2D

We now point out some of the important cases:

LINEAR MAP. This case is when $V(q) = \omega^2 q^2/2$ and $f(p) = p^2/2$. We have already seen how *any* forced harmonic oscillator leads to linear maps, the kicked harmonic oscillator is no exception, but now the stroboscopic map is absolutely straightforward to study:

$$\begin{aligned} q_{n+1} &= q_n + T p_n \\ p_{n+1} &= p_n - T\omega^2 q_{n+1} = p_n(1-\omega^2 T^2) - T\omega^2 q_n. \end{aligned} \tag{1.14}$$

The trace of the Jacobian, $\mathrm{tr}(J) = 2 - T^2\omega^2$, is an important quantity in this case and depending on whether $|\mathrm{tr}(J)| <$ or > 2 we have either stability (ellipses) or instability (hyperbolae). The phase space is the plane.

THE STANDARD MAP. This is the case of the kicked pendulum, $f(p) = p^2/2$ and $V(q) = -g\cos(2\pi q)/(2\pi)^2$. The stroboscopic map becomes:

$$\begin{aligned} q_{n+1} &= q_n + p_n \pmod 1 \\ p_{n+1} &= p_n - (K/2\pi)\sin(2\pi q_{n+1}). \end{aligned} \tag{1.15}$$

Here we have rescaled momentum: $T p \to p$, and $K = T^2 g$ is a rescaled effective parameter. This is the only parameter the kicked pendulum depends on. This map is one of the most widely studied of simple chaotic systems, called variously as the "standard map", the "Chirikov map" or the "Chirikov-Taylor" map. The modulo operation is necessary as the coordinate is cyclic, an angle, that has been scaled to lie in $[0, 1)$. Thus the phase space is a cylinder, cyclic along q and infinitely extended along the p or the angular momentum direction.

THE HARPER MAP. This is the case of the kicked Harper Hamiltonian, $f(p) = \cos(2\pi p)/(2\pi)$ and $V(q) = g\cos(2\pi q)/(2\pi)$. The stroboscopic map becomes:

$$\begin{aligned} q_{n+1} &= q_n - T\sin(2\pi p_n) \pmod 1 \\ p_{n+1} &= p_n + g T\sin(2\pi q_{n+1}) \pmod 1. \end{aligned} \tag{1.16}$$

Thus this is a two parameter map (T and gT), defined on a *torus* which is a square which has its opposite sides identified, the topology is that of a south-Indian "medu vada", the only popular type of vada north of the Vindhyas. This map also has been used in many studies.

As you may imagine, choosing any $f(p)$ and $V(q)$ and possibly imposing different boundary conditions, such as above, will lead to a plethora of maps. In fact it is quite a challenge finding any that are *not* chaotic in some parameter range. Try it! There do exist such systems, and for the sake of recording a very rare nonlinear but nonchaotic map we state the following system.

AN INTEGRABLE MAP.

$$\begin{aligned} q_{n+1} &= q_n + p_n \\ p_{n+1} &= p_n + q_{n+1}(A - 2q_{n+1}^2)/(B + q_{n+1}^2). \end{aligned} \tag{1.17}$$

Here A and $B > 0$ are real constants. You can find the corresponding kicking potential easily and it represents an exact discretization of the quartic double-well potential. The integrability of such maps is intimately connected to very special properties of Elliptic functions. But such maps are very rare and even less understood. It is not clear how to check whether a given map is *not* chaotic, i.e. integrable. This forms an active area of research in Mathematical Physics.

Exercises.

(a) Find the fixed points of all the maps stated above, and analyze their stability as function of system parameters. Fixed points are those that do not move, that is $q^0_{n+1} = q^0_n$, $p^0_{n+1} = p^0_n$. The stability is checked by find the Jacobian at these points and evaluating their eigenvalues. If the eigenvalues have a real part greater than unity in magnitude, the point is unstable. For 2D area-preserving maps such as above, the eigenvalues that are complex have modulus unity and are elliptic fixed points, *while those whose eigenvalues are real (one larger than unity in modulus) are* hyperbolic fixed points.

(b) Plot all of the maps above for various parameters and initial conditions. Get a feel for how easy it is to get pretty pictures. You will later see how difficult it is to make sense of them!

(c) Show that translation along p by one unit $S = (p \to p+1,\ q \to q)$ is a symmetry of the standard map. This operation commutes with the map itself, if we call the map M then $M \circ S = S \circ M$. Show that the reflection about the center of the unit square: $(q \to 1-q, p \to 1-p)$ is also a discrete symmetry of the standard map. What about the other maps? What effect do these symmetries have on the way the phase space looks?

In Fig. (1.5) is shown many orbits for the standard map for a few parameter values. The standard map is plotted as if the phase-space was a torus, that is the modulo condition is applied on the momentum as well. This gives us a true picture of what is happening on the cylinder as this unit cell repeats indefinitely along the cylinder. This follows from the fact that translation along p by one unit is a *symmetry* of the standard map (see exercise).

The standard map is one of the earliest models to have their *quantum mechanics* studied, a topic we will later touch on. Here it is enough to say that if you plotted the standard map on the cylinder, you will see a diffusion like behaviour in the momentum direction: exactly like a random walker in real space. This diffusion leads to increasing energy to the pendulum indefinitely. It was found that quantizing the system lead to a suppression of this diffusion, which lead to the phrase "quantum suppression of classical chaos".

Problem: **Classical Transport in the Standard Map***:*

Iterate the standard map on the cylinder *(no mod 1 on the momentum), and plot p as a function of time for various initial conditions for $K >> 6$, say $K = 10$. Notice the similarities between this graph and a 1-d random walker. Then find $< p^2(t) >$, where you first square the momentum and the average ove many initial conditions at a given time. The initial conditions could be for instance chosen to be uniformly spread along $p = 0$, $0 \le q < 1$. This is the " ensemble" averaging. Similarly find $< p(t) >$ and hence plot $< p^2(t) > - < p(t) >^2$ as a function of time t. You should observe a straight line with a slope approximately proportional to K^2, which can be predicted with simple arguments. However the exact value of the slope (the "diffusion" coefficient) is a very important quantity whose evaluation is a challenging and open problem in general. In particular there are K values where diffusion is violated, due to the presence of small islands, like those seen in the figure for $K = 5$, which don't fully disappear and lead to so-called "anomalous" diffusion, with diffusion mixed with purposeful marching, along so-called "accelerator modes". For further details see the references.*

The Fig. (1.5) shows how Hamiltonian chaos develops in typical low-dimensional systems. At $K = 0$, the dynamics is that of a *free rotator*, something called a twist map.

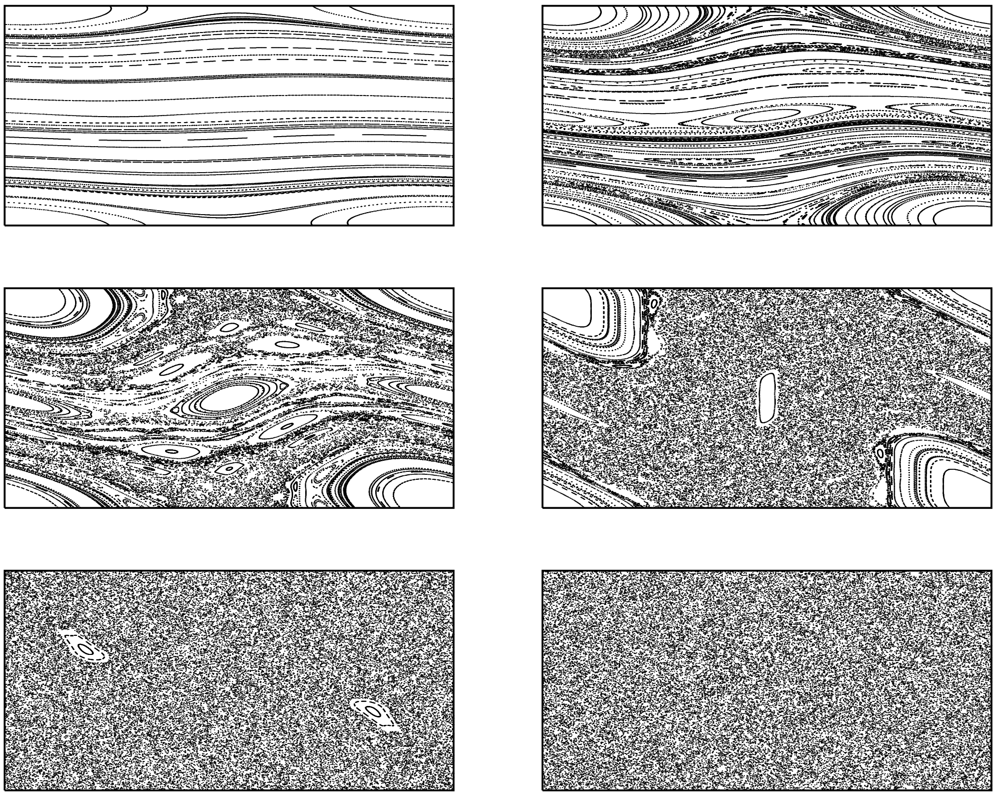

Figure 1.5: The standard map $(q-p)$ plot for parameter values $K = 0.1, 0.5, 1.0, 2.0, 5.0, 7.0$, increasing top left to bottom right for a random collection of 100 initial conditions followed 500 times. In all figures both the q and p directions go from 0 to 1.

1.4 Twist Map

The map we must begin with is something we can understand:

$$\begin{aligned} q_{n+1} &= q_n + p_n \,(\text{mod } 1) \\ p_{n+1} &= p_n. \end{aligned} \tag{1.18}$$

is an example of a *twist map*, in the sense that a radial line from the origin in phase-space will be twisted due to different rotation angles at different momenta (consider momenta to be radial coordinate and q to be the angle). This is a simple map and can be solved exactly:

$$\begin{aligned} q_n &= q_0 + n\, p_0 \,(\text{mod } 1) \\ p_n &= p_0. \end{aligned} \tag{1.19}$$

Exercises.

(a) Derive that Eq. (1.19) is in fact the solution.

(b) Show that if $p_0 = r/s$, where r and s are integers which don't have any common factor (i.e. they are "coprime"), the orbit consists of s distinct points that are periodic. Establish that the role of r is to skip $r-1$ points each time the map is iterated. Thus show that all rational values of p_0 lead to periodic orbits.

(c) Show that if p_0 is an irrational number the orbit will not be periodic. It will in fact uniformly cover the interval $0 \le q < 1$. It is said to be ergodic on the coordinate axis.

(d) Using the previous parts draw a phase-space portrait of this map. Compare it to the standard map at $K = 0.1$.

We have to see what happens to the twist map when we add terms that make it like the standard. The two types of orbits, the periodic ones and the non-periodic ones fare very differently. But first an objection may be raised that this is not general enough to be of interest: why the twist map? Actually, the twist map is also the *generic form of the PSOS for $d = 2$ separable Hamiltonian systems.*

1.4.1 Twist maps and Poincaré Surface of Sections

This is where the much maligned and largely ignored topic of classical mechanics courses, the Action-Angle variables show up for their wages. An important class of Hamiltonians are close to those that we can solve, so that some sort of perturbation theory can be used, and most of the solvable problems are separable in some appropriate coordinate systems. So let us start with a Hamiltonian of the form:

$$H(q_1, q_2, p_1, p_2) = H_1 + H_2 + V_{12}(q_1, q_2) \tag{1.20}$$

where $H_i = p_i^2/2 + V_i(q_i)$ is the Hamiltonian for the individual degrees of freedom while the potential V_{12} provides an interaction between them. As has been mentioned earlier the generic state of such Hamiltonian systems are chaotic.

However consider first the case $V_{12} = 0$, then what is the PSOS? For then instead of studying the effect of the potential in the full phase-space we can find the effect on the PSOS. Let us consider the case when V_1 and V_2 are confining potentials leading to periodic motions of period $T_i(E_i)$. The period can in general depend on the energies. Let us define the PSOS where $q_2 = 0$ and $p_2 > 0$. Therefore if

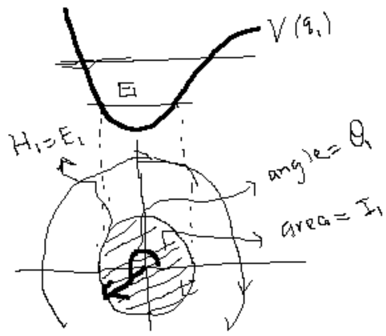

Figure 1.6: Illustrating Action-Angle

$(q_1(n), p_1(n))$ is a point on the PSOS we have to simply wait for a time T_2 to get $(q_1(n+1), p_1(n+1))$. Thus schematically we can write the PSOS as:

$$(q_1(n+1), p_1(n+1)) \; = \; f^{T_2}(q_1(n), p_1(n)) \tag{1.21}$$

where f^t evolves phase-space points in DoF 1. This mapping is in general nonlinear and can be quite complicated, although you know that the answer you get will have to be an integrable map, not chaotic! (We know the one constant of motion required, namely E_1.) You will however be able to write the PSOS for some simple cases, such as when the two oscillators are Harmonic, or when one or more of the confining potentials is hard wall like. If both are hard wall like, it is a rectangular "billiard". Thus this form of the PSOS is not revealing and not much perturbation theory can be done with this approach.

However the fact that the mapping is simple in some sense, tells us that there could exist coordinate systems in which the PSOS is simple. The "coordinate system" is the Action-Angle variables that we can get by means of a canonical transformation of the old (q_1, p_1) variables. Recall that if:

$$I_1 = \frac{1}{2\pi} \oint p_1 \, dq_1 \tag{1.22}$$

where the integral is taken over a closed phase space trajectory, then H is only a function of the action I_1, and not its conjugate variable θ_1. I_1 is the area under the curve $H_1 = E_1$ (except for the trivial factor 2π) and, serves like the radial marker in polar coordinates, while the angle tells you where on this constant area curve you actually are. Since the energy surfaces are nested, the actions uniquely determine (in 1D) the orbit, and the angle specifies where on the orbit the phase space point is. See the doodle in Fig. (1.6).

The Action-Angle transformation is a canonical one, in the sense that the the Hamiltonian written in this still generates the equations of morion through the canonical equations of motion, stated right at the beginning. Thus $H_1(I_1)$ is the Hamiltonian and we have

$$\frac{d\theta_1}{dt} \; = \frac{\partial H_1}{\partial I_1} \; = \omega_1(I_1) \tag{1.23}$$

$$\frac{dI_1}{dt} \; = \frac{\partial H_1}{\partial I_1} \; = 0, \tag{1.24}$$

where $\omega_1(I_1)$ is some in general nonlinear function. Thus in the Action-Angle coordinates, the Action is a constant, while the angle increases linearly, till of course it folds back. Thus in the Action-Angle space the PSOS is:

$$\begin{aligned} \theta_{n+1} &= \theta_n + T_2\,\omega_1(I_n)\,(\mathrm{mod}\ 2\pi) \\ I_{n+1} &= I_n, \end{aligned} \tag{1.25}$$

where we dropped the uniform subscript indicating DoF 1. Thus in these variables the PSOS is a generalized twist map, we had stated earlier the case when $\omega_1(I) = I$, a linear function. In general $\omega_1(I)$ is an increasing function of I, and the above map has all the properties we have already discussed. Notice that $T_2 = 2\pi/\omega_2$, where ω_2 is the corresponding frequency function for DoF 2. Thus depending on whether the *ratio of the frequencies of the two oscillators* is rational or not, we get closed or non-closed orbits. A little thought will show that this is not only reasonable, but in fact evident. The rational ratios result in a continuous family of orbits with the same behaviour, and these lie on *rational tori*, while the other orbits lie on *irrational tori.* On the maps, the rational tori show up as finite periodic orbits, while the irrational ones as continuous curves. The ratio of frequencies is the all important *winding number* and the action of the perturbation on it depends on this number crucially. Thus to summarize, twist maps are the generic form of not only the stroboscopic map of unkicked 1.5 degree of freedom systems (hence simply 1-d systems!), but also the PSOS of separable $d = 2$ DoF systems.

1.5 KAM, Birkhoff, Poincaré

The names in this section title are in the reverse chronological order, the order in which we discuss them, at least state the results to some extent. There are many books that deal adequately enough with these topics, which are really quite complex and form the crux of modern classical mechanics. The oustanding problem of the gravitational three-body problem spurred the major developments of classical mechanics. The question of the stability of the three-body gravitational systems was raised, and nothing less than the eventual stability of the solar system was in question. Today, it is understood that there are many solar system inhabitants that are chaotic, some more so than others. The 16^{th} satellite of Saturn, Hyperion, is known to be a tumbling piece of rock, about 140 Km wide, quite chaotically influenced by the big planet and its large satellites Titan. Its Lyapunov exponent is about $1/100$ (days)$^{-1}$, while its rotation period is 20 days. Two other moons of saturn, Pandora and Prometheus, that are said to "herd" the rings of saturn, are also believed from recent observational data to be chaotic. Pluto has been found to be mildly chaotic and would leave the solar system eventually. Despite all this chaos, it remains a mystery why there is not much more of it in the solar system, after all there are more than three bodies, and three is sufficient for chaos. The apparent stability of the solar system still remains unresolved in its entirety.

1.5.1 Kolmogorov (1954), Arnold (1960), Moser (1962)

KAM theorem address the problem of what happens to an integrable Hamiltonian system that is very slightly perturbed. Just how slightly, just by what perturbation etc. are also stated. KAM asserts that under the conditions of:

1. sufficiently small perturbation,
2. sufficiently smooth perturbation, and
3. for, loosely speaking, sufficiently "nonlinear" integrable Hamiltonians,

"sufficiently irrational" tori survive, that is they are topologically equivalent to the integrable (unperturbed) tori. Suffices to say that a complete proof of this theorem is difficult and involved, as may be judged from the fact it took three great mathematicians to do what Poincaré thought he had done about 60 years earlier: exorcised the small-denominator problem. While K&A were working with Hamiltonian flows, J. Moser addressed the problem from a perturbed twist-map angle.

The persistence of almost straight-line orbits in the first window of Fig. (1.5) corresponding to $K = 0.1$ is an evidence of the working of KAM theorem. In fact lets go over the KAM conditions: is $K = 0.1$ small enough? This is hardly clear, the original proof of Arnold reportedly requiring a perturbation that is less than 10^{-48}! The fact that tori survive almost up to $K = 1$ is certainly not explained by the KAM theorem. These highly non-perturbative regimes are little understood. Is the perturbation smooth? Yes, the sin function is C^{∞}, infinitely differentiable. The Moser proof required that the perturbation be at least C^{333}, again certainly a very odd number! Subsequent developments allow perturbations that are only $C^{2+\epsilon}$. Counterexamples are known for C^2 perturbations, so we may at least require that the perturbation and its derivative is continuous. Is the unperturbed system "sufficiently nonlinear"?

The unperturbed system is assumed to have good action angle coordinates, that is the Hamiltonian $H(I_1, I_2, \ldots, I_d)$ is only a function of actions. The frequencies corresponding to the actions are $\omega_i(I_i) = \partial H/\partial I_i$. The condition of nonlinearity actually requires that these frequencies not be degenerate. This can happen if the frequencies don't depend on the actions at all. This happens in the case of the harmonic oscillator. Recall that the frequency does not depend on the energy, and hence on the action, indeed the Hamiltonian is $H = \omega I$ for the 1-D oscillator. More generally it is required that

$$\mathrm{Det} \left| \frac{\partial \omega_i}{\partial I_j} \right| \neq 0.$$

Translated into English, this means that given a set of frequencies they locally determine a set of actions and hence we can specify the tori based on the frequency functions. The implicit function theorem (see books on calculus) guarantees this provided the determinant condition holds. Just think $d = 1$, this is not valid for the harmonic oscillator but valid for generic potentials. This explains why we were only "loosely speaking" when we said that the unperturbed system is "nonlinear", it has to be nonlinear and nondegenerate.

The unperturbed system for the standard map is the twist map, and the angle is q, while the action is p and we see that the frequency function is $\omega(I) = I$, therefore the unperturbed system is not degenerate, and the KAM conditions are satisfied. But note that the condition of sufficient nonlinearity excludes the applicability of KAM to many physically interesting problems, including perturbed Harmonic oscillators. Non-KAM behaviour may or may not be seen if any of these conditions are violated. Non-KAM systems are even less understood, although examples abound.

1.5.2 Poincaré and Birkhoff.

The theorem associated with the French founder of modern dynamics, Henri Poincaré and his American follower Georg Birkhoff, explains the fate of *rational tori.* While KAM said "nothing much" happened to the irrational ones, the rational ones undergo dramatic change, it is an example of a bifurcation, where marginal orbits are replaced by a chain of stable (elliptic) and unstable (hyperbolic) orbits.

The proof the PB theorem is in fact much easier than the KAM and is largely geometrical. Again, we simply state the result. Let the unperturbed rational tori have a winding number $\omega = r/s$. Then on perturbation this will be replaced by a chain of alternating hyperbolic and elliptic periodic orbits of

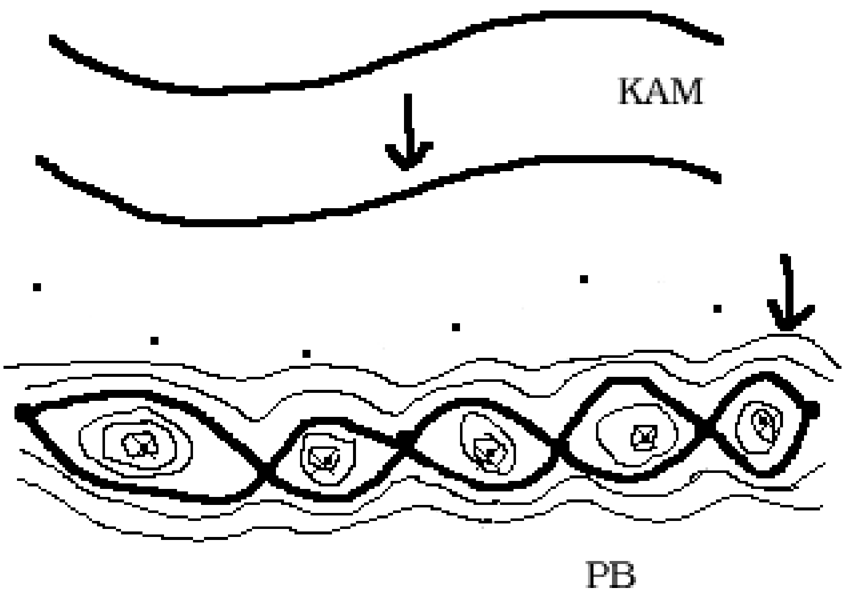

Figure 1.7: A doodle of the KAM and PB theorems. An irrational tori survives the perturbation, while a rational torus (here $s = 6$) breaks into a resonance chain. Shown here as a sequence of six dots is only a representative orbit of the unperturbed rational tori, which has an infinite number of them.

period s, with a winding number of r/s. It should be emphasized that the unperturbed rational tori supports an *infinity* of periodic orbits of period s (the whole line, in the case of the twist maps), but the perturbed system has only *one*. around the elliptic periodic orbits there are closed stable orbits, while around the hyperbolic orbits something very strange occurs that eventually matures to chaos.

The PB scenario for rational tori, is a frequency matching commensuration condition and this is therefore called a "resonance", an $r : s$ resonance is said to be occur. The smaller the s is, that is smaller the period, on perturbation the larger is the elliptic or the resonance zone. As perturbation increases the resonance region, which resemble the simple pendulum phase space, grows. The fattening resonances overlap and this gives rise to global chaos in one of the scenarios of Hamiltonian chaos, (due to Chirikov, the "chirikov overlap criterion").

Let us take the example of the standard map, Eq. (1.15). At $K = 0$, the twist map has a $0 : 1$ resonance all along the line $p = 0$. This entire line is a line of *fixed* points, that is points of period 1. For $K \gtrsim 0$ there are only *two* fixed points, the stable one at $(0, 0)$ and the unstable one at $(0.5, 0)$, and the region becomes like a simple pendulum. For increasing K this region grows, till it eventually collapses, as can also be seen from the Fig.(1.5). The PB scenario can be seen in abundance in the standard map.

But what gives rise to the splatter of points? If KAM and PB were the whole story then the phase space should not look anything much more complicated than that of a pendulum. One key factor in the differences between KAM and PB was the rationality of otherwise of the winding number; but on the real line, *both the sets of rational and irrational numbers are dense.* This means that arbitrarily close to any point we can find a rational number, we can also find an irrational number. This means that the resonances are also dense. However each resonance has some width, and therefore we can expect that resonances will generically intersect even for very small perturbations, and result in complex dynamics.

Therefore it seems reasonable that *chaos begins on the boundaries of resonances*, especially in the neighbourhood of the hyperbolic periodic orbits.

1.5.3 The Homoclinic Tangle or $1 \Rightarrow \infty$.

In a 2D area-preserving map the neighbourhood of a hyperbolic periodic point, say x^* contains the seeds of chaos. There are a set of points that approach the hyperbolic points ever more closely, while there is a set that was very close to it in the ever receding past. The first set is called the *stable manifold*, denoted $W^s(x^*)$, while the second is called the *unstable manifold*, denoted $W^u(x^*)$. In general These "manifolds" (just think of manifolds as smooth nonintersecting curves for our purpose) are a collection of an infinity of orbits.

Exercise.

FIND THE EQUATION FOR THE STABLE AND UNSTABLE MANIFOLDS OF THE SIMPLE (UNFORCED!) PENDULUM.

Firstly, the stable and unstable manifolds do not intersect each other. Remember that the manifolds can consist of many orbits. Only in a $d = 1$ Hamiltonian flow the manifolds coincide with orbits themselves. Therefore for such systems (or in general flows in 2D phase space) the fact that the stable and unstable manifolds do not self-intersect is a direct consequence of uniqueness of solutions, something we have already seen. For higher dimensions, the manifolds are themselves not orbits, this argument is not directly applicable.

However let us say that an unstable manifold intersects itself as in Fig. (1.8), then from *continuity* of the transformation ("nearby points go to nearby points") it follows that such a self intersecting point must be mapped to another self intersecting point, which gets mapped to another one and so on ad-infinitum. But also the self-intersecting point must have *come* from such a point etc. to the distant past when the orbit was arbitrarily close to x^*. Thus self-interesecting points must accumulate to this point. This is not possible, as from a fundamental theorem of dynamical systems, the Hartman-Grobman theorem, the unstable manifold is tangential to an eigenvector of the linear stability matrix at that point (the *local* unstable manifold). Similar argument for the stable manifold, reversing time now, and going forward. Thus indeed the sets of stable and unstable manifolds are *manifolds.*

This nonintersection also follows from invertibility and continuity, as two points cannot be mapped to the same. Refer to the Fig. (1.8), where we have marked a segment of an orbit as $p0 \rightarrow p1 \rightarrow p2 \rightarrow p3 \rightarrow p4 \rightarrow p5$. The point $p4$ "jumps" over the point $p1$ to reach $p5$ (remember this is a map). However from continuity the segments of orbits in $p0 - p1$ gets mapped to $p1 - p2$ etc., and therefore there must be some point in the segment $p3 - p4$ that gets mapped into $p1$. But $p1$ came from $p0$ and cannot have two immediate predecessors and therefore the envisioned scenario is prohibited.

If the unstable manifolds belong to two different periodic points, then they clearly cannot intersect each other, as in the distant past there would be a conflict of interest and similarly for stable manifolds in the distant future.

Surprisingly, the stable and unstable manifolds *can* and do intersect each other, with dramatic consequences. If they belong to the same orbit such an intersection is called *homoclinic* and if they belong to two different orbits it is *heteroclinic*. Neither of the two arguments against intersection hold here. The first argument about one intersection implying another and so on also holds here. If a point belongs to both the stable and unstable manifold, its distant past and distant future is sealed, it must be in the

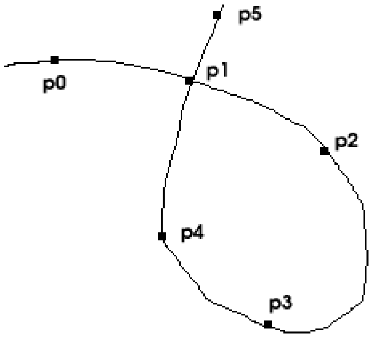

Figure 1.8: If an unstable (or stable) manifold intersects itself ...

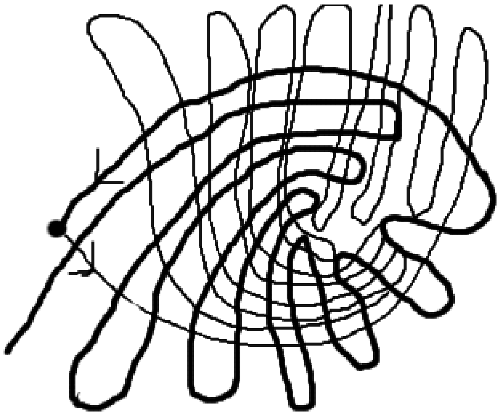

Figure 1.9: A homoclinic tangle doodle. The dark line is the stable manifold, while the other is the unstable one. Notice how they have to arrange themselves in order not to self intersect.

vicinity of x^*, therefore all its iterates also have this property and hence lie on intersections. Combined with the area preserving nature of the transformations (Fig. (1.10), the homoclinic intersections give rise to a complex network. Phase space points that are in this network behave in a apparently random manner, although their dynamics is completely deterministic.

If you think that the homoclinic tangle is a mess, you are in good company,

"It may be futile to even try to represent the figure formed by these two curves and their infinite intersections, each of which corresponds to a doubly asymptotic solution [to the equations of motion]. The intersections form a kind of trellis, a tissue, an infinitely tight lattice; each of the curves must never self-intersect, but it must fold itself in a very complex way, so as to return and cut the lattice an infinite number of times. The complexity of this figure is so astonishing that I cannot even attempt to draw it. Nothing is more appropriate to give us an idea of the complexity of the three-body problem and in general of all the problems in Dynamics where there is no uniform integral."

Henri Poincaré, 1899 on homoclinic orbits.

Exercise. *Draw the homoclinic tangle. Draw an heteroclinic tangle. Does area conservation along*

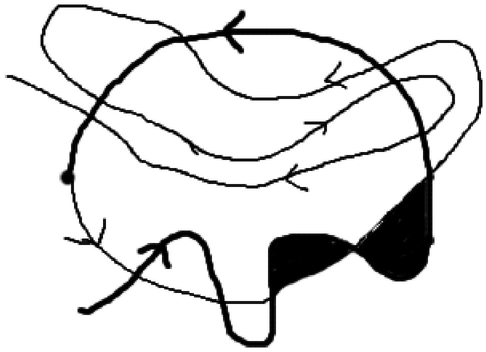

Figure 1.10: The shaded areas are successive mappings.

with nonintersection lead to a contradiction? Won't the shaded areas such as in Fig. (1.10) not be able to intersect itself, yet not go away and therefore fill a finite area infinitely, which is clearly absurd. The answer is in this figure itself. Go figure.

The neighbourhood of each of the hyperbolic points in the PB scenario is in fact a homoclinic tangle. To understand the tangle is to understand the genesis of Hamiltonian chaos. As physicists we look to abstract this object, make it so simple that it cannot get simpler without destroying what we study. The dissipative abstraction of the tangle is called the Smale (pron.: Small a) horseshoe, after its originator Stephen Smale and the shape of the areas on iterations, horseshoes. We will however look at a simple model that is still globally area preserving: the baker map, named after the generic humble baker who quite oblivious of the homoclinic tangle is engaged in baking the daily bread.

1.6 The Baker Map

"The baker's map is the harmonic oscillator of chaos"
–Predrag Cvitanovic.

On the lightly floured surface, flatten the dough slightly into a disk-shape. Use the heels of your hands to PUSH the dough away. Pick up the edge furthest away from you and FOLD it toward you, sliding the dough back to its original spot on the counter. TURN the dough a quarter-turn. Vigorously repeat "push, fold, and turn" steps.

– From www.baking911.com. (without permission).

So whats all this fuss about? The baker does it every day, and while making chappathis we adopt similar strategy to mix thoroughly the *atta* with the water. Looking at the instructions for baking we see two crucial ingredients, PUSH, and FOLD. Pushing provides the instability, while folding provides the confinement, the classic "stretch and fold" mantra of chaos. (For the moment we ignore the instruction of the baker to "turn"). We also assume that the dough is 2D and a perfect square!

Baker Map.

$$\left.\begin{aligned} q_{n+1} &= 2\,q_n \\ p_{n+1} &= p_n/2 \end{aligned}\right\} 0 \le q_n < 1/2; \quad \left.\begin{aligned} q_{n+1} &= 2\,q_n - 1 \\ p_{n+1} &= (p_n+1)/2 \end{aligned}\right\} 1/2 \le q_n < 1. \tag{1.26}$$

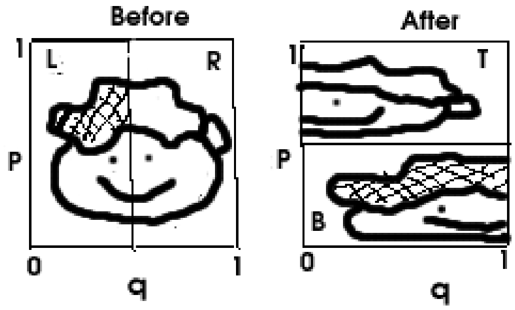

Figure 1.11: The dough before and after. Notice how the baker's smile becomes a bit wane, as his face is stretched in the q direction and compressed in the p, both by a factor of 2, cut in the center and stacked with the right half on top of the left, so that $L \to B$ and $R \to T$. It is a wonder that the baker is still smiling at all.

The baker map is area preserving, its Jacobian is simply $\mathrm{diag}(2, 1/2) = \{(2,0),(0,1/2)\}$ everywhere, the eigenvalues are 2 and 1/2. The map is said to uniformly hyperbolic, the stretching is the same throughout phase space. Hamiltonian systems of d DoF are always characterized by a maximum of d pairs of stretching and compressing directions as the overall area (and in fact various other quantities known as Poincaré Cartan integral invariants) has to be preserved. This leads to the sum of the d Lyapunov exponents being zero. Thus the lyapunov exponents for the baker map are $\log(2)$ and $-\log(2)$. Thus with a positive nonzero Lyapunov exponent the map is a candidate for chaos. It is in fact a paradigm of chaos, and this becomes clear if we work in the binary representation of numbers.

Let (q_0, p_0) be an initial phase space point that is evolved by the baker map in Eq. (1.26). How is the phase space point after n iterations (q_n, p_n) related to the initial conditions? In short can we *solve* the baker map? If you look more closely at the baker map, you realize that the evolution of q has nothing to do with p, while the evolution of p is dependent on q. Thus we could solve for q_n for instance, and in fact the q map is known as the doubling or the sawtooth map. It is simply $q' = 2q \,(\mathrm{mod}\, 1)$, whose solution is $q_n = 2^n\, q_0 \,(\mathrm{mod}\, 1)$. What have we achieved? Actually not much. Although we have "solved" for q_n the solution does not leave us much wiser. This is a good illustration that *chaos is not about the lack of analytical solutions.* Chaos has little to do with our labels of "numerical", "analytical" etc., it is a statement about dynamics.

To "understand" the baker any further, we need to do something more than solve it. Let the phase space points be specified in the binary representation, say as $q_0 = 0.a_0 a_1 a_2 \ldots$ and $p_0 = 0.a_{-1} a_{-2} a_3 \ldots$, where $a_i = 0, 1$. Recall that this means

$$q_0 \;=\; \frac{a_0}{2} + \frac{a_1}{2^2} + \frac{a_2}{2^3} + \ldots;\; p_0 \;=\; \frac{a_{-1}}{2} + \frac{a_{-2}}{2^2} + \frac{a_{-3}}{2^3} + \ldots. \tag{1.27}$$

Note that $a_0 = 0$ if q_0 lies in left half L and it is 1 otherwise. Thus $q_1 = 2\,q_0 - a_0$ whether $a_0 = 0\,\mathrm{or}\,1$. Similarly $p_1 = (p_0 + a_0)/2$ in either case. We get

$$q_1 \;=\; \frac{a_1}{2} + \frac{a_2}{2^2} + \frac{a_3}{2^3} + \ldots;\; p_1 \;=\; \frac{a_0}{2} + \frac{a_{-1}}{2^2} + \frac{a_{-2}}{2^3} + \ldots. \tag{1.28}$$

If we write Eq. (1.27) as a *bi-infinite* sequence of the following form

$$(p_0|q_0) \;=\; \ldots a_{-3} a_{-2} a_{-1} \circ a_0 a_1 a_2 \ldots \tag{1.29}$$

then

$$(p_1|q_1) \;=\; \ldots a_{-2}a_{-1}a_0 \circ a_1 a_2 a_3 \ldots \tag{1.30}$$

The notation $(p|q)$ is to indicate a phase space point, the right side is to be thought of symbolically, with the small circle separating the p in the left from the q on the right. Thus given the right side, we can read off q and p. Thus the action of the baker dynamics is transparent. It shifts the entire sequence of a_i to the left by one place. Iterating the map simply shifts it further and futher. Thus the small circle, dividing q from p, also acquires the significance of the *present moment.* This dynamics is known as a *left shift.* Although this appears to be very special it is some form of left shit on possibly infinite symbols (not just 0 and 1) that underlies chaos, including that found in many body problems. The left shift is in many senses the heart of chaos, Hamiltonian or otherwise.

This representation then reveals many features of the baker map:

1. Proliferation of errors. The left shift reveals the alarming nature of chaos and eventually the limitations of mathematical modelling for prediction. We would know the initial conditions only up to some precision, say we have an accuracy of $10^{-20} \approx 2^{-67}$, that is we know $(a_0, a_{\pm 1}, \ldots, a_{\pm 66})$ and a_{-67}. The rest of the binary expansion coefficients are inaccessible to us. On iterating the baker map, we lose one bit of information every time, and after 66 times the following is the case:

$$\begin{aligned}(p_0|q_0) \;&=\; [u]\, a_{-67}\ldots a_{-1} \circ a_0 \ldots a_{66}\, [u] \longrightarrow \\ (p_{66}|q_{66}) \;&=\; [u]\, a_{-67}\ldots a_0 \ldots a_{65} \circ a_{66}\, [u].\end{aligned} \tag{1.31}$$

We have indicated the any unknown bit strings uniformly as $[u]$. The initial area of ignorance is a square of size $2^{-67} \times 2^{-67}$, whose left-bottom corner is at $(q = 0.a_0 \ldots a_{66},\ p = 0.a_{-1}a_{-2}\ldots a_{-67})$.

What do know about $(p_{66}|q_{66})$? About q_{66} we only know the first significant bit which is a_{66}, we are at the edge of our knowledge. Thus all we can say about q_{66} is whether it is in the left half $(a_{66} = 0)$, or the right half $(a_{66} = 1)$ of the square. We seem to have compensated for our q losses in p, we now know it to a *greater(!)* accuracy of about 10^{-40} now. After one more iteration we have no clue where q_{67} is, we can only make the trivial, but consoling, statement that it is somewhere in the square, we are not losing any dough, and the accuracy of p is at its best. The area of ignorance is now the rectangle of size (1×2^{-134}), with the left-bottom corner being at $(q = 0, p = 0.a_{66}a_{65}\ldots a_0 a_{-1}\ldots a_{-67}.)$

What next? Only *now* does chaos rear its head. The situation described in the previous paragraph is really only a consequence of instability, the PUSHING action of the baker. It is true for unstable nonchaotic systems, like a ball rolling down a hill, as well. the unknown bits of q now become the *most significant* bits of p due to FOLDING. Now we have a peculiar situation that we know some of the less significant bits of p, but the most significant ones are being lost, or rather are being taken over by the unknown bits of q. What is the error in p? Remember that the error in q is now the maximum possible, namely 1.

Lets take stock after $n = 68$ steps.

$$(p_{68}|q_{68}) \;=\; [u]a_{-67}\ldots a_{66}u_1 \circ [u], \tag{1.32}$$

where we denote by u_k, one of the 2^k unknown bit strings of length k, u_1 could be 0 or 1. Thus the area of ignorance is now *two* rectangles, each of area 1×2^{-68}, one whose left-bottom corner is at $(q = 0,\ p = 0.0a_{66}\ldots a_{-67})$ and the other at $(q = 0,\ p = 0.1a_{66}\ldots a_{-67})$. After one more time step there are *four* areas of ignorance of size 1×2^{-69} etc. Thus it is clear that the area of ignorance remains a constant, after this *is* an are preserving transformation! However the area of ignorance after a critical

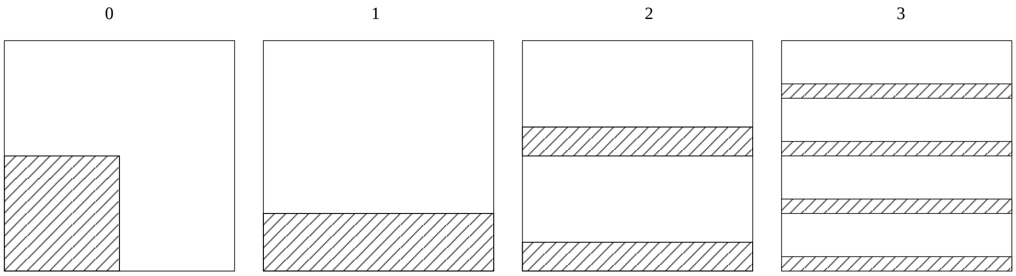

Figure 1.12: Evolution of an area in the baker map

time, which depends on the original area, starts taking on such complex and proliferating branches, typically exponentially large in number, that it loses the typical meaning of "error bars" anymore.

Naturally a picture is in order here. See Fig. (1.12) for an illustration where the initial area of ignorance is pretty large, being one quarter of the square (some really bad equipment here!), this size meaning we don't wait inordinately long for things to happen. The evolution of this area is $[u]0 \circ 0[u] \to [u]00 \circ [u] \to [u]00u_1 \circ [u] \to [u]00u_2 \circ [u]$. The two possibilities for u_1 is reflected as the two horizontal strips at $n = 2$ (the one at the top is $u_1 = 1$, while the one below is $U_1 = 0$); similarly the four possibilities for u_2 results in four strips at $n = 3$.

Thus while the area of ignorance remains constant, its shape changes in such a way that its boundaries are not practical to keep track of any longer. In the case of the baker, the error along the q direction initially increases till it reaches a constant (1), while the error along p decreases till it reaches a constant, such that the total area is always preserved. However these errors are not practical error bars any longer as the region is not a simple one. In fact if we have as a possibility on measurement a scatter of points, we are sure about the result being one of them, then the area of error is zero, but this is quite absurd as a practical source of error measurement.

On the other hand, the baker map is very special in that it singles out q and p axes, in general the error will increase along a direction that itself changes in a complex way along the orbit, this infact being the unstable manifold, and the error will decrease along the stable manifold. We have seen that the geometry of these is so complicated that all practical observables will experience an increase in the error and it is quite right to say that *errors proliferate, typically exponentially, in the case of chaotic systems.*

Sensitivity to Initial Conditions. Closely related to the proliferation of errors is this property that is often taken to be synonymous with chaos. Two initially close points will share a very long common number of bits in both p and q, but the differences will come to the fore, exponentially fast, they will fly farther apart along q, while coming together along p till they separate also on p.

Mixing. The evolution of areas shown above also illustrates the important property of mixing, the shaded region has the same area but tends to get thoroughly mixed in the background. This is of course why the baker was interested in this transformation in the first place. Mixing was properly described mathematically by Hopf, who also invented the baker map. It is characterized by certain numbers that describe how fast it occurs, the so called Ruelle-Pollicot resonances, something we will not expand upon here.

Periodic Orbits Everywhere. From pictures such as we saw for the kicked pendulum and the standard map, we may think that chaos is some formless mess. This is not necessarily the case, in this mess there is a backbone of periodicity, a periodicity that is more prolific than even for regular systems. Consider the fate of points such as

$$(p_0|q_0) = \ldots u_k\, u_k \circ u_k\, u_k \ldots \tag{1.33}$$

where u_k is any binary string of length k. It is then clear from the left shift dynamics that $(p_k|q_k) = (p_0|q_0)$, that is this initial point comes back to itself after k steps. It also immediately follows that after any multiple of k the point recurs, in short we have a *periodic point* of period k. As there are 2^k possible u_k strings for any k, there are exactly 2^k possible periodic points for the baker map of period k. The repeating string is often denoted by an overbar, thus $(p_0|q_0) = \overline{u_k} \circ \overline{u_k}$.
For example the point $\overline{01} \circ \overline{01}$ is a periodic point of period 2, and in usual decimal representation it is $(q_0 = 1/3\,, p_0 = 2/3)$.
Exercise.

1. *Enumerate all periodic points of period* 1, 2, 3 *and* 4, *writing them out in binary and decimal forms. Note how period* 4 *points include period* 2 *points and how all of them include period* 1 *(fixed) points.*

2. *Prove that the decimal representation of* $(p_0|q_0) = \overline{u_k} \circ \overline{u_k}$, *is*

$$q_0 = d(u_k)/(2^k - 1),\; p_0 = Rd(u_k)/(2^k - 1). \tag{1.34}$$

If the string $u_k = a_0 a_1 \ldots a_{k-1}$ *then* $d(u_k) = 2^{k-1} a_0 + 2^{k-2} a_1 + 2^{k-2} a_2 + \ldots + a_{k-1}$ *is the value of the binary string* u_k, *and* $Rd(u_k) = 2^{k-1} a_{k-1} + 2^{k-2} a_{k-2} + \ldots a_0$ *is the value of the string that is obtained by reversing the string* u_k, *with the least significant bit becoming the most significant bit etc. Note that this is different from the bit-reversal operation that interchanges the* 0 *and* 1 *bits. Getting* Rd *from* d *is quite a nontrivial, nonlocal, operation that has in it an element of the complexity of the baker map. In an (apparently) totally unrelated event, this operation is central to the Fast Fourier Transform (FFT) and occurs as the scrambling of the output frequencies.*

The exercise shows how to find the periodic orbits. Where are they? The *periodic orbits are dense*, that is *arbitrarily close to any phase space point there is some periodic orbit.* The proof is also easy from the left shift dynamics. If we take as the random point $(p0|q0) = \ldots a_{-1} \circ a_0 a_1 \ldots$, and we want to find a periodic point within a radius $\epsilon < 2^{-K}$ for some large and positive K, we will consider the periodic point with the repeating string $u_{2K} = a_0 a_1 \ldots a_K a_{-K} a_{-K+1} \ldots a_{-1}$. At $n = 0$ this will be within 2^{-K} distance from the chosen random point, but it will be an periodic orbit of period $2K$. Thus it is clear that periodic orbits are dense.

Exercise.

Show that there is a dense orbit in the baker map. This is an orbit such that it comes arbitrarily close to any other phase space point. In fact dense orbits are dense in phase space. Dense orbits imply and are implied by ergodicity. Roughly speaking ergodicity guarantees that time averages can be calculated by suitable phase space averages, because any typical trajectories explores all the nooks and corners of the phase space, so to speak.

Stable and Unstable Manifolds. Homoclinic and Heteroclinic Points. For any point or orbit in the baker map the stable and unstable manifolds are easily found using the left shift. For instance for the fixed point at the origin any point whose position (in binary) ends in an infinite string of zeros is in the stable manifold. In general for a periodic orbit of period k characterized by the string u_k the following is easily seen:

1. Stable Manifold: $something \circ somethingelse\,\overline{u_k}$.
2. Unstable Manifold: $\overline{u_k}\,something \circ somethingelse$.
3. Homoclinic points: $\overline{u_k}\,something \circ somethingelse\,\overline{u_k}$.
4. Heteroclinic points: $\overline{u'_l}\,something \circ somethingelse\,\overline{u_k}$.

Here the heteroclinic points approach the periodic orbit characterized by u_k in the infinite future, but came from a different periodic orbit characterized by a different string u'_l, which could also have a different period $l \neq k$. *something* and *somethingelse* are arbitrary strings of 0 and 1. For example $\overline{01} \circ 10\overline{01}$ is a point that is homoclinic to the period 2 point $(2/3|1/3) = \overline{01} \circ \overline{01}$, while $\overline{101} \circ 00101\overline{10}$ is an heteroclinic *connection* between the period 2 orbit $\overline{10} \circ \overline{10} = (1/3|2/3)$, to which it comes arbitrarily close in the future and the period 3 orbit $\overline{101} \circ \overline{101} = (5/7|5/7)$, from which it deviated arbitrarily closely the sufficiently distant past.

Therefore if both p and q coordinates were rational numbers, then the orbit is either itself a periodic orbit, or is homoclinic to a periodic orbit, or is an heteroclinic connection between two periodic orbits. All other phase space points densely fill the phase space. We also know that irrational numbers are of measure one in the real number line. This means that if we were to select at random a real number it is, with probability 1, an irrational number. Thus although *periodic orbits are dense in the phase space, they are of measure zero.* While these statements are very easy to see for the baker map, they are also believed to be widely applicable for any Hamiltonian system. Rigorous proof of these, even for particular systems is very difficult.

Prime Periodic Orbits. Counting. If $p(n)$ denotes the total number of periodic points of period n, for the baker map we found that

$$p(n) \;=\; 2^n \;=\; e^{\ln(2)\,n}. \tag{1.35}$$

There are an exponentially large number of periodic points, for example there are about a million periodic points of period 20, all jostling for space on the unit square. The rate of growth of the number of periodic points with period which is $\ln(2)$ for the baker map is an important dynamical indicator, and in general this quantity is called the *topological entropy.*

Each such periodic point lies on a *periodic orbit* of period n. Thus we may say that there are $p(n)/n$ periodic orbits. We see that this is not exactly true as the periodic point may also lie on orbits whose periods are *divisors* of n. For instance all the fixed points are of period n for any n. All period 2 orbits are orbits of even periods etc. So we may ask how many genuine periodic orbits of period n are there? By genuine we mean those that don't have a lesser period that is a factor of n. Such orbits are called *primitive* periodic orbits. Points on the primitive orbits are primitive periodic points. Let $P(n)$ denote the number of primitive periodic points of period n, will this also increase exponentially with the period? This is a more harder and interesting question, whose answer is yes. To evaluate $P(n)$ we encounter an interesting function of number theory that seems as chaotic as the baker map, the Möbius function. A little thought shows that:

$$\sum_{k|n} P(k) \;=\; 2^n, \tag{1.36}$$

where the notation $k|n$ is for those k that divide n including 1 and n. The inversion of such formulae for arithmetic functions ($P(n)$ is an arithmetic function, it maps integers to integers) is achieved by the Möbius inversion formula.

Möbius Inversion Formula. If

$$\sum_{k|n} f(k) \;=\; g(n), \text{ then} f(n) \;=\; \sum_{k|n} \mu(k)\, g(n/k). \tag{1.37}$$

Here $\mu(k)$ is the Möbius function defined as:

$$\mu(n) = \begin{cases} 0 \;\text{ if } n \text{ has one or more repeated prime factors.} \\ 1 \;\text{ if } n = 1 \\ (-1)^k \;\text{ if } n \text{ is the product of } k \text{ distinct prime factors.} \end{cases} \tag{1.38}$$

A proof the inversion formula is found in many standard books on number theory.

Using the Möbius inversion formula we can write

$$P(n) \;=\; \sum_{k|n} \mu(n/k)\, 2^k. \tag{1.39}$$

While this cannot be summed up to any simpler form, it provides an efficient way of calculating $P(n)$. It is found that $P(n) \sim 2^n$ also, so that the number of periodic orbits $\sim 2^n/n$. This generalizes to the important rule:

$$\#\text{ of Periodic Orbits of Period } T \sim \frac{e^{h\,T}}{T}. \tag{1.40}$$

The constant h is the topological entropy.

Exercise. *Find $P(1), \ldots, P(10)$. Write a computer program to find $P(n)$ and plot $\ln(P(n))$ vs n, verify that it is a straight line with a slope that approaches $\ln(2)$ for large n. The author found the "Mathematica" software ideal to do such calculations, as this package has in-built in it arithmetical functions such as the Möbius.*

In Fig. (1.13) we see all the periodic orbits of periods 5, 10 and 15, there are 32, 1024 and 32768 points in each respectively. It is also clear that the periodic orbits are *isolated*, they do not form continuous families. This distinguishes chaotic systems from most regular ones. The stability of periodic orbits is of course of central importance. In the baker map all the isolated periodic orbits are *unstable*. If the baker map were not exactly solvable in terms of an explicit left shift, we would not have a ghost of a chance finding "long" periodic orbits even of length as small as 15. Numerical errors of deviation from the periodic orbit will take us far afield.

The arrangement of periodic orbits in the phase space is important, and for area preserving maps and for PSOS of $d = 2$ Hamiltonian systems it is believed that they are uniformly spread over the phase space. The periodic orbits of the baker map hold out intriguing patterns, as yet unexplored, of course to the best of the authors' knowledge.

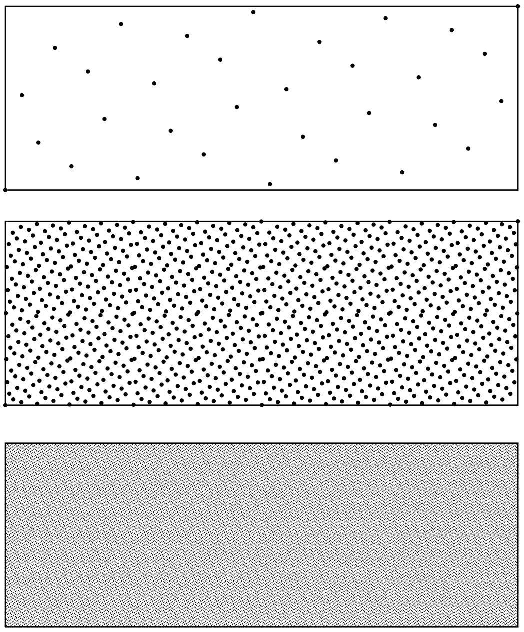

Figure 1.13: All periodic points of the baker map of periods 5, 10 and 15 from top to bottom. The plots are all on unit (q, p) squares.

Exercise.

1. *Prove that all the periodic orbits of the baker map are uniformly unstable with a Lyapunov exponent of* $\ln(2)$.
2. *Devise an algorithm to find all the periodic orbits of a given period in the baker map.*
3. *Devise an algorithm for only primitive periodic orbits.*

Exercise. The 3D baker map.

While the baker map discussed above is very illuminating from the point of view of 2 DoF Hamiltonian system, it unfortunately must leave a real baker bewildered, no piece of dough, however flat is in flatland. For the baker map not to get pie on its face in the pastry industry, we propose that you study the 3D version. Indeed what we will do is to take the "TURN" exhortation of the baker, from the quotation at the beginning of the baker discussion, to heart. Thus devise a model from a cube into itself, that incorporates the "PUSH", "FOLD" and "TURN" instructions and analyze it for chaos. You may take the FOLD step to be as in the 2D baker, to be a "cut and translate" step.

As can be seen from above the baker map has many features of chaotic systems in a completely transparent manner and helps us understand features of what is called "hard chaos". In particular the dense set of unstable periodic orbits plays a very important role in both classical as well as semiclassical mechanics. The fact that they exponentially proliferate $P(T) \sim \exp(hT)/T$ and are uniformly spread in phase space are also of crucial import.

While there are more aspects of this map that can be usefully studied, we turn to another system which is better suited for our purposes now, the so called " cat map". We wish to turn attention away from individual orbits to collections of orbits, or densities. The relevant classical mechanics equation will then be the Liouville equation rather than Hamiltonian equations. These two formulations, while mathematically distinct, are of equal importance, and are complementary descriptions of the same dynamical system.

Statistical mechanics deals with collections of orbits, or ensembles, and during the early days of statistical physics, ergodicity was discussed extensively. During the momentous developments of the last century, these questions were relegated to relatively dark corners, as important models of equilibrium statistical physics, such as the Ising model, took the centerstage. There is now renewed interest in the foundations of nonequilibrium statistical physics and its relationship, if any, with dynamical chaos. For instance one issue that comes up with regularity is whether chaos can explain the lack of time-reversibility in the macroscopic world, despite the fundamental equations of motion possessing this property.

1.6.1 The cat map

The cat map was introduced by Arnold and Avez (1967) in their study of ergodicity in classical mechanics. It is also a 2D area preserving map defined on the unit square or torus. Unlike the baker map it is a smooth system, no discontinuity exists. It is linear, the nontriviality of the map arises solely from the re-injection of trajectories thanks to the periodic boundary conditions. It is given by the map:

$$\begin{aligned} q_{n+1} &= a\, q_n + b\, p_n \,(\mathrm{mod}\ 1) \\ p_{n+1} &= c\, q_n + d\, p_n (\mathrm{mod}\ 1) \end{aligned} \tag{1.41}$$

There are four parameters (a, b, c, d) and the map will be continuous if these are integers, in fact they are smooth dynamical systems in this case. We also assume that $ad - bc = 1$, which makes them area preserving and if $|tr| = |a + d| > 2$ then the map is also hyperbolic and completely chaotic. The map with ($a = 2$, $b = c = d = 1$) is usually referred to as the cat map, or the Arnold cat map, but we will call this generalization as the family of cat maps. The two eigenvalues of the matrix $\{(a, b), (c, d)\}$, $\lambda_\pm = (tr \pm \sqrt{tr^2 - 4})/2$ provide the expansion and contraction rates, and the positive Lyapunov exponent is $\ln(\lambda_+)$.

The cat map is so called, because its inventors illustrated its action on a set of points by displaying what happens to its image as the map is iterated. However since the cat should hardly be credited for the development of chaos in this world, we illustrate it with another picture instead. See Fig. (1.14).

Consider what happens to a collection of initial conditions described by the density function $\rho(q, p; 0)$. This means that $\rho(q, p; 0)\, dq\, dp$ is the fraction of initial conditions in the area $dq\, dp$ around (q, p) at time 0. After a time n the initial condition is at say (q_n, p_n) and the area is now $dq_n\, dp_n = dq\, dp$, due to area preservation. Thus we have that

$$\rho(q_n, p_n; n) = \rho(q, p; 0). \tag{1.42}$$

Symbolically if we write $(q_n, p_n) = f^n(q, p)$ as the time evolution we get

$$\rho(q, p; n) = \rho(f^{-n}(q, p); 0), \tag{1.43}$$

the Liouville condition of phase space incompressibility expressed in discrete language. Thus for evolving densities forward in time we need to evolve phase space points backward in time.

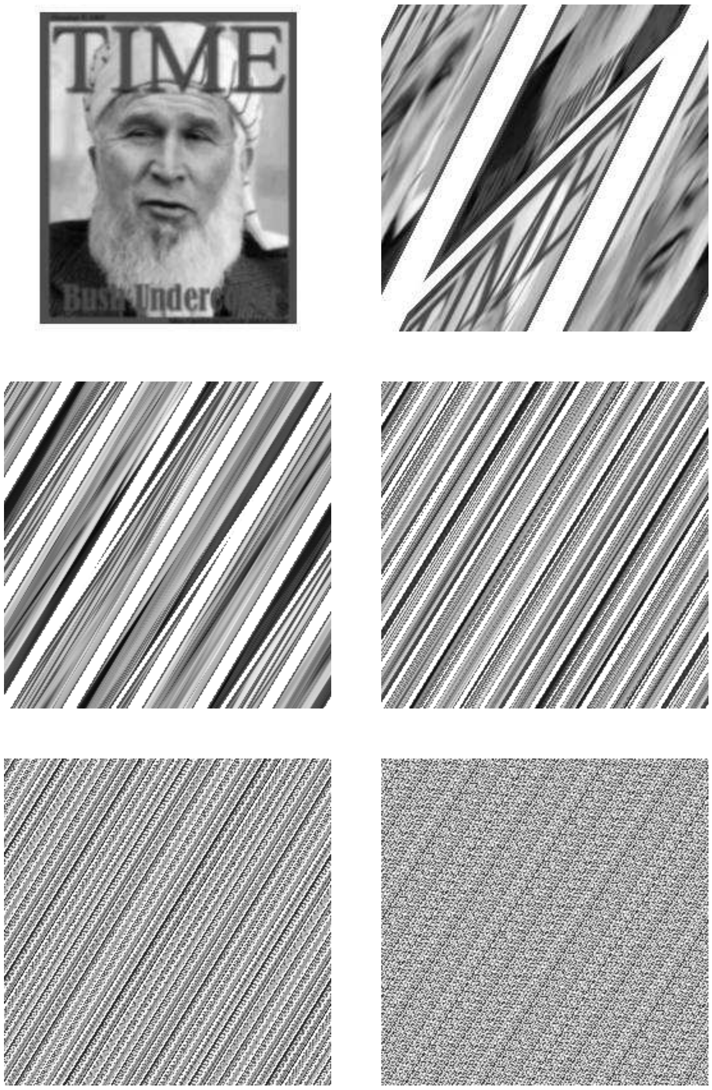

Figure 1.14: Dubya subject to the Arnold cat map for five iterations. Notice the unstable manifolds along which the pixels align, and how degeneration occurs with time. It is a peculiarity of the cat map though that there occurs a time when the initial image will exactly reappear, history will repeat endlessly. The first image appears smaller due to a white boundary, there is no loss of information in this process, the picture is merely scrambled. The original picture is taken without permission from http://politicalhumor.about.com/, where I highly recommend a visit to understand modern chaos in practice.

From the Liouville equation it is clear that if the initial density was uniform then it would remain uniform. That is the *uniform density is an invariant density or measure for all area preserving maps.* However if the map was not chaotic there exist other smooth invariant densities, and in general any initial density (that is not uniform) does not march on toward the uniform density as time goes by. Put in more technical language, in the space of densities, the uniform one is not an attractor, and there is general no attractor. However for chaotic systems it is almost as good as an attractor, and we illustrate this, not only by making use of Dubya but also by the following analysis.

The Dubya picture shows how complicated the outcome of the Liouville equation could be if the underlying dynamics f is chaotic. It appears from the picture that Dubya is uniformly spread all over the phase space. It is as if a "macroscopic" equilibrium has been reached after an initial scrambling. It is widely believed that this is the way in which thermodynamic equilibrium is reached, due to the mixing behaviour of the underlying dynamics. The evolution of densities such as Dubya's is in general difficult to track, as indeed it is tantamount to solving the equations of motion. However for the cat map this is possible, despite the presence of hard chaos. Since any density on the torus is doubly periodic we can write:

$$\rho(q,p;0) = \sum_{kl} a_{k_1 k_2}(0)\, \exp\left(2\pi i k^T v\right), \tag{1.44}$$

where we have introduced the integer vector $k \equiv (k_1, k_2)^T$ and phase space $v \equiv (q,p)^T$. Here T in the superscript stands for the transpose. We note that from normalization of the density $a_{00}(0) = 1$. For a typical smooth function ρ the Fourier coefficients $a_{k_1k_2}(0)$ will decrease with wavenumbers sufficiently fast for the series to converge.

The solution of the cat map is: $v_n = M^n\, v \,(\mathrm{mod}\ 1)$, where M is the 2×2 matrix $\{(a,b),(c,d)\}$. Note that this is only possible because M is an *integer* matrix, otherwise the act of taking powers of M do not commute with the modulo operation: the fact that the cat is a "diffeomorphism" is important here. Thus we have from Liouville equation Eq. (1.43) that:

$$\rho(q,p;n) = \sum_{kl} a_{k_1k_2}(0)\, \exp\left(2\pi i k^T\, M^{-n} v\right) \;=\; \sum_{kl} a_{k_1k_2}(n)\, \exp\left(2\pi i k^T\, v\right), \tag{1.45}$$

where $a_{k_1k_2}(n) = a_{M^n k}(0)$. From the fact that M has real eigenvalues, one larger than 1, implies that $||M^n k||$ increases with time n for chaotic maps, for all k except $(0,0)$. (We have assumed for simplicity that M is symmetric, this is not of course essential). That is $a_{00}(n) = a_{00}$ for all n.

What we have done is transfer the cat map dynamics to a map on the "dual" Fourier space wavenumber lattice, on which the dynamics is a simple linear hyperbolic map. Note in particular that there is no "modulo 1" in this map. Therefore the small wavenumber coefficients get rapidly destroyed, as some higher wavenumber ones get "excited". In fact all this occurs exponentially rapidly. Thus the smooth density with predominantly small wavenumbers tends to be a highly oscillatory one, except for $a_{00} = 1$ for all time. Thus it is *not strictly true that the density will tend to the uniform density* ($\rho = 1$), however, it does so in a *weak* sense. that is

$$\int_\Omega f(q,p)\, \rho(q,p;n)\, dq\, dp \longrightarrow \int_\Omega f(q,p)\, dq\, dp. \tag{1.46}$$

as $n \to \infty$, for sufficiently smooth functions of phase space $f(q,p)$.

Thus the approach to equilibrium in Hamiltonian systems proceed in somewhat subtle ways, the complex network that Poincaré talked about, the homoclinic tangle leaves its imprint on the evolving density by means of high wavenumber features that would get observationally blurred, leaving behind an appearance of a smooth uniform, "microcanonical" ensemble.

1.6.2 Afterword

These last few pages, there has been a short overview of Hamiltonian dynamics in relation to chaos. Note that we have not really gone beyond 2 DoF or 2D area preserving maps. There is much more to be said, and much more to be found! 4D symplectic maps that are of relevance to 3 DoF Hamiltonian systems are only now being explored. “Arnold diffusion” is a process that is found to occur in these systems that is absent in lower dimensions.

Chapter 2

Hamiltonian Chaos: Quantum Mechanics

2.1 Introduction

The founders of quantum mechanics were adepts at the classical. In many cases classical intuition guided them along, till they reluctantly were forced to give in to notions that were genuinely alien then. For instance Schrödinger was guided by the analogy between wave optics and geometric (ray) optics, and made use of the Hamilton Jacobi theory heavily. It was with great reluctance that he introduced the imaginary unit $\sqrt{-1} = i$ fundamentally into physics. When he first wrote the equation $H\psi = E\psi$ and passed this on to Lorentz, Lorentz said it couldn't be quite right as an equation with H, that is energy must have somewhere time in it. See our very first Hamiltonian equations of motion, the Hamiltonian was crucially involved in finding time derivatives. After Schrödinger went back to the drawing board, he apparently came up with $H\psi = i\hbar\,\partial\psi/\partial t$, and was very unhappy with it, as it involved i. After one year he resolved this by applying H *twice* to get the real equation $H^2\psi = -\hbar^2\partial^2\psi/\partial t^2$. Only to realize that this cannot be right in general as the Hamiltonian can after all contain time explicitly, such as in the 1.5 DoF Hamiltonians we have been discussing. Thus it seemed that with reluctance he accepted the now famous Schrödinger equation which is our starting point.

The quantization of chaotic systems must need no motivation, considering the centrality of Hamiltonians in physics, considering the fundamental nature of quantum mechanics, and the alleged ubiquitousness of chaos, even in Hamiltonian systems. For instance going beyond the simplest atom, the hydrogen atom, to the Helium atom at once forces us to consider a problem in quantum chaos, as the two electrons in the field of the protons in the nucleus, is equivalent to a restricted three-body problem that is known to be chaotic. Even in the simplest of atoms, the H atom, if a sufficiently strong magnetic field was applied the electronic motion when treated classically is chaotic. If time dependent fields are applied almost anything (except the harmonic oscillator) is chaotic. All of these situations have also been realized experimentally.

More recently, the effects of quantum chaos on transport has been studied through measurements of magneto-resistance in quantum dots. These are simple generalizations of the 1D wells that we study in a first quantum mechanics course, only now they are 2D and can have different shapes. The motion of the electrons inside these is like the motion of a ball on billiard tables, and this class of billiard problems have been at the center of many classical as well as quantum studies. Experimental work on such systems has been on for more than a decade now. Recent explorations of the possibility of a quantum computer, has also brought to the forefront issues of the effect of chaos on the functioning of many-body quantum computers. In particular the “entangling” power of quantum chaos is a current research topic. Entanglement which measure how nonseparable quantum systems are in a genuinely quantum way, is influenced by chaos in an apparently very nontrivial manner. Apart from all these “systems”, the fundamental nature of quantized chaotic systems could lie at the foundations of quantum statistical mechanics. There is also a suggestion that decoherence, which is the entanglement of a system with its environment, is strongly influenced by chaos in the system and/or environment.

The area of quantum chaos (we will call it that for simplicity, a certain school lead by Sir Michael Berry calls it “quantum chaology”) is dominated roughly by the following approaches:

1. **Phenomenology**: Numerical experiments abound and are central to our understanding, much like the classical case. This provides the basis of many theories and modelling efforts.

2. **Semiclassics**: The semiclassical theory of anything beyond 1D (no chaos!), involves nontrivial extensions of the WKB method. Gutzwiller’s periodic orbit theory developed in the late 60’s, early 70’s and refined over the years forms an important tool in understanding quantum chaos. Another semiclassical tool that has found practical applications and helped intuitive understanding is the technique of semiclassical wavepacket propagation.

3. **Statistical Modelling**: Chaos implies ergodicity, mixing, and an invariant measure classically. Thereby we can calculate averages knowing the invariant density. Quantum mechanically it has been found for about twenty years now that the methods originally devised for “complex” many body nuclei were applicable to low-dimensional chaotic systems. These methods fall under the class of problems which consider the Hamiltonian to be specific random matrices that obey the broad symmetries of the Hamiltonian of the system, such as parity, time-reversal symmetry etc. Thus modelling using random matrix theory (RMT) has been found to be of great importance and use in quantum chaos. RMT was developed initially by Wigner, Dyson and Mehta.

4. **Experiments**: Experiments from many fields (atomic, nuclear, mesoscopic, quantum optics) deal with quantum chaos, due to the basic character of the investigations, after all we are only talking of the Schrödinger equation. While the earliest experiments involved multiphoton ionization of hydrogen atoms in Rydberg states subjected to microwave radiation, recent controlled experiments range from quantum dots to laser cooled sodium atoms in pulsed fields, and resonant tunneling across quantum wells in magnetic fields. There are another class of experiments that are truly “electromagnetic” than quantum, in the sense that they simulate the Schrödinger equation with 2D microwave cavities (in which case the Helmoltz equation for the electric field becomes identical to the Schrödinger equation for the wavefunction of a particle freely moving inside a billiard whose shape is that of the 2D cavity.)

We may also classify the “objects” or “systems” of quantum chaos, that have been studied over the years. These are the central systems and are not exhaustive. The field of quantum chaos started with the independent and simultaneous publication of two papers, one on the quantized standard map by a combination of American (Joseph Ford), Italian (G. Casati) and Russian (B. Chirikov, F. M. Izrailev) efforts, while the other was on general planar 2D maps by a combination of American (N. L. Balazs), French (A. Voros) and British (M. V. Berry and M. Tabor) efforts, in 1979. Thus in fact the earliest quantized chaotic systems where quantizations of 1.5 DoF systems, and area preserving abstract maps that we have looked at classically in the previous chapter. Thus we begin the classification with these.

1. **Quantum Maps**: These come in two flavours: (a) quantizations of 1.5 DoF systems, mostly of the "kicked" variety that we saw lead to explicit stroboscopic maps; (b) quantization of abstract dynamical systems, such as the baker map, and the cat map. Although in some cases (like the cat map) there have been mappings on to kicked systems. Almost all studies so far on this have been restricted to 2D area preserving mappings.

   Experimentally these have been studied using pulsed fields that provide a very good approximations to delta function impulses. One important phenomenon studied here is the dynamical localization of wavepackets. Experimental realizations of the baker map have been proposed using simple quantum gates.

2. **Billiards**: Billiards are variously shaped cavities inside which particles travel freely and suffer specular reflections at the boundary. Mainly, 2D billiards have been studied. Apart from the circular, elliptical and rectangular 2D cavities, which are integrable, others studied are either chaotic or what is called "psuedo integrable". This is an intriguing set of models with application to quantum dots, where experiments using various shaped billiards have revealed that the presenc or absence of chaos has effects on conductance in ballistic dots.

3. **Nonlinear Oscillators**: Nonlinear oscillators, again mostly two oscillators have been studied. The phenomena of localization has been found here as well. These are of great importance in the study of atoms in strong external fields. In suitable coordinates these problems can be reduced to chaotic nonlinear oscillators.

4. **The Riemann Zeta function**: This rather odd addition to the "systems" is the tantalizing connections between number theory, analysis and chaos. The celebrated, largely unresolved, Riemann hypothesis conjectures that the (nontrivial) zeros of the zeta function lie on the $Re(z) = 1/2$ line. The zeta function obeys certain functional equations that look (almost) like the Gutzwiller semiclassical formulas, and the zeros, when treated as energy eigenvalues, are distributed according to a signature RMT distribution that is obeyed by time-reversal violating system. The millions of zeros of the zeta function have been used for statistical analysis, as if they are from a quantized chaotic system. Also the extensive theory of the zeta function has been used to gain insights into the semiclassics of quantum chaos.

   A spirited hunt was on to find the Hamitonian whose eigenvalues are the nontrivial (imaginary parts of) zeros of the zeta function, with the clues that its classical limit is chaotic and that it was not time reversal invariant, that its periodic orbits had periods that were the prime numbers and actions that were the log of the primes! The hunt is still on, although there are some developments on certain other parallel lines.

5. **Scattering systems**: We mention these separately, as we have not really talked about scattering, but chaotic scattering is quite common and has been studied mostly with the help of billiards. Experiments have been done using 2D microwave cavities.

6. **Spin Chains**: These are not really well studied models. But potentially interesting problems for the future include many body systems, such as spin chains studied in condensed matter physics. The Hubbard model, the Ising model in transverse field etc. are largely unexplored areas where quantum chaos could be found.

7. **Quantum Chromodynamics**: There has been some work that indicates that fundamental theories such as QCD would have connections to quantum chaos. As may be imagined, since we

have not really gone much beyond 2DoF, a field theory is quite far. However again evidence from RMT statistics implies that chaos is present in QCD. This should not really come as a surprise, the very first application and motivation for RMT came from excited states of heavy nuclei.

We will concentrate on quantum maps in the following, due to their simplicity and usefulness.

2.2 Quantum Maps: Generalities

Quantum maps are quantizations of classical maps. Classical 2D area preserving maps are *symplectic* or what is more commonly called *canonical* transformations. Thus quantum maps may be thought of as the quantum equivalents of canonical transformations. The task is, given a canonical quantization, to find its quantum equivalent. The quantum equivalent is an unitary operator, and it is not immediately clear whether this is possible. For the class of maps derived from kicked Hamiltonians we can derive the quantum map quite easily as will be shown below.

We will first deal with the broad class of canonical transformations (maps) that comes from kicked systems. Consider the Hamiltonian:

$$H \;=\; H_0 \;+\; V \sum_{n=-\infty}^{\infty} \delta(t/T - n). \tag{2.1}$$

H_0 and V are time independent operators. There is no need to assume anything about the number of DoF. The Schrödinger equation we want to solve is

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle \;=\; H_0|\psi\rangle \;+\; V\delta_T(t)|\psi\rangle; \tag{2.2}$$

given an initial state $|\psi(0)\rangle$, we wish to solve for $|\psi(t)\rangle$. Recall that $\delta_T(t)$ is an abbreviation for the train of delta impulses. Recall that the classical map related phase space variables just after consecutive kicks. Therefore we may consider the quantum map to be that operator, say U, that connects states just after consecutive kicks. Due to the periodicity of the perturbation, this is independent of the kick number itself, and from elementary quantum mechanics this is an unitary operator. Thus if we write the state just after kick n as $|\psi(n^+)\rangle$ we are seeking that U such that

$$U\,|\psi(n^+)\rangle \;=\; |\psi(n+1^+)\rangle. \tag{2.3}$$

From just after kick n to just before kick $n+1$, the delta function term is effectively absent in Eq. (2.2). Thus we have:

$$|\psi(n+1^-)\rangle \;=\; \exp(-iH_0T/\hbar)\,|\psi(n^+)\rangle. \tag{2.4}$$

Now we have to deal with integration over a kick, during which time the wavefunction changes abruptly. Integrating the schrödinger equation over the infinitesimal time about the kick, eliminates the H_0 part of the Hamiltonian, or alternatively we could say that the kick dominates the Hamiltonian during this time. Therefore consider the general equation:

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle \;=\; V\,g(t)|\psi\rangle, \tag{2.5}$$

where $g(t)$ is any function of time t. It is easy to verify that it is solved by

$$|\psi(t')\rangle \;=\; \exp\left(-\frac{iV}{\hbar}\int_t^{t'} g(t)\,dt\right)|\psi(t)\rangle, \tag{2.6}$$

this effectively being a (dynamic) rescaling of time. In our case $g(t) = \delta_T(t)$ and we get using $t' = n+1^+$, $t = n+1^-$,

$$|\psi(n+1^+)\rangle = \exp(-iVT/\hbar)\,|\psi(n+1^-)\rangle. \tag{2.7}$$

Combining this with Eq. (2.4) we get:

$$|\psi(n+1)\rangle = \exp(-iVT/\hbar)\,\exp(-iH_0T/\hbar)\,|\psi(n)\rangle, \tag{2.8}$$

where we have dropped all the + superscripts, all the states are now understood to be immediately after the stated times. Thus we have the quantum map to be the unitary operator:

$$U = \exp(-iVT/\hbar)\,\exp(-iH_0T/\hbar) \tag{2.9}$$

2.2.1 Comments

The form of the unitary operator, or quantum map, is as a product of two unitary operators, the first one is the "free" evolution corresponding to the Hamiltonian H_0, while the other is the kick. If $[H_0, V] = 0$, that is these two operators commute then the evolution operator is simply $\exp(-i(H_0+V)T/\hbar)$, equivalent to a continuous flow. The most interesting, and general case is when this does not happen. If the system has 1DoF (so that the whole Hamiltonian has 1.5 DoF), then this can mean the difference between order and chaos. Without the kicks the 1D Hamiltonian is simply H_0+V, there is no classical chaos, the unitary operator over a time T is also $\exp(-i(H_0+V)T/\hbar)$. Thus for 1D quantum systems the difference between e^{A+B} and $e^A\,e^B$ could spell the difference between order and chaos.

It must be noted that but for the impulsive time dependence we would be hard put to write explicitly the quantum map. For general time dependences, fully numerical integration has to be resorted to to write the corresponding quantum map or the Floquet operator. Since the Hamiltonian is time dependent the usual description of stationary states and energy eigenvalues does not exist. However the quantum map, is stationary in the sense that it does not depend on the kick number, and is a special case of the Floquet operator for general time dependence.

Iterating the classical map is equivalently done in quantum maps as repeated multiplication by the operator U, thus:

$$|\psi(n)\rangle = U^n\,|\psi(0)\rangle. \tag{2.10}$$

The powers of an operator is essentially determined by its eigenvalues and vectors and hence the problem of time evolution is here also solved by an eigenvalue problem. The eigenangles of U take the role of the energies and the eigenvectors of U are the "stationary" states. Since U is an unitary operator its eigenvalues lie on the unit circle, the eigenvalue equation may be written as:

$$U|\phi_k\rangle = \exp(i\phi_k)|\phi_k\rangle. \tag{2.11}$$

where $0 \le \phi_k < 2\pi$ are real numbers, the eigenangles, and also referred to as the "quasi-energies". The index k may be discrete, or continuous, as the eigenangles are discrete or continuous. In fact the nature of the spectrum of operators such as U even for 1D systems is notoriously difficult to predict, it may also be of a singular continuous kind, where the spectrum is a Cantor set, a fractal. These different kinds of spectra impact crucially properties of quantum transport.

Note that

$$|\psi(n)\rangle = U^n\,|\psi(0)\rangle = \sum_k \exp(i\phi_k\,n)|\phi_k\rangle\langle\phi_k|\psi(0)\rangle. \tag{2.12}$$

From the reality of the eigenangles it follows that quantum evolution is quasi-periodic, especially if the spectrum is discrete. If the spectrum is continuous this need not be the case.

We now quantize the maps that were displayed in the classical section 1.3.1.

2.3 Quantum maps on the plane and cylinder

Quantum Linear Map. The quantum map corresponding to the classical map in Eq. (1.14) is

$$U = \exp\left(-\frac{iT}{\hbar}\omega^2 q^2\right) \exp\left(-\frac{iT}{2\hbar}p^2\right), \tag{2.13}$$

where of course p and q are operators satisfying the Heisenberg commutation relation: $[q,p] = i\hbar$. The quantum linear map is completely solvable, just like the classical linear map. This can be seen from the fact that an application of the Campbell-Baker-Hausdorff (CBH) theorem will reduce the product of the two exponentials to a single exponential with an effective quadratic Hamiltonian. Therefore for cases where the classical map is filled with elliptic orbits, the quantum spectrum is identical to the Harmonic oscillators, the eigenangles are equispaced.

Quantum Standard Map. The quantum map corresponding to the classical map in Eq. (1.15) is

$$U = \exp\left(\frac{igT}{(2\pi)^2\hbar}\cos(2\pi q)\right) \exp\left(-\frac{iT}{2\hbar}p^2\right). \tag{2.14}$$

While the classical map was shown to depend on only one (scaled) parameter, $K = T\,g$, in the case of the quantum map we see that there are *two* effective parameters: $gT/\hbar$ and $T/\hbar$. Thus $\hbar$ enters in a crucial manner, and a scaled Planck constant determines many behaviours of the standard map. We will return to the standard map shortly, but note that we have not taken into account any modulo operation so far. As it exists the above would be the quantization of the standard map on the entire plane. The nature of the spectrum of the above operator (whether discrete, continuous, singular) has been the topic of much research and the there has been a mapping of this map to an tight-binding model of condensed matter physics. It has been at the center of many quantum chaos studies including atom-optics experiments.

Quantum Harper Map. It immediately follows from the above that a quantization of the Harper map without the modulo conditions is

$$U = \exp\left(-\frac{igT}{(2\pi\hbar}\cos(2\pi q)\right) \exp\left(-\frac{iT}{2\pi\hbar}\cos(2\pi p)\right). \tag{2.15}$$

2.3.1 Standard map on the cylinder

While both the standard and Harper maps were easy to study classically, at least in terms of their phase space trajectories, the quantum maps pose severe problems, they are infinite dimensional and there is no guarantee that the spectrum is discrete. The classical maps lived on cylinders and tori and thereby simplified matters considerably. For instance the kicked pendulum configuration space is the circle S^1 and not the line. Therefore we could quantize these maps on cylinders and tori. Cylindrical phase spaces we are more familiar with. There is an angle $0 \leq q < 1$, and an angular momentum $-\infty < p < \infty$ pair, If $|q\rangle$ are angle kets, the angular momentum kets are $|m\rangle$ such that $p|m\rangle = mh$

$$|m\rangle = \int_0^{2\pi} e^{2\pi imq}|q\rangle\, dq;\; m = 0, \pm 1, \pm 2 \ldots, \tag{2.16}$$

the transformation function between momentum and angle is:

$$< q|m\rangle = e^{2\pi imq}. \tag{2.17}$$

Thus the standard map on the cylinder is given the infinite dimensional matrix

$$U_{mm'} = \langle m| \exp\left(\frac{igT}{(2\pi)^2\hbar}\cos(2\pi q)\right) \exp\left(-\frac{iT}{2\hbar}p^2\right)|m'\rangle. \tag{2.18}$$

Inserting complete $|q\rangle$ states, we get

$$e^{-i2\pi^2 Tm'^2\hbar)}\frac{1}{2\pi}\int_0^{2\pi} e^{igT\cos(\theta)/(4\pi^2\hbar)}e^{i\theta(m'-m)}\, d\theta. \tag{2.19}$$

We have made the substitution $2\pi q = \theta$ and used the eigenvalues of the momentum operator $(2\pi m\hbar)$. Using the standard definition of the Bessel (J) function:

$$J_n(z) = \frac{1}{2\pi}\int_0^{2\pi} \exp\left(-i(n\theta - z\sin(\theta))\right)\, d\theta,$$

and the standard property of integer order Bessel functions: $J_{-n}(z) = (-1)^n J_n(z)$ we get:

$$U_{mm'} = (-i)^{m'-m}J_{m'-m}(gT/4\pi^2\hbar)\exp\left(-i2\pi^2Tm^2\hbar\right), \tag{2.20}$$

$$= (-i)^{m'-m}J_{m'-m}(K/\tau\hbar)\exp\left(-i\tau m^2\hbar/2\right). \tag{2.21}$$

Here we have reintroduced the *classical* effective parameter $K = gT^2$ (see the classical map), and introduced $\tau = 4\pi^2T$ to show that there is effectively one more parameter.

Note that we have already chosen our units so that the moment of inertia, I, of the rotator is unity, and the units of $\hbar$ are of I/τ, which may be considered a characteristic action in the system. Therefore one may define an effective scaled dimensionless Planck constant as $\hbar\tau/I = \hbar\tau$, as $I = 1$, which measures roughly "how many classical actions are there in an $\hbar$". Thus the classical limit is the limit $\hbar\tau \to 0$. Since always the scaled Planck constant appears in the combination $\hbar\tau$, we may set $\tau = 1$ and loosely talk of $\hbar \to 0$. Often one is bewildered how fundamental constants are blithely treated as variables and limits are taken, it is always implied in these cases that some scaled constant is involved. This can always be done as long as the fundamental constant is *not dimensionless.*

This matrix U is the quantum standard map on the cylinder. All the complications of the classical standard map, from the KAM theorem, the Poincaré Birkhoff theorem, to the homoclinic tangle and hard chaos, all illustrated in Fig. (1.5), must appear as $\hbar \to 0$ from this matrix, and must be in some quantized avatar otherwise. One of the first, and enduring, questions, of quantum chaos, was exactly how this happens. As M. V. Berry points out, there are two questions that are often conflated here: (a) How does the classical limit emerge from the quantum. The answer, if complicated, is already known in the sense that the classical limit is known. (b) Do any new phenomena occur in the semiclassical regime, something that is not classical, that perhaps survives from the quantum regime? Can this even

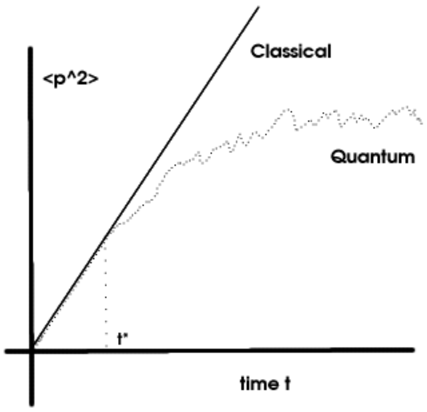

Figure 2.1: A doodle of the quantum and classical diffusion of the energy of the rotator.

survive the classical limit? As Berry again points out, this question would be nonsensical as long as the limit were not *singular*. The classical-quantum limit is completely different from say the relativistic-nonrelativistic limit in the sense that we cannot set $\hbar = 0$ and get the classical limit (as we may set $c = \infty$ and get the nonrelativistic limit).

The structure of the unitary operator U is that of a *banded matrix*. This follows from $|U_{mm'}| = |J_{m-m'}(K/\tau\hbar)|$. From properties of the Bessel function we know that $J_n(z)$ decays exponentially for $n > z$, thus the effective (half) band width of U is $K/\tau\hbar$. We see from this that in the classical limit the matrix tends to become full, so also in the large classical chaos limit when K is large. A full matrix has much more complicated spectra, at least potentially, than a banded one.

One of the first questions asked of the quantum standard map, is whether it allows unlimited diffusion of the momentum of the pendulum. We know (see also “problem” in classical standard map section) that classically $< p^2(t) >= D\,t$, the kinetic energy, ensemble averaged over an initial conditions ensemble, increases linearly. Quantum mechanically an initial ensemble is already provided by a state, say take $|m = 0\rangle$ state, which is one of angular momentum zero. It is uniformly spread in the q space, and therefore we can think of this as the quantum equivalent of an ensemble of initial conditions with $p = 0$ and uniform spread in angle. Therefore we evaluate:

$$|\psi(t)\rangle = U^t|0\rangle;\ \langle p^2\rangle \;=\; \langle 0|U^{-t}p^2U^t|0\rangle \;=\; 4\pi^2\hbar^2\sum_m m^2|\langle 0|U^t|m\rangle|^2, \tag{2.22}$$

where in the last equality we have inserted momentum states. Shown below is a doodle of the quantum-classical cases. Note that this is an “easy” computation these days with powerful computers, however we have to truncate the infinite dimensional matrix somewhere, and this determines the time t till which our numerical calculation can be done. This is checked by ensuring that the norm of the vector $|\psi(t)\rangle$ is reasonably close to 1. A truncation leads to nonunitary matrices. The truncation becomes effective only if the matrix is banded and therefore from the above we see the difficulty posed by both the large chaos, and the semiclassical regimes.

The kinetic energy (actually twice the kinetic energy is shown in figure) of the quantum pendulum (or rotator) increases nearly linearly along with the classical till a time t^* after which it deviates, falls short and starts to oscillate. Whether this will continue to be bounded or will increase depends on the nature of the quantum spectrum and there are very few rigorous results on this. It is believed from many numerical investigations that the energy does not indefinitely increase. The fact that the energy of the rotator is bounded implies that all the eigenstates of the quantum map are *localized* in momentum space. This among things gave rise to the understanding that quantum mechanics somehow smoothens classical chaos, and makes it less random.

Problem.

1. *Establish that U is indeed an unitary matrix.*
2. *Write a program in your favourite language to calculate the matrix elements of U.*
3. *Find the powers of U by repeated multiplication and for the initial state $|m = 0\rangle$ find how the expectation value of the kinetic energy behaves in time. Note that one does not have to store the matrix elements if the elements are easy to find each time. Keep track of the normalization to see that it is not tending to* 0. *Suggested parameters are $\hbar\tau = 1$, $K = 5$, $N = 1000$, where N is the matrix dimension to which U is truncated. Note that for these parameters the band width is* 5. *if we go to a smaller $\hbar\tau$ like* 0.01, *the half width will be* 500 *and $N = 1000$ would be too small. Try it!*

The time t^* at which quantum-classical correspondence breaks down is an important time scale in much of quantum chaos. The general understanding is that it is at this time that the discreteness of the quantum spectrum is resolved. It is the so called Heisenberg time. There are more time scales in quantum chaos and a detailed study of these is quite involved and even incomplete. We do not attempt that here. It may be mentioned finally that such quantum localization of classical chaos was found experimentally by pulsing cold sodium atoms and the break time agreed well with theoretical predictions. Localization and delocalization remains a topic of research. One way the localization can be understood is by mapping the eigenvalue problem to a tight-binding model and show that the onsite potential is psuedo-random and invoke Anderson localization. The connections between transport properties in such disordered systems, and "simple" chaotic systems is intriguing and has been studied to some extent.

2.4 Quantum maps on the torus

The quantum standard map on the cylinder is a scattering system, in the sense that unlimited diffusion in momentum can take place. If we want to study 2D Hamiltonian systems, the PSOS at any given energy in bound systems is finite, and therefore if we wish to study the effects of chaos, without the complication of scattering we have to study area preserving maps on compact phase spaces, such as tori. Indeed the two modulo conditions, on both q and p are possible for the standard map, the Harper map and is the natural phase space of the the baker and cat maps. This quantum maps on tori have been studied fruitfully as models of quantum 2 DoF nonintegrable Hamiltonian systems.

2.4.1 Quantum kinematics on the torus

Consider the unit $q-p$ torus $[0,1) \times [0,1)$ as the classical phase space. Since the restriction of both q and p to be angle like variables leads to finite quantum mechanics that is not often treated in standard books, we will develop this to the extent possible here. Imposing periodic boundary conditions on both position and momentum, results in a state space of finite dimensions. Let the position and momentum eigenstates be $|q_n\rangle$, and $|p_n\rangle$, $n = 0, 1, \ldots, N-1$, where N is the dimensionality of the Hilbert space. Assume that these form orthonormal basis sets. Recall from continuum quantum mechanics that $\exp(-ipa/\hbar)$ is the position translation operator in the sense that $\exp(-ipa/\hbar)|q\rangle = |q+a\rangle$,, while $\exp(iqb/\hbar)$ is the momentum translation (or boost) operator. Here a and b are arbitrary real numbers. Since there are only N discrete states, it is finite translation operators that take on special significance for finite quantum mechanics. Strictly speaking we should deal with unitary operators rather than the generating Hermitian ones, as there are no infinitesimal translations of a finite number of states. Therefore rather than deal with position and momentum operators we deal with position and momentum *translation* operators.

The position translation operator is denoted by T_q. It is such that

$$\langle q_n|T_q = \langle q_{n+1}|, \quad \text{and} \quad \langle q_n|T_q^N = \langle q_{n+N}| = \exp(2\pi i\beta)\langle q_n|. \tag{2.23}$$

Here $0 \leq \beta < 1$, is the phase accumulated as one goes along the q direction. For periodic boundary conditions $\beta = 0$, for anti-periodic, it is $\beta = 1/2$. Phases such as these are very useful in controlling quantum symmetries. The physical interpretation of this phase is possible as a magnetic flux line threading the particles circular configuration space. The phase then appears as the Aharanov-Bohm phase and is useful in controlling time-reversal symmetry. The translation operator in momentum, T_p, is similarly defined.

$$T_p|p_n\rangle = |p_{n+1}\rangle, \quad \text{and} \quad T_p^N|p_n\rangle = |p_{n+N}\rangle = \exp(2\pi i\alpha)|p_n\rangle. \tag{2.24}$$

Here $0 \leq \alpha < 1$, similarly controls parity symmetry. We find the relationship between the two basis, the position and momentum, by requiring that the momentum states be eigenstates of the position translation operator and vice-versa; just as in continuum mechanics.

Exercises.

1. *Using the above definitions, prove that the translation operators T_p and T_q are indeed unitary. Write down the T_p operator in momentum basis and the T_q operator in position basis for $N = 4$.*

2. *Show by direct verification that*

$$|p_m\rangle \equiv \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \exp\left(2\pi i(n+\alpha)(m+\beta)/N\right)|q_n\rangle \tag{2.25}$$

is an eigenvector of T_q, that is

$$T_q|p_m\rangle = \exp\left(2\pi i(m+\beta)/N\right)|p_m\rangle. \tag{2.26}$$

Similarly

$$T_p|q_n\rangle = \exp\left(2\pi i(n+\alpha)/N\right)|q_n\rangle. \tag{2.27}$$

From this exercise we get the important transformation function which is nothing but a discrete version of the Fourier transform of continuum quantum mechanics.

$$\langle q_n|p_m\rangle = \frac{1}{\sqrt{N}} \exp\left(2\pi i(n+\alpha)(m+\beta)/N\right) \equiv G_{nm} \tag{2.28}$$

Thus although we avoid writing down position and momentum operators, the rest of the machinery is very much there on the torus, and appropriate discretization is involved. We may also identify "position" and "momentum" eigenvalues from the eigenvalues of the translation operators as $q_n = (n+\alpha)/N$ and $p_m = (m+\beta)/N)$.

Notice that we have now a 2 parameter family of quantizations and this freedom with boundary conditions is absent in ordinary quantum mechanics. It is interesting that the Aharanov-Bohm phase appears in finite quantum mechanics unobtrusively and in fact there is one more phase which comes from momentum periodicity.

Exercise.

One may ask what about the uncertainty relation $[q,p] = i\hbar$? As is well known this translates into the fact that unitary translation operators along q and p, do not commute, which is a reflection that there is no sensible phase space in quantum mechanics. Show that the analogue of the uncertainty relation is the non-commutativity of T_q and T_p described by

$$T_p T_q \;=\; e^{-2\pi i/N} T_q T_p. \tag{2.29}$$

For simplicity put $\alpha = \beta = 0$. Hence find λ_{rs} where $T_p^r T_q^s = \lambda_{rs} T_q^s T_p^r$ for some integers r and s. Also investigate the role of the phases.

Where is $\hbar$? From comparing the transformation function with the continuum formula for $\langle q|p\rangle$ we may infer that $N = 1/h$. This also follows from semiclassical arguments of state counting: as there are N states on the unit phase space, and there is one state per h, it follows that

$$h = \text{Total area of phase space/Total number of states} = 1/N. \tag{2.30}$$

This is of course the effective scaled Planck constant. The classical limit is then the large N limit, $N \to \infty$.

Problem.

G_N, the finite Fourier transform matrix is an unitary matrix (prove it!). We discussed that quantum maps of area preserving transformations were unitary operators. May G_N be the quantum map corresponding to some classical map? Indeed show that G_N corresponds to the simple classical transformation of a 90 degree rotation of the unit square about its center. Note how this dovetails with the fact that $G^4 = 1_N$, where 1_N is the N dimensional identity. Hence show that the eigenvalues of G_N are only ± 1 and $\pm i$. Thus G_N, the finite Fourier transform has an interesting and intuitive interpretation of a rotation, a simple operation that is at the bottom of integrable systems.

Coherent States on the Torus

Coherent states on the torus are the equivalent of the coherent states that one studies in quantum mechanics as eigenstates of the harmonic oscillator annihilation operator. We use them essentially to visualize quantum states in a "phase space", as coherent states are of minimal $q-p$ uncertainty and therefore come closest to being phase space points. They are the quantum goggles through which we hope to see the quantum-classical border with more precision.

First we need a "fiducial" state which is the analogue of the harmonic oscillator ground state, the first coherent state (recall $a|0\rangle = 0$, so that $0\rangle$ is a coherent state). Saraceno proposed using the ground state of the Hamiltonian

$$H_h = 2 - \frac{1}{2}\left(T_q + T_q^\dagger + T_p + T_p^\dagger\right), \tag{2.31}$$

which is the quantization of $2 - \cos(2\pi q) - \cos(2\pi p)$ on the torus (see this from the analogy of the translation operators on the torus to the usual translation operators). Examine the classical Hamiltonian to see that the energy is bounded between 0 and 4, which is also the bound for the eigenvalues of H_h. Expanding about $q = p = 0$ we see that it is a Harmonic oscillator in the linear approximation. Thus we can expect this state to be localized at the $q = p = 0$ and be one of minimal uncertainty. Calling this state $|00\rangle$ we may then define:

$$|pq\rangle = T_p^p T_q^{-q}|00\rangle, \quad 0 \le p, q \le N-1, \tag{2.32}$$

so that $|pq\rangle$ is the coherent state that we seek. In particular if ψ is any state $|\langle pq|\psi\rangle|^2$ tells us how this state is spread in momentum and position simultaneously.

Problem.

Analyse more carefully the fiducial state as defined above. Derive an approximate expression for this from the harmonic oscillator approximation. Diagonalize H_h exactly and compare this ground state with that found approximately. What about the excite states? For how long do you expect the harmonic oscillator approximation to be valid?

This ends our discussion of the kinematics on the toral phase space. We are now ready to quantize maps on tori.

2.4.2 General toral quantum maps

Consider the quantization of the kicked Hamiltonian in Eq. (1.7) and the resultant classical map of Eq. (1.12). Recall that the map is from just after a kick to just after the next kick. Therefore first there is the "free motion", and then the kick. This results, as discussed earlier, in the quantum map:

$$U = \exp(-iV(q)/\hbar)\exp(-if(p)/\hbar). \tag{2.33}$$

We now wish to treat the map restricted to a torus, which requires that f and V be periodic functions of unit period. Thus we write the quantum map in the position basis as:

$$U_{nn'} = \langle q_n|U|q_{n'}\rangle = \langle q_n|\exp(-if(p)/\hbar)|q_n'\rangle e^{-2\pi i N V\left(\frac{n'+\alpha}{N}\right)}, \tag{2.34}$$

where we have used $h = 1/N$ and inserting complete momentum states we get

$$\langle q_n|\exp(-if(p)/\hbar)|q_n'\rangle = \frac{1}{N}\sum_{m=0}^{N-1} e^{-2\pi i N f(\frac{m+\beta}{N})} e^{2\pi i(m+\beta)(n-n')/N)}. \tag{2.35}$$

Finally the whole caboodle is:

$$U_{nn'} = \frac{1}{N} e^{-2\pi i N V\left(\frac{n'+\alpha}{N}\right)} \sum_{m=0}^{N-1} e^{-2\pi i N f(\frac{m+\beta}{N})} e^{2\pi i(m+\beta)(n-n')/N)}. \tag{2.36}$$

While this may appear somewhat messy, its essential underlying simplicity must be appreciated. Nothing much further can be done with this form in this generality. The finite unitary U is the quantum map corresponding to the general family of maps in Eq. (1.12), with modulo 1 conditions in both q and p. An example is the Harper map for which both f and V are simply cosines.

Exercise.

Write a program for the quantum Harper map. Evaluate the matrix elements and explicitly verify that it is unitary, that is $U^\dagger U = I_N$.

2.4.3 Quantum standard map on the torus

What about the standard map on the torus? In this case $f(p) = p^2/2$ does not appear naturally as a periodic function. However we define the action of the free motion on an momentum eigenstate in the obvious manner:

$$\exp(-ip^2/2\hbar)|p_m\rangle \; = \; \exp(-\pi i(m+\beta)^2/N)|p_m\rangle. \tag{2.37}$$

and therefore we quantize the standard map on the torus in the position basis as ($V = -K\cos(2\pi q)/(2\pi)^2$):

$$U_{nn'} = \frac{1}{N} e^{\frac{iNK}{2\pi}\cos\left(\frac{2\pi(n'+\alpha)}{N}\right)} \sum_{m=0}^{N-1} e^{-\pi i\frac{(m+\beta)^2}{N}} e^{2\pi i(m+\beta)(n-n')/N}. \tag{2.38}$$

In the case that $\beta = 0$, we can do the sum exactly, as this was done by Gauss quite some time back and constitutes an example of an exact *Gaussian sum.* The objection that p^2 is not periodic is addressed in this case by restricted the value of N to even integers. This ensures that $e^{-i\pi m^2/N}$ has the periodicity of N. We get after the summation a simple formula for the standard map on the torus:

$$U_{nn'} = \frac{1}{\sqrt{iN}} e^{\frac{iNK}{2\pi}\cos\left(\frac{2\pi(n'+\alpha)}{N}\right)} e^{i\pi(n'-n)^2/N}. \tag{2.39}$$

2.4.4 Quantum bakers map

The bakers map was the simplest classical 2D area preserving transformation that we studied, in the sense that it was exactly solvable for all orbit types, periodic or otherwise, its Lyapunov exponent, topological entropy etc. are easy to find, it is in short an exactly solvable model of chaos. Therefore it is natural for us to seek a quantum version of the map. Perhaps it will also be exactly solvable? It was with this motivation that the bakers map was first quantized in 1988-89, however, despite its structural simplicity it is not exactly solvable in the sense that we do not yet know how to solve for the spectrum of the quantum problem.

One reason why the baker was quantized fairly late was that it does not have a kicked Hamiltonian generating it. However there is a generating function generating it. Here we will merely state the quantum baker map and restrict ourselves to some motivating comments. Given a particular choice of toral boundary conditions (α, β), recall that we have the finite Fourier transform which we denoted by G_N as the transformation function between position and momentum. This will form the central quantity in the quantum baker map which in the position representation is:

$$B \; = \; G_N^{-1} \begin{pmatrix} G_{N/2} & 0 \\ 0 & G_{N/2} \end{pmatrix}. \tag{2.40}$$

Here $G_{N/2}$ is the $N/2$ dimensional Fourier transform (FT), and we require that N be an even integer. Thus we see that the quantum baker map is a simple combination of finite Fourier transforms. In terms of signals, it instructs us to split the signal into two halves and do a FT in each part individually, then combine the two outputs and do an inverse FT on the whole lot. Indeed it seems a very simple transformation, but this is the quantized version of the paradigm chaotic system: the left shift dynamics.

The bakers map first quantized by Balazs and Voros has since undergone several versions of justifications and other operators have also been proposed. We will take a route to it through generating functions that also throw interesting light on quantum-classical correspondences. As we had noted earlier, quantum maps are quantizations of classical canonical transformations.

Canonical Transformations and Propagators: A digression.

Recall that a canonical transformation is specified by a generating function and this comes in 4 flavors (Goldstein!), F_1, F_2, F_3 and F_4, such that

$$F_1(q,Q):\ p=\partial_q F_1,\ P=-\partial_Q F_1;\ F_2(q,P):\ p=\partial_q F_2,\ Q=\partial_P F_2; \tag{2.41}$$

$$F_3(p,Q):\ q=-\partial_p F_3,\ P=-\partial_Q F_3;\ F_4(p,P):\ q=-\partial_p F_4,\ Q=\partial_P F_4. \tag{2.42}$$

The generating functions F_2 and F_3 are said to be of a "mixed" kind, referring to their dependencies on the position and momentum. For the sake of simplicity we treat 1DoF and time independent transformations, the extensions do not add any essential complication.

Now we write the corresponding quantum propagators:

$$\langle Q|K|q\rangle \sim \exp(-iF_1(q,Q)/\hbar);\ \langle P|K|q\rangle \sim \exp(-iF_2(q,P)/\hbar); \tag{2.43}$$

$$\langle Q|K|p\rangle \sim \exp(-iF_3(p,Q)/\hbar);\ \langle P|K|p\rangle \sim \exp(-iF_4(p,P)/\hbar). \tag{2.44}$$

The propagators have 4 possible representations, two of which are mixed, and correspond exactly to the 4 classical generating function types. Notice that this has the intuitive structure of the propagator "taking the old variables to the new". The classical relation between the generating functions is via Legendre transformations (for instance $F_2 = F_1 + PQ$, F_1 is Legendre transformed wrt Q), while the quantum propagators are related to each other via the Fourier transform. The "$\sim$" symbol is to indicate that the relationship is semiclassical. However *if the transformation is linear the relationship is exact* Upton normalizations.

For instance take the identity transformation ($Q = q$, $P = p$), which is generated by $F_2 = qP$ (verify it), then since a classical identity transformation can be expected to be a quantum identity transformation we get $\langle P|Id|q\rangle = \langle P|q\rangle \sim \exp(-iPq/\hbar)$, a result we know is an equality if we put in the factor $1/\sqrt{2\pi\hbar}$. Thus the FT is the identity in the mixed representation. Consider the exchange of q and P, ($Q = p$, $P = -q$), which is actually a 90 degree anticlockwise rotation in phase space generated by $F_1 = qQ$. The corresponding quantum map is $\langle Q|K|q\rangle \sim \exp(-iqQ/\hbar)$, which is again the FT. Thus the FT is a 90 degree rotation in the pure position representation. This is also the solution to a problem posed earlier in the context of quantum maps. As another example, we know that Hamiltonians generate infinitesimal time translations, which leads us to $\langle P|K(dt)|q\rangle \sim \exp(-iH(q,P)\,dt/\hbar)$, while its Fourier transform would give us the propagator in position representation; but as mentioned earlier the FT is classically (and semiclassically) a Legendre transform. The Legendre transform of the Hamiltonian is of course the Lagrangian and we can write $\langle Q|K(dt)|q\rangle \sim \exp(-iL(q,Q)\,dt/\hbar)$, which is the mysterious formula in Dirac's book that spurred Feynman to develop the path-integral formalism of quantum mechanics. It also explains the confusion we often fall into while asking why the Lagrangian should appear in the propagator rather than the Hamiltonian, the answer is that the Hamiltonian would appear in a mixed representation of the propagator. That should be expected as indeed Hamiltonians generate translations in the "mixed space" of phase space.

We return to the baker map. Recall that the $L \to B$ part of the baker map is $(q' = 2\,q\,p' = p/2)$, which is generated by the canonical transform $F_2(q,P) = 2qP$, where we identify $(q' \equiv Q, p' \equiv P)$. Therefore this half is given by the operator B whose mixed representation is $\langle P|B|q\rangle \sim \exp(-i2qP/\hbar)$, which is almost the FT but for the factor 2 in the exponent. On the torus, this becomes $G_{N/2}$, see that this indeed has the right structure. However this is only for those $(q < 1/2,\ P < 1/2)$, in the phase space. In the Hilbert space this translates to those $(q_n < 1/2,\ P_m < 1/2)$ or $(n < N/2,\ m < N/2)$. Similar arguments hold for the other half of the baker map and we get the quantum baker in the *mixed* representation by the matrix:

$$B_{\text{mixed (P-q) representation}} = \begin{pmatrix} G_{N/2} & 0 \\ 0 & G_{N/2} \end{pmatrix}, \tag{2.45}$$

from which we multiply by G_N^{-1} to take the baker to the pure position representation. This completes our motivation of why Eq. (2.40) should qualify as a quantum baker. Other arguments also favour this simple matrix. It is well known that quantization is not an unique process, and while there exist a few other quantizations, they are all equivalent (or believed to be) in the semiclassical regime. The simplicity of the Balazs-Voros baker makes it still the simplest model of quantum chaos. Saraceno found that antiperiodic boundary conditions ($\alpha = 1/2,\ \beta = 1/2$) maximally preserves the classical symmetry of reflection about the center of the square.

Exercise.

1. *Find explicitly the matrix elements of the quantum baker map in the position representation.*
2. *What is the quantum baker map in the momentum representation?*
3. *Define the operator R such that $R|q_n\rangle = |q_{N-n-1}\rangle$. Find the action of R on the momentum states. Hence prove that R corresponds classically to the act of reflection about the center of the square of the square: $(q \to 1-q,\ p \to 1-p)$. Show that the classical map commutes with this reflection.*
4. *Prove that $[R,B] = 0$ if $\alpha = 1/2, \beta = 1/2$.*
5. *Write a program to calculate the matrix elements of B and verify that indeed B is unitary and that it commutes with R.*

2.5 Quantum Chaos: Eigenfunctions

We can use any of the models we have developed in the previous section, such as the quantum standard map or the quantum baker map to finally study the effects of quantizing a chaotic system. In particular if there are special properties of eigenfunctions and eigenvalues, and what happens on time evolution? We very briefly describe here some of the phenomenology found so far. As a practical note, we emphasize that none of the operators discussed thus far have been analytically diagonalized. Use any of the standard matrix diagonalization routines to diagonalize the matrices for some fixed N (effective inverse Planck constant) and parameter values when studying the stationary states.

2.5.1 Scarring.

Eigenfunctions of quantized chaotic systems are very interesting beasts that are full of information and importance. It is important to understand that quantum eigenfunctions are semiclassically associated with classically invariant sets. For classically chaotic systems, the only such set with full measure is the energy shell. There are smaller invariant sets, for instance there are an infinite number (dense, recall the baker map!) of periodic orbits whose measure is zero. It was not expected that these influence the eigenfunctions. This gave rise to the Berry-Voros hypothesis which said that the Wigner function (a phase space representation) of typical eigenstates will be uniformly spread on the energy shell (like the microcanonical ensemble of statistical physics). A mathematical formulation of this is known as Schnirelmann's theorem.

However numerical investigation of the eigenfunctions of the chaotic stadium billiard by Eric Heller showed that most of the eigenfunctions were "decorated" with strong streaks that could be unambiguously identified with classical periodic orbits. Since this is a chaotic system, these orbits are isolated and unstable. Heller called these "scars" of periodic orbits in quantum wavefunctions.

Since these investigations many many examples have been found. Heller has put forward certain explanations for this phenomena based on wavepacket dynamics, while Bogomolny and Berry have advanced semiclassical theories based on Gutzwiller's periodic orbit theory. Today we know that apart from periodic orbits there are also scars of homoclinic and heteroclinic orbits. However our understanding is far from complete, in the sense that we cannot say which eigenfunction will be influenced by which classical orbits. Heller gave a criteria that restricts those periodic orbits that could scar the wavefunctions, which effectively cuts off long periodic orbits. Almost all scarring studies have been done with 2DoF systems or quantum maps. Experimental evidence exists from resonant tunneling experiments and microwave cavity billiards.

It is accurate to say that eigenfunctions remain poorly understood even for 2DoF systems. When the baker map was first quantized, the bakers looked at the eigenfunctions in the position representation and concluded that they were mostly erratic, or random looking. However when subsequently coherent states were used to look at the functions a bewildering variety of patterns became visible, most of which could be identified with some classical feature, such as periodic orbits, or homoclinic orbits, or stable and unstable manifolds, but the way they were appearing held no particular rule. With the techniques developed by us so far, this is quite easy to do, we diagonalize the quantum baker map, we have used $N = 50$ in the figure below, find all the N eigenfunctions $|\psi_i\rangle$, which would be in the position basis and then calculate the overlap:

$$|\langle pq|\psi_i\rangle|^2, \tag{2.46}$$

for each i, where $|pq\rangle$ is the coherent state discussed earlier and must simply be thought of as a minimum uncertainty wavepacket at (q, p). The overlap is sometimes called the *Husimi representation*. This will tell us how the eigenfunction is spread in "phase-space."

Figs (2.2) are 30 of the 50 eigenfunctions and will give some idea of what we are up against. Firstly notice that the wavefunctions are not really spread all over, there is prominent clumping to be seen, and that this is indeed associated with classical orbits is quite easily seen in the case of the bakers map, as the classical orbits are exactly known. For instance we can see the period 2 orbit $(2/3, 1/3)$, $(1/3, 2/3)$ prominently in some eigenfunctions, we can also see period 3 and 4. To really convince onceselves, we need to superimpose the orbits with the eigenfunctions, and they would fall on each other. However in this "eigenfunction zoo" we only know know *aposteriori* what orbits are scarring what functions. Besides it must be said that there is a lot of "grass" or small structure that is not immediately visible but which is nevertheless important.

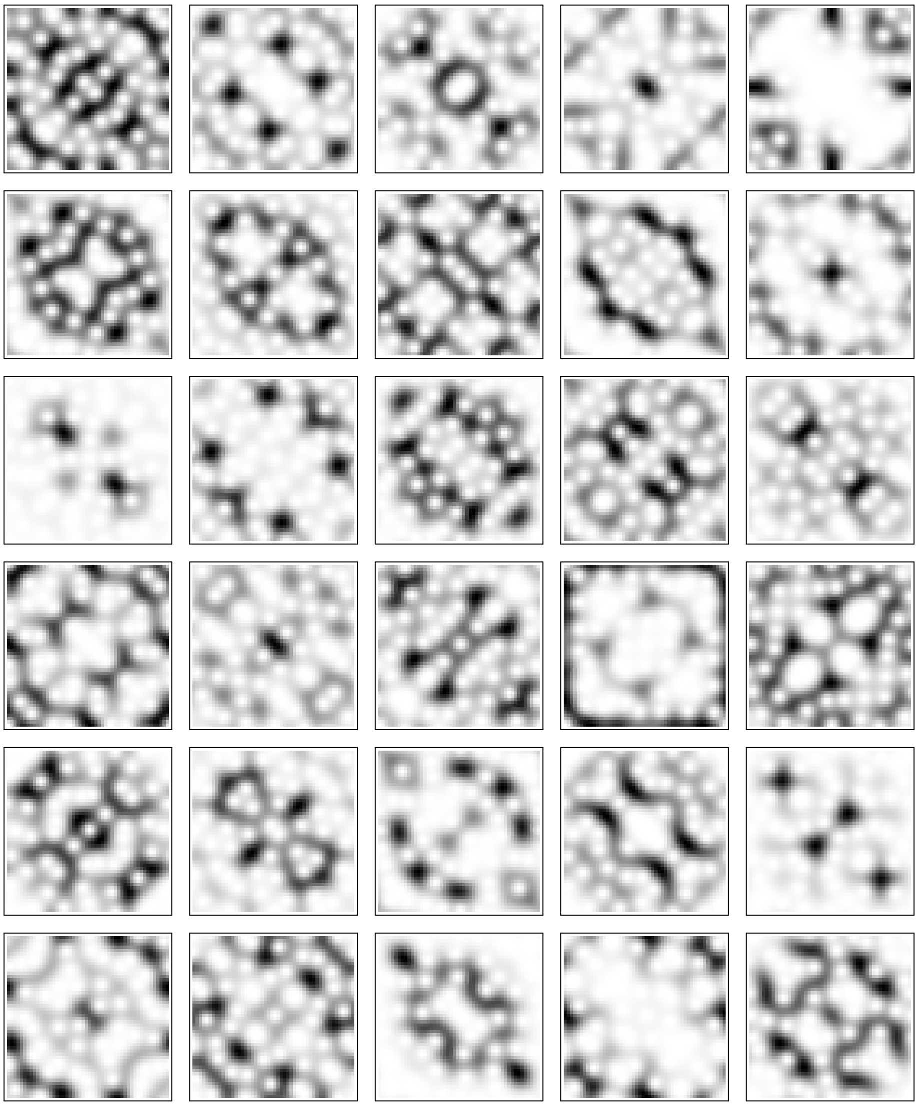

Figure 2.2: Quantum baker eigenfunctions for $N = 50$. The squares are the unit torus, notice intense scarring in some "clean" states by low period periodic orbits, 2, 3 and 4 orbit.

After the example of a "hard chaos" system, the baker map, lets look at the quantum standard map which could have a mixed phase space depending on the parameter K. Say we take $K = 2$, in which case we have a prominent elliptic island around the fixed point at the origin and a large chaotic sea. In Fig. (2.3) we again show 30 of the 50 eigenfunctions for $N = 50$ case. Firstly it appears overall "cleaner". It is useful now to go back to the classical standard map and look at the phase space for $K = 2$ in Fig. (**??**). See the remarkable classical-quantum correspondence that is there. Notice how there is a state that is only affected by the fixed point at the origin and how remarkably there is a state that is localized around the stable period 2 orbit $(0, 1/2), (1/2, 1/2)$. There are many that are affected by the elliptic orbits around the fixed point at the origin, and the rest are prominently located in the chaotic "sea" and look somewhat like the baker eigenfunctions. The other observation is that all the states seem to be either "scarred" by the regular orbits, or by the chaotic ones, not by both simultaneously. This was conjectured to be the case by Ian Percival in the early 1970's, and while it is seen to hold for many 2DoF systems, it is not clear if this is valid in higher dimensions. Violations of these have come to light in certain periodic systems, and states that are localized in both chaotic and regular regions have been called "amphibious".

A lot of work has gone into understanding functions, but there are many fundamental open questions concerning them. There is also a viewpoint that individual states may not be important, as there are too many and often they are too close in energy. Thus statistical and average properties may be of more experimental interest and indeed some finer semiclassical theories are possible if such averaging is done. We move on now to the eigenvalues.

2.6 Quantum Chaos: Semiclassics of Eigenvalues

The story of eigenvalues is somewhat more happier if not entirely so. The general aim of semiclassics is to provide quantum information from purely classical one. For instance everything about the quantum harmonic oscillator can be found from classical properties. It is not at all clear whether this is possible in general. It must be emphasized that calculating quantum quantities using classical ones, does not mean that the phenomena are classical, of course not. It also does not mean that when quantum-classical correspondence there is an end to the use of semiclassics.

The Gutzwiller trace formula which connects the trace of the energy Green's function to a weighted sum over the periodic orbits on energy shells is the central object. This however requires quite an extensive treatment, we will here restrict ourselves to a part of it and give a flavor of the issues involved. Using quantum maps, the trace formula is also usefully studied. As one central object we will deal with the trace of the propagator in time:

$$\mathrm{Tr}(U^T) = \sum_{i=0}^{N-1} \exp(iT\phi_i) \tag{2.47}$$

where U is some unitary map, the ϕ_i are the eigenangles. This implies that if we know the traces of the powers of U we can know the eigenangles. This is seen by Fourier transforming both sides:

$$\sum_{T=-\infty}^{\infty} e^{-i\omega T}\mathrm{Tr}(U^T) = \tag{2.48}$$

$$\sum_{m=-\infty}^{\infty} \sum_{i=0}^{N-1} \delta(\phi_i - \omega - 2\pi m) \tag{2.49}$$

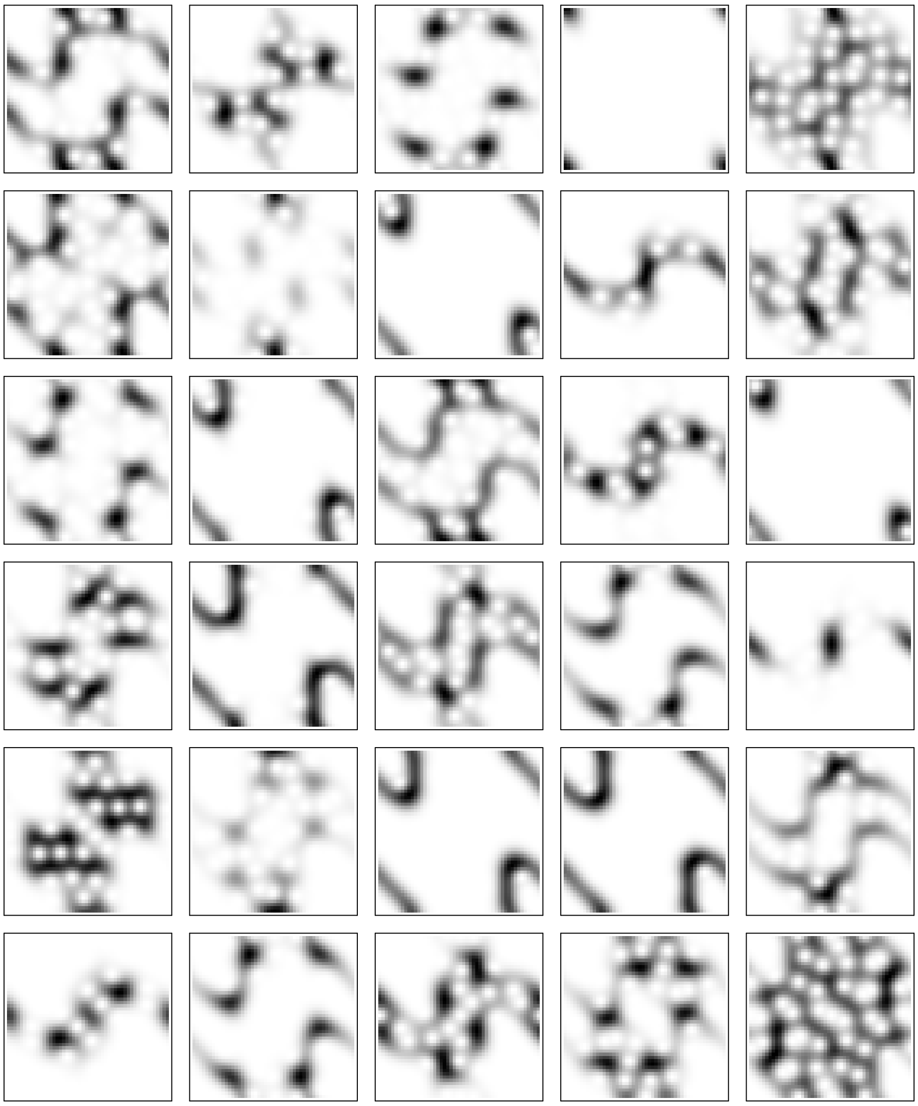

Figure 2.3: Quantum standard map eigenfunctions for $N = 50$. The squares are the unit torus, compare with the classical phase space in Fig. (1.5), and notice how all the eigenfunctions are either in the regular or in the chaotic regions.

where we have made use of the *Poisson identity*:

$$\sum_{n=-\infty}^{\infty} e^{2\pi i n x} = \sum_{m=-\infty}^{\infty} \delta(x-m) \tag{2.50}$$

an identity from the theory of Fourier transforms that is of singular importance, simplicity and power. If we multiply the above identity by a smooth function $f(x)$ and integrate we get the following *Poisson summation formula*:

$$\sum_{n=-\infty}^{\infty} \int_{n=-\infty}^{\infty} f(x) e^{2\pi i n x}\, dx = \sum_{m=-\infty}^{\infty} f(x). \tag{2.51}$$

Thus Fourier transforming the traces of the powers of the propagator will give us delta functions at the eigenangles.

Semiclassical theory then attempts to find $\mathrm{Tr}(U^T)$ from purely classical quantities. The general structure of this trace formula is

$$\mathrm{Tr}(U^T) \sim \sum_{\gamma(T)} A_\gamma \exp(2\pi i S_\gamma/\hbar) \tag{2.52}$$

where γ enumerates classical *periodic orbits* of period T, S_γ is the action of the periodic orbit, and A_γ is a weight that typically exponentially falls with the period T. This last statement may give rise to the expectation that the long orbits can be neglected, but remember that in chaotic systems there is an *exponential proliferation* of periodic orbits with period. Therefore this is a delicate problem that needs care and in fact while the trace of quantum maps on finite Hilbert spaces hardly poses a problem, whole of semiclassics is beset with convergence issues. There is also the question of *how long* the above approximation holds good, while a fair amount of work has gone into this it is again not very clear what exactly this time is and how it depends on the scaled Planck constant and the parameters of chaos. For instance one surprising result that has emerged is that *semiclassics can be more accurate for larger chaos!*.

Semiclassics has been described as a determined usage of the stationary phase approximation. To give an idea of what goes on, we can make use of the quantum map machinery we have already discussed. As a fair warning this may be somewhat heavy on first reading, but this is really "semiclassics-lite".

Consider the following map defined on the unit torus:

$$\begin{aligned} q_{j+1} &= q_j + p_j - l_j \\ p_{j+1} &= p_j - V'(q_{j+1}) - m_j, \end{aligned} \tag{2.53}$$

where $V(q)$ is the periodic "kicking" potential with unit periodicity, the prime indicates derivative, and the integers m_j and l_j are such that the map is restricted to the unit torus (winding numbers). They are the "modulo one" operations. As was discussed earlier the above map can be derived from a time dependent Hamiltonian system. Also there exists a generating function for the map on the torus given by

$$S(q_j, q_{j+1}; l_j, m_j) = \frac{1}{2}(q_{j+1} - q_j + l_j)^2 - V(q_{j+1}) - m_j q_{j+1} \tag{2.54}$$

from which the map can be derived as $p_j = -\partial S/\partial q_j$ and $p_{j+1} = \partial S/\partial q_{j+1}$. This is of the F_1 type we discussed earlier.

The quantum map corresponding to the Eqs.(26) is given by the finite dimensional unitary matrix

$$\langle n|U|n'\rangle = \frac{e^{-i\pi/4}}{\sqrt{N}} \exp\left(\frac{i\pi}{N}(n-n')^2 - 2\pi i N V\left(\frac{n}{N}\right)\right), \tag{2.55}$$

which generalizes the quantum standard map used before. This takes on the function of the propagator as it connects states after consecutive kicks. Here the representation is in the position basis and n and n' may take the integer values from 0 to $N-1$. N is itself the dimensionality of the Hilbert space and is also the inverse Planck constant, and is restricted to be even integers for preservation of toral boundary conditions. Semiclassics means the study of the unitary operator as $N \to \infty$.

The object of primary interest, the trace of the powers of the propagator, from which the spectrum may be derived by a Fourier transform can be written as

$$\mathrm{Tr}(U^T) = \frac{e^{-i\pi T/4}}{N^{T/2}} \sum_{n_i=0}^{N-1} \exp\left(\frac{2\pi i}{N}\sum_{j=1}^{T}\left(n_j^2 - n_j n_{j+1} - N^2\, V(\frac{n_j}{N})\right)\right), \tag{2.56}$$

with

$$n_{T+1} = n_1.$$

It is implied in the above that the outer sum is over the T variables n_i, $i = 1, 2, \ldots, T$. Using the Poisson summation formula we can rewrite the above as

$$\mathrm{Tr}(U^T) = e^{-i\pi T/4}\, N^{T/2} \sum_{k_i=-\infty}^{\infty} \int_{-\epsilon}^{1-\epsilon} dx_1 \ldots dx_T$$

$$\exp\left(2\pi i N \sum_{j=1}^{T}\left(k_j x_j + x_j^2 - x_j x_{j+1} - V(x_j)\right)\right), \tag{2.57}$$

with

$$x_{T+1} = x_1, \text{ and } \; k_{T+1} = k_1.$$

The stationary phase approximation, assuming that N is large, gives the following T conditions

$$x_{j+1} = 2x_j - x_{j-1} - V'(x_j) + k_j; \quad j = 1, \ldots, T, \;\; x_0 = x_T, \;\; x_1 = x_{T+1}, \tag{2.58}$$

with the further condition that

$$0 \le x_j < 1.$$

These are precisely the equations that determine the period T orbits of the map. The integers k_j are related to the integers l_j and m_j of Eqs. (2.53) by the relation $k_j = l_{j-1} - l_j - m_{j-1}$. With the assumption that they uniquely determine a periodic orbit of period an integer fraction of T, we restrict the infinite sum to only those that relate to such a periodic orbit labeled below by γ. This is the first approximation and the second one is that we will extend the ranges of integration to the whole real line. These approximations together are exact in the case of the quantum cat maps, which we have not discussed here, and the third related approximation is that we Taylor expand the potential about the periodic orbits retaining up to the quadratic terms. This approximation is unnecessary for the piecewise linear maps, but is necessary in general.

Therefore we define new variables y_j such that $x_j = q_j + y_j$ and q_j is the central periodic orbit.

$$\mathrm{Tr}(U^T) \sim e^{-i\pi T/4} N^{T/2} \sum_{\gamma} \exp\left(2\pi i N \sum_{j=1}^{T}\left(-q_j q_{j+1} + q_j^2 + q_j\, k_j - V(q_j)\right)\right) \times$$

$$\int_{-\infty}^{\infty} dy_1 \ldots dy_T \exp\left(2\pi i N \sum_{j=1}^{T}\left(y_j^2 - y_j y_{j-1} - y_j^2\, V''(q_j)/2\right)\right) \tag{2.59}$$

The sum

$$\sum_{j=1}^{T} \left(-q_j q_{j+1} + q_j^2 + q_j\, k_j - V(q_j)\right) \tag{2.60}$$

can be identified with the action of the periodic orbit, as one gets

$$S_\gamma = \sum_{j=1}^{T} (q_j^2 - q_j q_{j+1} - V(q_j) + q_j k_j + l_j^2/2), \tag{2.61}$$

We can neglect the term $l_j^2/2$, from the Lagrangian; this is legitimate as the action occurs as $e^{2\pi i N S}$, and since N is an even integer these terms do not matter.

The integral is evaluated by standard methods.

$$\int_{-\infty}^{\infty} d^T y \, \exp(i\pi N y^t A_\gamma y) = \frac{e^{i\pi T/4}}{N^{T/2}} \frac{e^{-i\pi \nu_\gamma/2}}{\sqrt{|\mathrm{Det}(A_\gamma)|}}. \tag{2.62}$$

Here y denotes the T component vector $\{y_j\}$ and y^t is its transpose. The real symmetric matrix A_γ is given by

$$A_\gamma = \begin{pmatrix} 2 - V''(q_1) & -1 & 0 & .. & .. & -1 \\ -1 & 2 - V''(q_2) & -1 & 0 & .. & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -1 & 0 & .. & .. & -1 & 2 - V''(q_T) \end{pmatrix}. \tag{2.63}$$

ν_γ is a "Maslov like" index, and is the number of negative eigenvalues of the matrix A_γ.

The nontrivial problem of evaluating the determinant is already solved and the results are known. The determinant can be related to the stability of the periodic orbit. If the residue of the periodic orbit, which is simply related to the trace of the stability matrix, is R_γ, then $R_\gamma = -\frac{1}{4}\mathrm{Det}(A_\gamma)$. or if we denote the stability matrix eigenvalues by λ_+^γ and λ_-^γ, $\mathrm{Det}(A_\gamma) = \lambda_+^\gamma + \lambda_-^\gamma - 2$.

Thus finally we can write the asymptotic periodic orbit sum, or the trace formula, for the toral maps as

$$\mathrm{Tr}(U^T) \sim \sum_\gamma \frac{\exp\left(2\pi i N S_\gamma - i\pi\nu_\gamma/2\right)}{\sqrt{|\lambda_+^{\gamma\, T} + \lambda_-^{\gamma\, T} - 2|}}. \tag{2.64}$$

The sum is over periodic orbits whose periods are integer fractions of T are labeled by γ. This is of the canonical Gutzwiller-Tabor form having in the exponent the *action* of the period T orbits, and the prefactor explicitly depending on the *stability* of these orbits. The piecewise linear maps such as the baker map, or the sawtooth map are such that the Maslov like phases are zero and the only type of periodic orbits are those of the direct hyperbolic kind. With this formula we can study the vast class of *mixed* systems, such as the well known standard map. It is then of interest to ask questions such as how long the semiclassical approximations are valid in such systems which one knows are generic. Not much is known on these issues due to difficulty of finding *classical* orbits.

A careful application of the above formula in the case of the standard map, and for the simplest possible trace, the time 1 trace, yields the following:

$$\mathrm{Tr}(U) = \frac{e^{-i\pi/4}}{\sqrt{N}} \sum_{n=0}^{N-1} \exp(-ikN\cos(2\pi n/N)) \sim \tag{2.65}$$

$$\frac{e^{-i\pi/4}}{\sqrt{2\pi}} \left[\frac{2\sin(Nk+\pi/4)}{\sqrt{k}} + \sum_{l=1}^{[k]} \frac{4\sin(\theta_N(l)+\pi/4)}{(k^2-l^2)^{1/4}} \right], \tag{2.66}$$

where

$$\theta_N(l) = N(\sqrt{k^2-l^2} + l\arcsin(l/k)). \tag{2.67}$$

We have defined $k \equiv K/(2\pi)$, taken all quantum boundary conditions to be 0, and [] denotes the integer value function. Notice how the quantum trace involves a sum containing N terms, which in the classical limit has infinite number of terms, while the semiclassical approximation has only $[k]$ terms, depending on the chaos parameter in the system! The sum is over all the fixed points of the standard map, there are $[k]$ of them. Thus semiclassics exposes a *duality* between classical periodic orbits and quantum traces, a duality that is deep and goes into modern areas of mathematical research.

Problem.

Verify if the semiclassical approximation for the trace of the standard map propagator, Eq. (2.66) is correct. Write a program that will do both the sums in this approximation, and evaluate the goodness of the approximation as a function k and N.

Semiclassical formulae such as these are an important analytical tool in understanding quantum chaotic systems. Poincarë had predicted that periodic orbits would be the way to penetrate the fortress of dynamics, and this has been borne out as the truth in the case of semiclassics.

2.7 Random Matrix Theory.

We will unfortunately not be able to go into details of this important aspect of quantum chaos. As has been said earlier, the statistical aspect of quantum chaos is well described by random matrix theory (RMT), and is widely used in many areas from nuclear to mesoscopic physics. These days RMT is being used in widely different areas such as time series analysis of EEG data (from the brain), analysis of weather patterns and study of fluid flows.

Wigner suggested that since complex many body Hamiltonians were hopelessly difficult to solve, we may as well assume that the Hamitonian matrix (in a generic representation) is a random matrix, that is a matrix whose elements are drawn from a distribution at random. The model that is most often used is when the distribution is a Gaussian and the matrix elements are independently drawn. This leads to the Gaussian ensembles. There are some fundamental symmetries that systems may obey despite all the complexity and chaos. For instance time-reversal (TR) symmetry is quite fundamental. What does this imply for the Hamiltonian matrix? It implies that given any arbitrary basis, we can find a related basis in which the Hamiltonian is real. Therefore TR symmetric Hamiltonians are generically real, while TR nonsymmetric Hamiltonians are in general complex.

We have till now talked of unitary matrices, maps rather than Hamiltonians. Therefore the appropriate ensembles are called circular, as the matrices are unitary. For the results we will recall, the most simplest, it does not make a difference.

2.7.1 Nearest neighbour spacing distribution. (NNS)

This is one of the earliest measures that was used and is quite simple. The question is how are the nearest neighbour energy differences distributed? Somewhat paradoxically, if the system were integrable the NNS is Poisson distributed, which will happen if the energy levels do not have any correlation between them. If the system is chaotic (in the classical limit) the distribution will be one of two types depending of if there is TR symmetry or no TR symmetry. These are *universal* distributions, independent of the system and once full chaos has been achieved seemingly also indifferent to the degree of chaos. First we have to normalize the energy differences so that we can compare different spectra. To do this we normalize the levels so that the mean energy spacing is unity.

In the case of the unitary operators such as quantum maps, the mean spacing is simply $2\pi/N$ as the eigenangles are uniformly distributed over $[0, 2\pi)$. Therefore define

$$s_i = \frac{N}{2\pi}(\theta_i - \theta_{i-1}), \tag{2.68}$$

and consider the set of normalized spacings $\{s_i, i = 1, \ldots, N-1\}$. If these are distributed according to the function $P(s)$, RMT says that for the Gaussian ensembles:

$$P(s) = \begin{cases} \exp(-s) \text{ Integrable.} \\ \frac{\pi}{2} s \exp(-\pi s^2/4) \text{ Chaotic. TR symmetric.} \\ \frac{32}{\pi^2} s^2 \exp(-4s^2/\pi) \text{ Chaotic. No TR symmetry.} \end{cases} \tag{2.69}$$

For mixed systems, distributions are found that are intermediate between the Poisson and the Wigner. Notice that small spacings are the rule in integrable systems, while for chaotic ones, the energy levels are very rarely found close together. The levels are said to *repel* each other in chaotic systems. Note that there is a linear repultion for TR symmetric systems and a quadratic repulsion for non-TR symmetric ones.

Exercise.

1. *Diagonalizing the quantum baker map using any algorithm, find the eigenangles. Normalize them so that the mean spacing is unity. Verify if the angles are uniformly distributed. Find the spacing distribution. You may take $N = 100$ or above for somewhat decent statistics. It has been found that while there is level repulsion, the quantum baker map has number theoretic properties that are not understood and leads to deviations from RMT predicted distributions.*

2. *Do the same exercise for the quantum standard map on the torus. Notice how for small K, where it is nearly integrable, the NNS distribution will be Poissonian ($\exp(-s)$), while for $K >> 5$, where complete classical chaos sets in the distribution will be RMT like. Show that if $\beta = 0$ the TR symmetric distribution is obtained, while if $\beta \neq 0$, the non-TR distribution is obtained. This shows how the phases may be used to make or break important symmetries that affect the spectrum dramatically. In fact this is a way in which one detect very weak TR violating effects in nuclear physics!*

RMT has also very important things to say about the eigenfunctions, this provides the base from which scarring is seen as deviations. We will not be able to go into these just now.

2.8 Afterword

We have given a somewhat whirlwind tour of the sights in this land of Hamiltonian chaos, but obviously a tourist's perspective is quite different from the natives'. I would like to end with a few topics of research that I see going on in quantum aspects of Hamiltonian chaos:

1. **Tunneling and Chaos:** While tunneling is uniquely quantum mechanical, it has been found that chaos has significant impact on tunneling rates. Tunneling rates are seen to be significantly enhanced in the presence of intervening chaos. Here again maps have been extensively used for these studies. The questions are quite involved as they must involve eigenfunctions.

2. **Fidelity Decay, Loschmidt Echo:** If we propagate an initial state by some Hamitonian H and reverse it by a slightly different Hamiltonian H' for the same time, the final state is not going to be the same. The fidelity, $F(t) = |\langle\psi| \exp(iH't/\hbar) \exp(-iHt/\hbar)|\psi\rangle|^2$, is a measure of how much it differs and is of practical significance in many situations. It may be imagined that if H is chaotic classically the fidelity will be more sensitive to how different H' is from H. The exact way in which $F(t)$ decays has been one topic of current research.

3. **Quantum information, entanglement, quantum computers, chaos:** The way in which quantum chaos impacts on quantum entanglement is being studied by several groups. This has larger ramifications in quantum information theory. Others have also studied if quantum chaos will aid or hinder a potential quantum computer. No definitive answers yet.

4. $\hbar \longrightarrow 0$ **or Decoherence?** The classical limit is still not completely clear, with one major school giving decoherence a place of central importance. Decoherence is the interaction of a pristine isolated system with a nebulous environment. The fact that there are strictly no closed systems in physics, implies that these influences could be very important. quantum chaotic systems have very short time of quantum-classical correspondence and therefore have been used in these studies.

5. **Mesoscopic physics, transport in quantum dots.** Quantum chaos shows up in tiny devices as characteristic conductance fluctuations. Many experimental and theoretical studies are underway in these aspects.

6. **Semiclassics and RMT.** While RMT works it is not at all clear why? Afterall the quantum baker map, or the quantum standard map are very simple and definite matrices, nothing random about them. So where is the random coming from? There have been successful derivations of RMT results from semiclassics such as the trace or more general formulas, however there are important unresolved issues in TR symmetric systems.

7. **Higher dimensional systems** That we have concentrated on 2D area preserving maps is because higher dimensions are hardly explored. Some work has begun on 4D symplectic mappings and many body systems, but it is very preliminary stages.

A careful study of this document is enough to start addressing many of these questions. Whether this will end is entirely up to you. Happy hunting!

Further References

Books

- R.L. Devaney, " An Introduction to Chaotic Dynamical Systems," Benjamin, Menlo Park, 1986. Still my favourite for classical chaos.
- M. Tabor, *Classical and quantum chaos??*. Good book to begin with.
- L. E. Reichl, *The transition to Chaos*. Springer Verlag. Book that has many research topics. Good source for reference, but lacks in-depth discussions. Few problems.
- M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics*. Springer Verlag. Excellent book to gain insights, but is difficult, as the trace formula is spread over many chapters. No problems of any sort.
- Fritz Haake, *Quantum Signatures of Chaos*. Springer Verlag. Exhaustive treatment of RMT. Concentrates on tops. Thorough book and will be a good reference in research.
- Stockmann Good book, concentration on billiards. He has done experiments on microwave billiards, nice discussions of "wave chaos", and understandable Gutzwiller- Tabor-Berry semiclassics.
- Predrag Cvitanovic and the Usual Gang of Cyclists. *Chaos. Classical and Quantum.* Webbook. Freely available from http://www.nbi.dk/ChaosBook/ Excellent doodles and written by authorities on cycle expansions, practical ways to use periodic orbit theory. Highly recommended. Downside is, it is heavily concentrated on the research in these groups; apart from developments due to Poincare, Birkhoff and Gutzwiller.
- A. M. Ozorio de Almeida, *Hamiltonian Systems: Chaos and quantization.* Cambridge Univ. Press. 88. Tough. Small. Written by a master of classical semiclassics.

Some papers on quantum maps

1. F. M. Izrailev, Phys. Rep. **196** (1990), 299. Review paper on "Simple Models in quantum chaos" Authoritative for standard map on cylinder. Sort of closed the show on this.
2. J.H. Hannay and M.V. Berry, *Physica* **1D** (1980), 267. First quantized the cat map.
3. N.L. Balazs and A. Voros, *Ann. Phys. (N.Y.)* **190** (1989), 1. First quantized the baker map.
4. M. Saraceno, *Ann. Phys. (N.Y)* **199** (1990), 37. Found scarring in bakers map.
5. A.M. Ozorio de Almeida and M. Saraceno, *Ann. Phys. (N.Y)* **210** (1991), 1. Semiclassical Periodic orbit theory for the quantum baker.

I have of course not even attempted any sembelance of a bibliography. But there is much available in these sources and on line. Look at the searchable physics archives: http://in.arxiv.org in nonlinear science and quantum physics.