Chapter 29

Prologue

> Anyone who uses words "quantum" and "chaos" in the same sentence should be hung by his thumbs on a tree in the park behind the Niels Bohr Institute.
>
> —Joseph Ford

(G. Vattay, G. Tanner and P. Cvitanović)

You have read the first volume of this book. So far, so good – anyone can play a game of classical pinball, and a skilled neuroscientist can poke rat brains. We learned that information about chaotic dynamics can be obtained by calculating spectra of linear operators such as the evolution operator of sect. 15.2 or the associated partial differential equations such as the Liouville equation (14.37). The spectra of these operators can be expressed in terms of periodic orbits of the deterministic dynamics by means of trace formulas and cycle expansions.

But what happens quantum mechanically, i.e., if we scatter waves rather than point-like pinballs? Can we turn the problem round and study linear PDE's in terms of the underlying deterministic dynamics? And, is there a link between structures in the spectrum or the eigenfunctions of a PDE and the dynamical properties of the underlying classical flow? The answer is yes, but . . . things are becoming somewhat more complicated when studying 2nd or higher order linear PDE's. We can find classical dynamics associated with a linear PDE, just take geometric optics as a familiar example. Propagation of light follows a second order wave equation but may in certain limits be well described in terms of geometric rays. A theory in terms of properties of the classical dynamics alone, referred to here as the *semiclassical theory*, will not be exact, in contrast to the classical periodic orbit formulas obtained so far. Waves exhibit new phenomena, such as interference, diffraction, and higher $\hbar$ corrections which will only be partially incorporated into the periodic orbit theory. [chapter 37]

29.1 Quantum pinball

In what follows, we will restrict the discussion to the non-relativistic Schrödinger equation. The approach will be very much in the spirit of the early days of quantum mechanics, before its wave character has been fully uncovered by Schrödinger in the mid 1920's. Indeed, were physicists of the period as familiar with classical chaos as we are today, this theory could have been developed 80 years ago. It was the discrete nature of the hydrogen spectrum which inspired the Bohr - de Broglie picture of the old quantum theory: one places a wave instead of a particle on a Keplerian orbit around the hydrogen nucleus. The quantization condition is that only those orbits contribute for which this wave is stationary; from this followed the Balmer spectrum and the Bohr-Sommerfeld quantization which eventually led to the more sophisticated theory of Heisenberg, Schrödinger and others. Today we are very aware of the fact that elliptic orbits are an idiosyncracy of the Kepler problem, and that chaos is the rule; so can the Bohr quantization be generalized to chaotic systems?

The question was answered affirmatively by M. Gutzwiller, as late as 1971: a chaotic system can indeed be quantized by placing a wave on each of the *infinity* of unstable periodic orbits. Due to the instability of the orbits the wave does not stay localized but leaks into neighborhoods of other periodic orbits. Contributions of different periodic orbits interfere and the quantization condition can no longer be attributed to a single periodic orbit: A coherent summation over the infinity of periodic orbit contributions gives the desired spectrum.

The pleasant surprise is that the zeros of the dynamical zeta function (1.9) derived in the context of classical chaotic dynamics,

[chapter 17]

$$1/\zeta(z) = \prod_p (1 - t_p) ,$$

also yield excellent estimates of *quantum* resonances, with the quantum amplitude associated with a given cycle approximated semiclassically by the weight

$$t_p = \frac{1}{|\Lambda_p|^{\frac{1}{2}}} e^{\frac{i}{\hbar} S_p - i\pi m_p/2} , \qquad (29.1)$$

whose magnitude is the square root of the classical weight (17.10)

$$t_p = \frac{1}{|\Lambda_p|} e^{\beta \cdot A_p - sT_p} ,$$

and the phase is given by the Bohr-Sommerfeld action integral S_p, together with an additional topological phase m_p, the number of caustics along the periodic trajectory, points where the naive semiclassical approximation fails.

[chapter 32]

In this approach, the quantal spectra of classically chaotic dynamical systems are determined from the zeros of dynamical zeta functions, defined by cycle expansions of infinite products of form

$$1/\zeta = \prod_p (1 - t_p) = 1 - \sum_f t_f - \sum_k c_k \tag{29.2}$$

with weight t_p associated to every prime (non-repeating) periodic orbit (or *cycle*) p.

The key observation is that the chaotic dynamics is often organized around a few *fundamental* cycles. These short cycles capture the skeletal topology of the motion in the sense that any long orbit can approximately be pieced together from the fundamental cycles. In chapter 18 it was shown that for this reason the cycle expansion (29.2) is a highly convergent expansion dominated by short cycles grouped into *fundamental* contributions, with longer cycles contributing rapidly decreasing *curvature* corrections. Computations with dynamical zeta functions are rather straightforward; typically one determines lengths and stabilities of a finite number of shortest periodic orbits, substitutes them into (29.2), and estimates the zeros of $1/\zeta$ from such polynomial approximations.

From the vantage point of the dynamical systems theory, the trace formulas (both the exact Selberg and the semiclassical Gutzwiller trace formula) fit into a general framework of replacing phase space averages by sums over periodic orbits. For classical hyperbolic systems this is possible since the invariant density can be represented by sum over all periodic orbits, with weights related to their instability. The semiclassical periodic orbit sums differ from the classical ones only in phase factors and stability weights; such differences may be traced back to the fact that in quantum mechanics the amplitudes rather than the probabilities are added.

[chapter 33]

The type of dynamics has a strong influence on the convergence of cycle expansions and the properties of quantal spectra; this necessitates development of different approaches for different types of dynamical behavior such as, on one hand, the strongly hyperbolic and, on the other hand, the intermittent dynamics of chapters 18 and 23. For generic nonhyperbolic systems (which we shall not discuss here), with mixed phase space and marginally stable orbits, periodic orbit summations are hard to control, and it is still not clear that the periodic orbit sums should necessarily be the computational method of choice.

Where is all this taking us? The goal of this part of the book is to demonstrate that the cycle expansions, developed so far in classical settings, are also a powerful tool for evaluation of *quantum* resonances of classically chaotic systems.

First, we shall warm up playing our game of pinball, this time in a quantum version. Were the game of pinball a closed system, quantum mechanically one would determine its stationary eigenfunctions and eigenenergies. For open systems one seeks instead complex resonances, where the imaginary part of the eigenenergy describes the rate at which the quantum wave function leaks out of the central scattering region. This will turn out to work well, except who truly wants to know accurately the resonances of a quantum pinball?

[chapter 34]

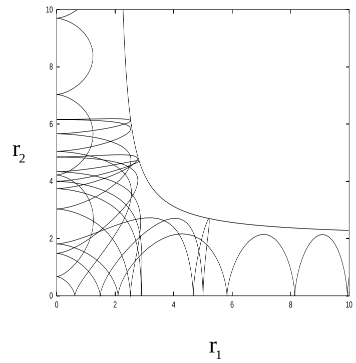

Figure 29.1: A typical collinear helium trajectory in the $r_1 - r_2$ plane; the trajectory enters along the r_1 axis and escapes to infinity along the r_2 axis.

29.2 Quantization of helium

Once we have derived the semiclassical weight associated with the periodic orbit p (29.1), we will finally be in position to accomplish something altogether remarkable. We are now able to put together all ingredients that make the game of pinball unpredictable, and compute a “chaotic” part of the helium spectrum to shocking accuracy. From the classical dynamics point of view, helium is an example of Poincaré’s dreaded and intractable 3-body problem. Undaunted, we forge ahead and consider the *collinear* helium, with zero total angular momentum, and the two electrons on the opposite sides of the nucleus.

We set the electron mass to 1, the nucleus mass to ∞, the helium nucleus charge to 2, the electron charges to -1. The Hamiltonian is [chapter 36]

$$H = \frac{1}{2}p_1^2 + \frac{1}{2}p_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_1 + r_2} . \qquad (29.3)$$

Due to the energy conservation, only three of the phase space coordinates (r_1, r_2, p_1, p_2) are independent. The dynamics can be visualized as a motion in the (r_1, r_2), $r_i \geq 0$ quadrant, figure 29.1, or, better still, by a well chosen 2-dimensional Poincaré section.

The motion in the (r_1, r_2) plane is topologically similar to the pinball motion in a 3-disk system, except that the motion is not free, but in the Coulomb potential. The classical collinear helium is also a repeller; almost all of the classical trajectories escape. Miraculously, the symbolic dynamics for the survivors turns out to be binary, just as in the 3-disk game of pinball, so we know what cycles need to be computed for the cycle expansion (1.10). A set of shortest cycles up to a given symbol string length then yields an estimate of the helium spectrum. This simple calculation yields surprisingly accurate eigenvalues; even though the cycle expansion was based on the *semiclassical approximation* (29.1) which is expected to be good only in the classical large energy limit, the eigenenergies are good to 1% all the way down to the ground state. [chapter 36]

Before we can get to this point, we first have to recapitulate some basic notions of quantum mechanics; after having defined the main quantum objects of interest, the quantum propagator and the Green's function, we will relate the quantum propagation to the classical flow of the underlying dynamical system. We will then proceed to construct semiclassical approximations to the quantum propagator and the Green's function. A rederivation of classical Hamiltonian dynamics starting from the Hamilton-Jacobi equation will be offered along the way. The derivation of the Gutzwiller trace formula and the semiclassical zeta function as a sum and as a product over periodic orbits will be given in chapter 33. In subsequent chapters we buttress our case by applying and extending the theory: a cycle expansion calculation of scattering resonances in a 3-disk billiard in chapter 34, the spectrum of helium in chapter 36, and the incorporation of diffraction effects in chapter 37.

Commentary

Remark 29.1 Guide to literature. A key prerequisite to developing any theory of "quantum chaos" is solid understanding of Hamiltonian mechanics. For that, Arnol'd monograph [36] is the essential reference. Ozorio de Almeida's monograph [11] offers a compact introduction to the aspects of Hamiltonian dynamics required for the quantization of integrable and nearly integrable systems, with emphasis on periodic orbits, normal forms, catastrophy theory and torus quantization. The book by Brack and Bhaduri [1] is an excellent introduction to the semiclassical methods. Gutzwiller's monograph [2] is an advanced introduction focusing on chaotic dynamics both in classical Hamiltonian settings and in the semiclassical quantization. This book is worth browsing through for its many insights and erudite comments on quantum and celestial mechanics even if one is not working on problems of quantum chaos. More suitable as a graduate course text is Reichl's exposition [3].

This book does not discuss the random matrix theory approach to chaos in quantal spectra; no randomness assumptions are made here, rather the goal is to milk the deterministic chaotic dynamics for its full worth. The book concentrates on the periodic orbit theory. For an introduction to "quantum chaos" that focuses on the random matrix theory the reader is referred to the excellent monograph by Haake [4], among others.

Remark 29.2 The dates. Schrödinger's first wave mechanics paper [3] (hydrogen spectrum) was submitted 27 January 1926. Submission date for Madelung's 'quantum theory in hydrodynamical form' paper [2] was 25 October 1926.